

Coordination Contents:

- (1) X/M(111)
- (2) 2X/M(111)
- (3) 3X/M(111)
- (4) 4X/M(111)
- (5) CO on Ni(111)
- (6) CO on Cu(111)
- (7) CO on Pd(111)
- (8) CO on Pt(111)
- (9) CO on nX/M(111)

(1) X/M(111)						
Cu/Ni(111)	1.0000000000000000					
	8.6223998537762050	-4.9781448766382850	0.0000000000000000			
	0.0000000000000000	9.9562897532765700	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292765422760382			
	Ni	Cu				
	79	1				
	Selective dynamics					
	Direct					
	0.0000000000000000	0.0000000000000000	0.1392871528000015	F	F	F
	0.9999996353090737	0.0000003646909263	0.4015356392611125	T	T	T
	0.1666666667000030	0.083333332999970	0.0514193316000018	F	F	F
	0.1671641961507788	0.0835294659453254	0.3144309256610143	T	T	T
	0.0833951807452422	0.1668094904869051	0.2269490183652394	T	T	T
	0.2500000000000000	0.0000000000000000	0.1392871528000015	F	F	F
	0.2499788741524256	0.9999577483048512	0.4011537014791813	T	T	T
	0.4166666667000030	0.083333332999970	0.0514193316000018	F	F	F
	0.4163652698945555	0.0835294659453254	0.3144309256610143	T	T	T
	0.3333220459778303	0.1666440920556767	0.2267720598664624	T	T	T
	0.5000000000000000	0.0000000000000000	0.1392871528000015	F	F	F
	0.5000007293818527	0.0000003646909263	0.4015356392611125	T	T	T
	0.6666666667000030	0.083333332999970	0.0514193316000018	F	F	F
	0.6665989505370291	0.0832994752185101	0.3147256647665913	T	T	T
	0.5834143096416540	0.1668094904869051	0.2269490183652394	T	T	T
	0.7500000000000000	0.0000000000000000	0.1392871528000015	F	F	F
	0.7501639755912350	0.0003279511824630	0.4014705770530185	T	T	T
	0.9166666667000030	0.083333332999970	0.0514193316000018	F	F	F
	0.9167005247814899	0.0832994752185101	0.3147256647665913	T	T	T
	0.833333332999970	0.1666666667000030	0.2270260577509617	T	T	T
	0.0000000000000000	0.2500000000000000	0.1392871528000015	F	F	F
	0.9996720488175370	0.2498360244087650	0.4014705770530185	T	T	T
	0.1666666667000030	0.333333332999970	0.0514193316000018	F	F	F
	0.1667308177071831	0.3333654088035871	0.3147501377505932	T	T	T
	0.0833951807452422	0.4165856903583460	0.2269490183652394	T	T	T
	0.2500000000000000	0.2500000000000000	0.1392871528000015	F	F	F
	0.2476548320323033	0.2478315111036054	0.4011527674267512	T	T	T
	0.4166666667000030	0.333333332999970	0.0514193316000018	F	F	F
	0.4169281104481470	0.3338562207962852	0.3150367052614413	T	T	T

0.3332324143382763	0.4166162072191426	0.2270989424456857	T	T	T
0.5000000000000000	0.2500000000000000	0.1392871528000015	F	F	F
0.5001766790713020	0.2478315111036054	0.4011527674267512	T	T	T
0.6666666667000030	0.3333333332999970	0.0514193316000018	F	F	F
0.6666345911964129	0.3333654088035871	0.3147501377505932	T	T	T
0.5833837927808574	0.4166162072191426	0.2270989424456857	T	T	T
0.7500000000000000	0.2500000000000000	0.1392871528000015	F	F	F
0.7501639755912350	0.2498360244087650	0.4014705770530185	T	T	T
0.9166666667000030	0.3333333332999970	0.0514193316000018	F	F	F
0.9167005247814899	0.3334010494629709	0.3147256647665913	T	T	T
0.8331905095130949	0.4165856903583460	0.2269490183652394	T	T	T
0.0000000000000000	0.5000000000000000	0.1392871528000015	F	F	F
0.9999996353090737	0.4999992706181473	0.4015356392611125	T	T	T
0.1666666667000030	0.5833333332999970	0.0514193316000018	F	F	F
0.1671641961507788	0.5836347301054445	0.3144309256610143	T	T	T
0.0833693268135960	0.6667386537272009	0.2269291701193197	T	T	T
0.2500000000000000	0.5000000000000000	0.1392871528000015	F	F	F
0.2476548320323033	0.4998233209286980	0.4011527674267512	T	T	T
0.4166666667000030	0.5833333332999970	0.0514193316000018	F	F	F
0.4169281104481470	0.5830718895518530	0.3150367052614413	T	T	T
0.3333220459778303	0.6666779540221697	0.2267720598664624	T	T	T
0.5000000000000000	0.5000000000000000	0.1392871528000015	F	F	F
0.6666666667000030	0.5833333332999970	0.0514193316000018	F	F	F
0.6661437792037148	0.5830718895518530	0.3150367052614413	T	T	T
0.5833837927808574	0.6667675856617237	0.2270989424456857	T	T	T
0.7500000000000000	0.5000000000000000	0.1392871528000015	F	F	F
0.7521684888963946	0.4998233209286980	0.4011527674267512	T	T	T
0.9166666667000030	0.5833333332999970	0.0514193316000018	F	F	F
0.9164705340546746	0.5836347301054445	0.3144309256610143	T	T	T
0.8333559079443233	0.6666779540221697	0.2267720598664624	T	T	T
0.0000000000000000	0.7500000000000000	0.1392871528000015	F	F	F
0.0000422516951488	0.7500211258475744	0.4011537014791813	T	T	T
0.1666666667000030	0.8333333332999970	0.0514193316000018	F	F	F
0.1666666667000030	0.8333333332999970	0.3145553644534616	T	T	T
0.0833693268135960	0.9166306731864040	0.2269291701193197	T	T	T
0.2500000000000000	0.7500000000000000	0.1392871528000015	F	F	F
0.2499788741524256	0.7500211258475744	0.4011537014791813	T	T	T
0.4166666667000030	0.8333333332999970	0.0514193316000018	F	F	F
0.4163652698945555	0.8328358038492212	0.3144309256610143	T	T	T
0.3332613462727991	0.9166306731864040	0.2269291701193197	T	T	T
0.5000000000000000	0.7500000000000000	0.1392871528000015	F	F	F
0.5001766790713020	0.7523451679676967	0.4011527674267512	T	T	T
0.6666666667000030	0.8333333332999970	0.0514193316000018	F	F	F
0.6666345911964129	0.8332691822928169	0.3147501377505932	T	T	T
0.5834143096416540	0.9166048192547578	0.2269490183652394	T	T	T
0.7500000000000000	0.7500000000000000	0.1392871528000015	F	F	F
0.7521684888963946	0.7523451679676967	0.4011527674267512	T	T	T
0.9166666667000030	0.8333333332999970	0.0514193316000018	F	F	F
0.9164705340546746	0.8328358038492212	0.3144309256610143	T	T	T
0.8331905095130949	0.9166048192547578	0.2269490183652394	T	T	T
0.5000000000000000	0.5000000000000000	0.4063775809481172	T	T	T

Ag/Ni(111)	1.0000000000000000			
	8.6223998537762050	-4.9781448766382850	0.0000000000000000	
	0.0000000000000000	9.9562897532765700	0.0000000000000000	
	0.0000000000000000	0.0000000000000000	23.1292765422760382	
	Ni	Ag		
	79	1		
	Selective dynamics			
	Direct			
	0.0000000000000000	0.0000000000000000	0.1392871528000015	F F F
	0.0001072651808158	0.9998927348191842	0.4012285508306377	T T T
0.1666666667000030	0.0833333332999970	0.0514193316000018	F F F	
0.1671697837766999	0.0833699561892445	0.3140581462795708	T T T	
0.0834543857270234	0.1669631498197433	0.2268478174539581	T T T	
0.2500000000000000	0.0000000000000000	0.1392871528000015	F F F	
0.2495865740936409	0.9991731481872819	0.4008450602789893	T T T	
0.4166666667000030	0.0833333332999970	0.0514193316000018	F F F	
0.4162001725125606	0.0833699561892445	0.3140581462795708	T T T	
0.3334729038491702	0.1669458077983563	0.2268366898520071	T T T	
0.5000000000000000	0.0000000000000000	0.1392871528000015	F F F	
0.4997854696383754	0.9998927348191842	0.4012285508306377	T T T	
0.6666666667000030	0.0833333332999970	0.0514193316000018	F F F	
0.6665833452495349	0.0832916725747594	0.3145411569705416	T T T	
0.5835087639927110	0.1669631498197433	0.2268478174539581	T T T	
0.7500000000000000	0.0000000000000000	0.1392871528000015	F F F	
0.7506395137622306	0.0012790275244541	0.4014100650814498	T T T	
0.9166666667000030	0.0833333332999970	0.0514193316000018	F F F	
0.9167083274252406	0.0832916725747594	0.3145411569705416	T T T	
0.8333333332999970	0.1666666667000030	0.2267996291097631	T T T	
0.0000000000000000	0.2500000000000000	0.1392871528000015	F F F	
0.9987209724755459	0.2493604862377694	0.4014100650814498	T T T	
0.1666666667000030	0.3333333332999970	0.0514193316000018	F F F	
0.1667613930014085	0.3333806964506962	0.3147526525605073	T T T	
0.0834543857270234	0.4164912360072890	0.2268478174539581	T T T	
0.2500000000000000	0.2500000000000000	0.1392871528000015	F F F	
0.2426913890313500	0.2432175835001047	0.4010419324083188	T T T	
0.4166666667000030	0.3333333332999970	0.0514193316000018	F F F	
0.4172651265252938	0.3345302529505787	0.3162190421803146	T T T	
0.3334557634387565	0.4167278817693827	0.2274495811952804	T T T	
0.5000000000000000	0.2500000000000000	0.1392871528000015	F F F	
0.5005261944687476	0.2432175835001047	0.4010419324083188	T T T	
0.6666666667000030	0.3333333332999970	0.0514193316000018	F F F	
0.6666193035493038	0.3333806964506962	0.3147526525605073	T T T	
0.5832721182306173	0.4167278817693827	0.2274495811952804	T T T	
0.7500000000000000	0.2500000000000000	0.1392871528000015	F F F	
0.7506395137622306	0.2493604862377694	0.4014100650814498	T T T	
0.9166666667000030	0.3333333332999970	0.0514193316000018	F F F	
0.9167083274252406	0.3334166547504651	0.3145411569705416	T T T	
0.8330368501802567	0.4164912360072890	0.2268478174539581	T T T	
0.0000000000000000	0.5000000000000000	0.1392871528000015	F F F	
0.0001072651808158	0.5002145303616246	0.4012285508306377	T T T	
0.1666666667000030	0.5833333332999970	0.0514193316000018	F F F	

	0.1671697837766999	0.5837998274874394	0.3140581462795708	T	T	T
	0.0833145094617862	0.6666290190235813	0.2266708385337566	T	T	T
	0.2500000000000000	0.5000000000000000	0.1392871528000015	F	F	F
	0.2426913890313500	0.4994738055312524	0.4010419324083188	T	T	T
	0.4166666667000030	0.583333332999970	0.0514193316000018	F	F	F
	0.4172651265252938	0.5827348734747062	0.3162190421803146	T	T	T
	0.3334729038491702	0.6665270961508298	0.2268366898520071	T	T	T
	0.5000000000000000	0.5000000000000000	0.1392871528000015	F	F	F
	0.6666666667000030	0.583333332999970	0.0514193316000018	F	F	F
	0.6654697470494213	0.5827348734747062	0.3162190421803146	T	T	T
	0.5832721182306173	0.6665442365612435	0.2274495811952804	T	T	T
	0.7500000000000000	0.5000000000000000	0.1392871528000015	F	F	F
	0.7567824164998953	0.4994738055312524	0.4010419324083188	T	T	T
	0.9166666667000030	0.583333332999970	0.0514193316000018	F	F	F
	0.9166300438107555	0.5837998274874394	0.3140581462795708	T	T	T
	0.8330541922016437	0.6665270961508298	0.2268366898520071	T	T	T
	0.0000000000000000	0.7500000000000000	0.1392871528000015	F	F	F
	0.0008268518127181	0.7504134259063591	0.4008450602789893	T	T	T
	0.1666666667000030	0.833333332999970	0.0514193316000018	F	F	F
	0.1666666667000030	0.833333332999970	0.3140469388232248	T	T	T
	0.0833145094617862	0.9166854905382138	0.2266708385337566	T	T	T
	0.2500000000000000	0.7500000000000000	0.1392871528000015	F	F	F
	0.2495865740936409	0.7504134259063591	0.4008450602789893	T	T	T
	0.4166666667000030	0.833333332999970	0.0514193316000018	F	F	F
	0.4162001725125606	0.8328302162233001	0.3140581462795708	T	T	T
	0.3333709809764187	0.9166854905382138	0.2266708385337566	T	T	T
	0.5000000000000000	0.7500000000000000	0.1392871528000015	F	F	F
	0.5005261944687476	0.7573086109686500	0.4010419324083188	T	T	T
	0.6666666667000030	0.833333332999970	0.0514193316000018	F	F	F
	0.6666193035493038	0.8332386069985915	0.3147526525605073	T	T	T
	0.5835087639927110	0.9165456142729766	0.2268478174539581	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392871528000015	F	F	F
	0.7567824164998953	0.7573086109686500	0.4010419324083188	T	T	T
	0.9166666667000030	0.833333332999970	0.0514193316000018	F	F	F
	0.9166300438107555	0.8328302162233001	0.3140581462795708	T	T	T
	0.8330368501802567	0.9165456142729766	0.2268478174539581	T	T	T
	0.5000000000000000	0.5000000000000000	0.4230056162900766	T	T	T
Au/Ni(111)	1.0000000000000000					
	8.6223998537762050	-4.9781448766382850	0.0000000000000000			
	0.0000000000000000	9.9562897532765700	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292765422760382			
	Ni	Au				
	79	1				
	Selective dynamics					
	Direct					
	0.0000000000000000	0.0000000000000000	0.1392871528000015	F	F	F
	0.0000990621841552	0.9999009378158448	0.4013740292999444	T	T	T
	0.1666666667000030	0.083333332999970	0.0514193316000018	F	F	F
	0.1670961155463928	0.0833456909702264	0.3143396813759054	T	T	T
	0.0833878219781141	0.1668527806013032	0.2269115547669855	T	T	T
	0.2500000000000000	0.0000000000000000	0.1392871528000015	F	F	F

0.2494254249027748	0.9988508498055495	0.4010459421035861	T	T	T
0.4166666667000030	0.0833333332999970	0.0514193316000018	F	F	F
0.4162495755238353	0.0833456909702264	0.3143396813759054	T	T	T
0.3333806967087085	0.1667613935174259	0.2268475366011700	T	T	T
0.5000000000000000	0.0000000000000000	0.1392871528000015	F	F	F
0.4998018756316824	0.9999009378158448	0.4013740292999444	T	T	T
0.6666666667000030	0.0833333332999970	0.0514193316000018	F	F	F
0.6665248582436831	0.0832624290718371	0.3145960987897354	T	T	T
0.5834649585231801	0.1668527806013032	0.2269115547669855	T	T	T
0.7500000000000000	0.0000000000000000	0.1392871528000015	F	F	F
0.7507033942075125	0.0014067884150322	0.4014413973472202	T	T	T
0.9166666667000030	0.0833333332999970	0.0514193316000018	F	F	F
0.9167375709281629	0.0832624290718371	0.3145960987897354	T	T	T
0.8333333332999970	0.1666666667000030	0.2269372126857192	T	T	T
0.0000000000000000	0.2500000000000000	0.1392871528000015	F	F	F
0.9985932115849678	0.2492966057924875	0.4014413973472202	T	T	T
0.1666666667000030	0.3333333332999970	0.0514193316000018	F	F	F
0.1664490249040398	0.3332245124020119	0.3147565374456960	T	T	T
0.0833878219781141	0.4165350414768199	0.2269115547669855	T	T	T
0.2500000000000000	0.2500000000000000	0.1392871528000015	F	F	F
0.2434199349086299	0.2437200602193172	0.4016411174109109	T	T	T
0.4166666667000030	0.3333333332999970	0.0514193316000018	F	F	F
0.4166122171172759	0.3332244341345429	0.3152649241256285	T	T	T
0.3332731385116361	0.4166365693058225	0.2272723990870489	T	T	T
0.5000000000000000	0.2500000000000000	0.1392871528000015	F	F	F
0.5003001253106873	0.2437200602193172	0.4016411174109109	T	T	T
0.6666666667000030	0.3333333332999970	0.0514193316000018	F	F	F
0.6667754875979881	0.3332245124020119	0.3147565374456960	T	T	T
0.5833634306941775	0.4166365693058225	0.2272723990870489	T	T	T
0.7500000000000000	0.2500000000000000	0.1392871528000015	F	F	F
0.7507033942075125	0.2492966057924875	0.4014413973472202	T	T	T
0.9166666667000030	0.3333333332999970	0.0514193316000018	F	F	F
0.9167375709281629	0.3334751417563169	0.3145960987897354	T	T	T
0.8331472193986968	0.4165350414768199	0.2269115547669855	T	T	T
0.0000000000000000	0.5000000000000000	0.1392871528000015	F	F	F
0.0000990621841552	0.5001981243683176	0.4013740292999444	T	T	T
0.1666666667000030	0.5833333332999970	0.0514193316000018	F	F	F
0.1670961155463928	0.5837504244761647	0.3143396813759054	T	T	T
0.0833290671972051	0.6666581344944191	0.2267924300196498	T	T	T
0.2500000000000000	0.5000000000000000	0.1392871528000015	F	F	F
0.2434199349086299	0.4996998746893127	0.4016411174109109	T	T	T
0.4166666667000030	0.5833333332999970	0.0514193316000018	F	F	F
0.4166122171172759	0.5833877828827241	0.3152649241256285	T	T	T
0.3333806967087085	0.6666193032912915	0.2268475366011700	T	T	T
0.5000000000000000	0.5000000000000000	0.1392871528000015	F	F	F
0.6666666667000030	0.5833333332999970	0.0514193316000018	F	F	F
0.6667755658654571	0.5833877828827241	0.3152649241256285	T	T	T
0.5833634306941775	0.6667268614883639	0.2272723990870489	T	T	T
0.7500000000000000	0.5000000000000000	0.1392871528000015	F	F	F
0.7562799397806828	0.4996998746893127	0.4016411174109109	T	T	T
0.9166666667000030	0.5833333332999970	0.0514193316000018	F	F	F

	0.9166543090297736	0.5837504244761647	0.3143396813759054	T	T	T
	0.8332386064825741	0.6666193032912915	0.2268475366011700	T	T	T
	0.0000000000000000	0.7500000000000000	0.1392871528000015	F	F	F
	0.0011491501944505	0.7505745750972252	0.4010459421035861	T	T	T
	0.1666666667000030	0.8333333332999970	0.0514193316000018	F	F	F
	0.1666666667000030	0.8333333332999970	0.3141415157668632	T	T	T
	0.0833290671972051	0.9166709328027949	0.2267924300196498	T	T	T
	0.2500000000000000	0.7500000000000000	0.1392871528000015	F	F	F
	0.2494254249027748	0.7505745750972252	0.4010459421035861	T	T	T
	0.4166666667000030	0.8333333332999970	0.0514193316000018	F	F	F
	0.4162495755238353	0.8329038844536072	0.3143396813759054	T	T	T
	0.3333418655055809	0.9166709328027949	0.2267924300196498	T	T	T
	0.5000000000000000	0.7500000000000000	0.1392871528000015	F	F	F
	0.5003001253106873	0.7565800650913701	0.4016411174109109	T	T	T
	0.6666666667000030	0.8333333332999970	0.0514193316000018	F	F	F
	0.6667754875979881	0.8335509750959602	0.3147565374456960	T	T	T
	0.5834649585231801	0.9166121780218859	0.2269115547669855	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392871528000015	F	F	F
	0.7562799397806828	0.7565800650913701	0.4016411174109109	T	T	T
	0.9166666667000030	0.8333333332999970	0.0514193316000018	F	F	F
	0.9166543090297736	0.8329038844536072	0.3143396813759054	T	T	T
	0.8331472193986968	0.9166121780218859	0.2269115547669855	T	T	T
	0.5000000000000000	0.5000000000000000	0.4176911382026134	T	T	T
Ni/Cu(111)	1.0000000000000000					
	8.8905944857135406	-5.1329871195825199	-0.0000000000000010			
	0.0000000000000000	10.2659742391650006	0.0000000000000010			
	0.0000000000000000	0.0000000000000000	23.3821328661704015			
	Ni	Cu				
	1	79				
	Selective dynamics					
	Direct					
	0.5000000000000000	0.5000000000000000	0.3795757109775479	T	T	T
	0.0000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.0000120110479997	0.9999879889520003	0.3832768680248790	T	T	T
	0.1666666667000030	0.0833333332999970	0.0259047434999999	F	F	F
	0.1668003148177348	0.0836315997847521	0.2945116459540458	T	T	T
	0.0833220919608166	0.1666987079936106	0.2050336998382676	T	T	T
	0.2500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.2501675867419593	0.0003351734839185	0.3834111862314913	T	T	T
	0.4166666667000030	0.0833333332999970	0.0259047434999999	F	F	F
	0.4168312850670262	0.0836315997847521	0.2945116459540458	T	T	T
	0.3333712529243158	0.1667425059486476	0.2050446258927323	T	T	T
	0.5000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.4999759779040005	0.9999879889520003	0.3832768680248790	T	T	T
	0.6666666667000030	0.0833333332999970	0.0259047434999999	F	F	F
	0.6665929121651359	0.0832964560325635	0.2944656615515200	T	T	T
	0.5833766159327993	0.1666987079936106	0.2050336998382676	T	T	T
	0.7500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.7497569360200345	0.9995138720400831	0.3833117013257805	T	T	T
	0.9166666667000030	0.0833333332999970	0.0259047434999999	F	F	F
	0.9167035439674365	0.0832964560325635	0.2944656615515200	T	T	T

0.833333332999970	0.166666667000030	0.2050272403659861	T	T	T
0.000000000000000	0.250000000000000	0.1155258754999977	F	F	F
0.0004861279599169	0.2502430639799655	0.3833117013257805	T	T	T
0.166666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.1668574729385597	0.3334287364192718	0.2944031056378051	T	T	T
0.0833220919608166	0.4166233840672007	0.2050336998382676	T	T	T
0.250000000000000	0.250000000000000	0.1155258754999977	F	F	F
0.2519783305529657	0.2518785527096767	0.3834400493455732	T	T	T
0.416666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.4168624711113438	0.3337249421226858	0.2941302298100155	T	T	T
0.3331832765271230	0.4165916383135695	0.2047266732899189	T	T	T
0.500000000000000	0.250000000000000	0.1155258754999977	F	F	F
0.4999002221567110	0.2518785527096767	0.3834400493455732	T	T	T
0.666666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.6665712635807282	0.3334287364192718	0.2944031056378051	T	T	T
0.5834083616864305	0.4165916383135695	0.2047266732899189	T	T	T
0.750000000000000	0.250000000000000	0.1155258754999977	F	F	F
0.7497569360200345	0.2502430639799655	0.3833117013257805	T	T	T
0.916666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.9167035439674365	0.3334070878348641	0.2944656615515200	T	T	T
0.8333012920063894	0.4166233840672007	0.2050336998382676	T	T	T
0.000000000000000	0.500000000000000	0.1155258754999977	F	F	F
0.0000120110479997	0.5000240220959995	0.3832768680248790	T	T	T
0.166666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.1668003148177348	0.5831687149329738	0.2945116459540458	T	T	T
0.0833287759239099	0.6666575519478215	0.2050618687929955	T	T	T
0.250000000000000	0.500000000000000	0.1155258754999977	F	F	F
0.2519783305529657	0.500097778432890	0.3834400493455732	T	T	T
0.416666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.4168624711113438	0.5831375288886562	0.2941302298100155	T	T	T
0.3333712529243158	0.6666287470756842	0.2050446258927323	T	T	T
0.500000000000000	0.500000000000000	0.1155258754999977	F	F	F
0.666666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.6662750578773142	0.5831375288886562	0.2941302298100155	T	T	T
0.5834083616864305	0.6668167234728770	0.2047266732899189	T	T	T
0.750000000000000	0.500000000000000	0.1155258754999977	F	F	F
0.7481214472903233	0.500097778432890	0.3834400493455732	T	T	T
0.916666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.9163684002152479	0.5831687149329738	0.2945116459540458	T	T	T
0.8332574940513524	0.6666287470756842	0.2050446258927323	T	T	T
0.000000000000000	0.750000000000000	0.1155258754999977	F	F	F
0.9996648265160815	0.7498324132580407	0.3834111862314913	T	T	T
0.166666667000030	0.833333332999970	0.0259047434999999	F	F	F
0.166666667000030	0.833333332999970	0.2945436853376791	T	T	T
0.0833287759239099	0.9166712240760901	0.2050618687929955	T	T	T
0.250000000000000	0.750000000000000	0.1155258754999977	F	F	F
0.2501675867419593	0.7498324132580407	0.3834111862314913	T	T	T
0.416666667000030	0.833333332999970	0.0259047434999999	F	F	F
0.4168312850670262	0.8331996851822652	0.2945116459540458	T	T	T
0.3333424480521785	0.9166712240760901	0.2050618687929955	T	T	T
0.500000000000000	0.750000000000000	0.1155258754999977	F	F	F

	0.4999002221567110	0.7480216694470343	0.3834400493455732	T	T	T
	0.6666666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.6665712635807282	0.8331425270614403	0.2944031056378051	T	T	T
	0.5833766159327993	0.9166779080391905	0.2050336998382676	T	T	T
	0.7500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.7481214472903233	0.7480216694470343	0.3834400493455732	T	T	T
	0.9166666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.9163684002152479	0.8331996851822652	0.2945116459540458	T	T	T
	0.8333012920063894	0.9166779080391905	0.2050336998382676	T	T	T
Pd/Cu(111)	1.0000000000000000					
	8.8905944857135406	-5.1329871195825199	-0.0000000000000010			
	0.0000000000000000	10.2659742391650006	0.0000000000000010			
	0.0000000000000000	0.0000000000000000	23.3821328661704015			
	Pd	Cu				
	1	79				
	Selective dynamics					
	Direct					
	0.5000000000000000	0.5000000000000000	0.3865501900938568	T	T	T
	0.0000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.0000416759687383	0.9999583240312617	0.3831679805830746	T	T	T
	0.1666666667000030	0.0833333332999970	0.0259047434999999	F	F	F
	0.1665823817276575	0.0832163840723510	0.2942365368931519	T	T	T
	0.0833705785525396	0.1667996748837197	0.2050135136619176	T	T	T
	0.2500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.2496520067597814	0.9993040135195486	0.3832760717019781	T	T	T
	0.4166666667000030	0.0833333332999970	0.0259047434999999	F	F	F
	0.4166340024447024	0.0832163840723510	0.2942365368931519	T	T	T
	0.3334698460465262	0.1669396921930542	0.2050039569563751	T	T	T
	0.5000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.4999166480625234	0.9999583240312617	0.3831679805830746	T	T	T
	0.6666666667000030	0.0833333332999970	0.0259047434999999	F	F	F
	0.6666216321471410	0.0833108160235696	0.2943068739297132	T	T	T
	0.5834290962311712	0.1667996748837197	0.2050135136619176	T	T	T
	0.7500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.7502905552753063	0.0005811105506197	0.3832496292077607	T	T	T
	0.9166666667000030	0.0833333332999970	0.0259047434999999	F	F	F
	0.9166891839764304	0.0833108160235696	0.2943068739297132	T	T	T
	0.8333333332999970	0.1666666667000030	0.2049045666083131	T	T	T
	0.0000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
	0.9994188894493803	0.2497094447246937	0.3832496292077607	T	T	T
	0.1666666667000030	0.3333333332999970	0.0259047434999999	F	F	F
	0.1669465399407315	0.3334732699203542	0.2945176382690491	T	T	T
	0.0833705785525396	0.4165709037688288	0.2050135136619176	T	T	T
	0.2500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
	0.2465060743216014	0.2464151925312805	0.3836747765038524	T	T	T
	0.4166666667000030	0.3333333332999970	0.0259047434999999	F	F	F
	0.4163394789369264	0.3326789577738367	0.2942020995202199	T	T	T
	0.3332710661060148	0.4166355331030118	0.2048473830162507	T	T	T
	0.5000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
	0.4999091182096791	0.2464151925312805	0.3836747765038524	T	T	T
	0.6666666667000030	0.3333333332999970	0.0259047434999999	F	F	F

	0.6665267300796458	0.3334732699203542	0.2945176382690491	T	T	T
	0.5833644668969882	0.4166355331030118	0.2048473830162507	T	T	T
	0.7500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
	0.7502905552753063	0.2497094447246937	0.3832496292077607	T	T	T
	0.9166666667000030	0.333333332999970	0.0259047434999999	F	F	F
	0.9166891839764304	0.3333783678528590	0.2943068739297132	T	T	T
	0.8332003251162803	0.4165709037688288	0.2050135136619176	T	T	T
	0.0000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.0000416759687383	0.5000833519374766	0.3831679805830746	T	T	T
	0.1666666667000030	0.583333332999970	0.0259047434999999	F	F	F
	0.1665823817276575	0.5833659975552976	0.2942365368931519	T	T	T
	0.0833147454941994	0.6666294910884218	0.2048557255063486	T	T	T
	0.2500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.2465060743216014	0.5000908817903209	0.3836747765038524	T	T	T
	0.4166666667000030	0.583333332999970	0.0259047434999999	F	F	F
	0.4163394789369264	0.5836605210630736	0.2942020995202199	T	T	T
	0.3334698460465262	0.6665301539534738	0.2050039569563751	T	T	T
	0.5000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.6666666667000030	0.583333332999970	0.0259047434999999	F	F	F
	0.6673210422261633	0.5836605210630736	0.2942020995202199	T	T	T
	0.5833644668969882	0.6667289338939852	0.2048473830162507	T	T	T
	0.7500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.7535848074687195	0.5000908817903209	0.3836747765038524	T	T	T
	0.9166666667000030	0.583333332999970	0.0259047434999999	F	F	F
	0.9167836159276490	0.5833659975552976	0.2942365368931519	T	T	T
	0.8330603078069458	0.6665301539534738	0.2050039569563751	T	T	T
	0.0000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.0006959864804514	0.7503479932402186	0.3832760717019781	T	T	T
	0.1666666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.1666666667000030	0.833333332999970	0.2941676316630151	T	T	T
	0.0833147454941994	0.9166852545058006	0.2048557255063486	T	T	T
	0.2500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.2496520067597814	0.7503479932402186	0.3832760717019781	T	T	T
	0.4166666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.4166340024447024	0.8334176182723425	0.2942365368931519	T	T	T
	0.3333705089115782	0.9166852545058006	0.2048557255063486	T	T	T
	0.5000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.4999091182096791	0.7534939256783986	0.3836747765038524	T	T	T
	0.6666666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.6665267300796458	0.8330534600592685	0.2945176382690491	T	T	T
	0.5834290962311712	0.9166294214474604	0.2050135136619176	T	T	T
	0.7500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.7535848074687195	0.7534939256783986	0.3836747765038524	T	T	T
	0.9166666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.9167836159276490	0.8334176182723425	0.2942365368931519	T	T	T
	0.8332003251162803	0.9166294214474604	0.2050135136619176	T	T	T
Pt/Cu(111)	1.0000000000000000					
	8.8905944857135406	-5.1329871195825199	-0.0000000000000010			
	0.0000000000000000	10.2659742391650006	0.0000000000000010			
	0.0000000000000000	0.0000000000000000	23.3821328661704015			
	Pt	Cu				

Selective dynamics

Direct

0.5000000000000000	0.5000000000000000	0.3844384201297970	T	T	T
0.0000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.9999989773712485	0.0000010226287515	0.3832555484970968	T	T	T
0.1666666667000030	0.083333332999970	0.0259047434999999	F	F	F
0.1666303021149247	0.0834475002824107	0.2944864613748805	T	T	T
0.0833063005886743	0.1666770856778541	0.2049781189451281	T	T	T
0.2500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.2496434669959626	0.9992869339919181	0.3833550849367597	T	T	T
0.4166666667000030	0.083333332999970	0.0259047434999999	F	F	F
0.4168171982674949	0.0834475002824107	0.2944864613748805	T	T	T
0.3333641918937218	0.1667283838874596	0.2049722568582197	T	T	T
0.5000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.5000020452575171	0.0000010226287515	0.3832555484970968	T	T	T
0.6666666667000030	0.083333332999970	0.0259047434999999	F	F	F
0.6665960227947139	0.0832980113473525	0.2943690297427963	T	T	T
0.5833707849891852	0.1666770856778541	0.2049781189451281	T	T	T
0.7500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.7502499418392858	0.0004998836785788	0.3832506585998274	T	T	T
0.9166666667000030	0.083333332999970	0.0259047434999999	F	F	F
0.9167019886526475	0.0832980113473525	0.2943690297427963	T	T	T
0.833333332999970	0.1666666667000030	0.2049958779990320	T	T	T
0.0000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.9995001163214212	0.2497500581607142	0.3832506585998274	T	T	T
0.1666666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.1663537393860324	0.3331768696430117	0.2944656541599997	T	T	T
0.0833063005886743	0.4166292150108148	0.2049781189451281	T	T	T
0.2500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.2474773131071686	0.2473361188672669	0.3843872439735918	T	T	T
0.4166666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.4157704420008059	0.3315408839016030	0.2935782344053095	T	T	T
0.3330377001888181	0.4165188501444135	0.2046830540510030	T	T	T
0.5000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.4998588057600983	0.2473361188672669	0.3843872439735918	T	T	T
0.6666666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.6668231303569883	0.3331768696430117	0.2944656541599997	T	T	T
0.5834811498555865	0.4165188501444135	0.2046830540510030	T	T	T
0.7500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.7502499418392858	0.2497500581607142	0.3832506585998274	T	T	T
0.9166666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.9167019886526475	0.3334039772052861	0.2943690297427963	T	T	T
0.8333229143221459	0.4166292150108148	0.2049781189451281	T	T	T
0.0000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.9999989773712485	0.4999979547424829	0.3832555484970968	T	T	T
0.1666666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.1666303021149247	0.5831828017325051	0.2944864613748805	T	T	T
0.0833159325916952	0.6666318652833851	0.2049777327966993	T	T	T
0.2500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.2474773131071686	0.5001411942399017	0.3843872439735918	T	T	T

0.416666667000030	0.5833333332999970	0.0259047434999999	F	F	F	
0.4157704420008059	0.5842295579991941	0.2935782344053095	T	T	T	
0.3333641918937218	0.6666358081062782	0.2049722568582197	T	T	T	
0.5000000000000000	0.5000000000000000	0.1155258754999977	F	F	F	
0.666666667000030	0.5833333332999970	0.0259047434999999	F	F	F	
0.6684591160983970	0.5842295579991941	0.2935782344053095	T	T	T	
0.5834811498555865	0.6669622998111819	0.2046830540510030	T	T	T	
0.7500000000000000	0.5000000000000000	0.1155258754999977	F	F	F	
0.7526638811327331	0.5001411942399017	0.3843872439735918	T	T	T	
0.916666667000030	0.5833333332999970	0.0259047434999999	F	F	F	
0.9165524997175893	0.5831828017325051	0.2944864613748805	T	T	T	
0.8332716161125404	0.6666358081062782	0.2049722568582197	T	T	T	
0.0000000000000000	0.7500000000000000	0.1155258754999977	F	F	F	
0.0007130660080819	0.7503565330040374	0.3833550849367597	T	T	T	
0.166666667000030	0.8333333332999970	0.0259047434999999	F	F	F	
0.166666667000030	0.8333333332999970	0.2942552419374564	T	T	T	
0.0833159325916952	0.9166840674083048	0.2049777327966993	T	T	T	
0.2500000000000000	0.7500000000000000	0.1155258754999977	F	F	F	
0.2496434669959626	0.7503565330040374	0.3833550849367597	T	T	T	
0.416666667000030	0.8333333332999970	0.0259047434999999	F	F	F	
0.4168171982674949	0.8333696978850753	0.2944864613748805	T	T	T	
0.3333681347166149	0.9166840674083048	0.2049777327966993	T	T	T	
0.5000000000000000	0.7500000000000000	0.1155258754999977	F	F	F	
0.4998588057600983	0.7525226868928314	0.3843872439735918	T	T	T	
0.666666667000030	0.8333333332999970	0.0259047434999999	F	F	F	
0.6668231303569883	0.8336462606139676	0.2944656541599997	T	T	T	
0.5833707849891852	0.9166936994113257	0.2049781189451281	T	T	T	
0.7500000000000000	0.7500000000000000	0.1155258754999977	F	F	F	
0.7526638811327331	0.7525226868928314	0.3843872439735918	T	T	T	
0.916666667000030	0.8333333332999970	0.0259047434999999	F	F	F	
0.9165524997175893	0.8333696978850753	0.2944864613748805	T	T	T	
0.8333229143221459	0.9166936994113257	0.2049781189451281	T	T	T	
(2) 2X-S1						
2Cu/Ni(111)	1.0000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni	Cu				
	78	2				
	Selective dynamics					
	Direct					
	0.0000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.0000725444057821	0.0021507519474540	0.4009851174421186	T	T	T
	0.1666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.1671625139084441	0.0833899710905470	0.3143538692610335	T	T	T
	0.0834521118154896	0.1667673491848305	0.2268654956235778	T	T	T
	0.2500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.2520154992745418	0.0024607583670857	0.4009983678140472	T	T	T
	0.4166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.4163791451791212	0.0833772108405029	0.3142022620711842	T	T	T
	0.3333048000507901	0.1666033333924020	0.2267003916851351	T	T	T

0.5000000000000000	0.0000000000000000	0.1392870000000030	F F F
0.4996781596847697	0.9998385798423826	0.4012740924560561	T T T
0.6666669999999968	0.0833330000000032	0.0514190000000028	F F F
0.6665312248866115	0.0832651124433070	0.3145679101564838	T T T
0.5834318455385343	0.1669015305606507	0.2268603604355661	T T T
0.7500000000000000	0.0000000000000000	0.1392870000000030	F F F
0.7500096869153410	0.0001515905359710	0.4011114182638806	T T T
0.9166669999999968	0.0833330000000032	0.0514190000000028	F F F
0.9162941307761514	0.0830564220133994	0.3143388335803579	T T T
0.8333197283507872	0.1666603641753923	0.2268380255461153	T T T
0.0000000000000000	0.2500000000000000	0.1392870000000030	F F F
0.9995163973333092	0.2497581986666546	0.4012377695923846	T T T
0.1666669999999968	0.3333330000000032	0.0514190000000028	F F F
0.1666383659613899	0.3333186829806962	0.3144970213946863	T T T
0.0834521118154896	0.4166847626306520	0.2268654956235778	T T T
0.2500000000000000	0.2500000000000000	0.1392870000000030	F F F
0.2477782636875148	0.2482924581934611	0.4010920064305239	T T T
0.4166669999999968	0.3333330000000032	0.0514190000000028	F F F
0.4169310849229859	0.3336855005659558	0.3149161932911753	T T T
0.3333331605532166	0.4166665802766047	0.2270084296748180	T T T
0.5000000000000000	0.2500000000000000	0.1392870000000030	F F F
0.5003669280535092	0.2479831525359089	0.4011189768470587	T T T
0.6666669999999968	0.3333330000000032	0.0514190000000028	F F F
0.6667902461902813	0.3334660072586999	0.3142578085819068	T T T
0.5834167091181186	0.4167451716685235	0.2269947879866621	T T T
0.7500000000000000	0.2500000000000000	0.1392870000000030	F F F
0.7500096869153410	0.2498580963793700	0.4011114182638806	T T T
0.9166669999999968	0.3333330000000032	0.0514190000000028	F F F
0.9162941307761514	0.3332367087627546	0.3143388335803579	T T T
0.8332403376607260	0.4166289364494986	0.2267379666950120	T T T
0.0000000000000000	0.5000000000000000	0.1392870000000030	F F F
0.0000725444057821	0.4979207924583307	0.4009851174421186	T T T
0.1666669999999968	0.5833330000000032	0.0514190000000028	F F F
0.1671625139084441	0.5837725428178970	0.3143538692610335	T T T
0.0834068300929758	0.6669768277578498	0.2270476860199366	T T T
0.2500000000000000	0.5000000000000000	0.1392870000000030	F F F
0.2477782636875148	0.4994858054940536	0.4010920064305239	T T T
0.4166669999999968	0.5833330000000032	0.0514190000000028	F F F
0.4169310849229859	0.5832455843570372	0.3149161932911753	T T T
0.3333048000507901	0.6667014666583881	0.2267003916851351	T T T
0.5000000000000000	0.5000000000000000	0.1392870000000030	F F F
0.6666669999999968	0.5833330000000032	0.0514190000000028	F F F
0.6662734833303716	0.5831367416651858	0.3150031023009348	T T T
0.5834167091181186	0.6666715374495880	0.2269947879866621	T T T
0.7500000000000000	0.5000000000000000	0.1392870000000030	F F F
0.7497055296258495	0.4979338032939822	0.4009553906938521	T T T
0.9166669999999968	0.5833330000000032	0.0514190000000028	F F F
0.9168981422004236	0.5841378601629117	0.3147208832544521	T T T
0.8334064694495709	0.6667032347247854	0.2268840745485363	T T T
0.0000000000000000	0.7500000000000000	0.1392870000000030	F F F
0.1666669999999968	0.8333330000000032	0.0514190000000028	F F F

	0.1664669400200296	0.8332329700100161	0.3150259455204321	T	T	T
	0.0834068300929758	0.9164310023351305	0.2270476860199366	T	T	T
	0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.2520154992745418	0.7495547409074490	0.4009983678140472	T	T	T
	0.4166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.4163791451791212	0.8330019343386184	0.3142022620711842	T	T	T
	0.3333973268201262	0.9166991634100654	0.2268264324973188	T	T	T
	0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.5003669280535092	0.7523837755176004	0.4011189768470587	T	T	T
	0.6666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.6667902461902813	0.8333232389315839	0.3142578085819068	T	T	T
	0.5834318455385343	0.9165303149778907	0.2268603604355661	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.7497055296258495	0.7517717263318602	0.4009553906938521	T	T	T
	0.9166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.9168981422004236	0.8327602820375191	0.3147208832544521	T	T	T
	0.8332403376607260	0.9166114012112274	0.2267379666950120	T	T	T
	0.0003385268539731	0.7501692634269830	0.4063156779272390	T	T	T
	0.4994097768988865	0.4997048884494433	0.4063754647250306	T	T	T
2Ag/Ni(111)	1.0000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni	Ag				
	78	2				
	Selective dynamics					
	Direct					
	0.0000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.9994901784246224	0.0062568810289250	0.4007260376976873	T	T	T
	0.1666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.1670328046980742	0.0832218869558545	0.3140012544548512	T	T	T
	0.0836478950474699	0.1667464364411657	0.2266443018938915	T	T	T
	0.2500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.2557165758309665	0.0062273805525379	0.4003990687922467	T	T	T
	0.4166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.4160947550709011	0.0832231796735812	0.3132090773617051	T	T	T
	0.3333944989534317	0.1671151416992345	0.2266684666466574	T	T	T
	0.5000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.4998977984541852	0.9999483992270939	0.4000546537504093	T	T	T
	0.6666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.6664019608988028	0.0832004804493991	0.3136806781377715	T	T	T
	0.5833948978935695	0.1669484986544774	0.2264181730540429	T	T	T
	0.7500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.7499360149658258	0.0019795341170976	0.4005232004492854	T	T	T
	0.9166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.9162304071289213	0.0830415362096488	0.3136745224767736	T	T	T
	0.8333997499788524	0.1667003749894178	0.2263588077124155	T	T	T
	0.0000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.9984661140156703	0.2492330570078423	0.4009419681182891	T	T	T
	0.1666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.1666503539261797	0.3333246769630946	0.3141796963854304	T	T	T

0.0836478950474699	0.4169014586063042	0.2266443018938915	T	T	T
0.2500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.2434182982047730	0.2449887490813794	0.4008330716893909	T	T	T
0.4166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.4174870586958548	0.3348269100520014	0.3160147301793472	T	T	T
0.3333981983427208	0.4166990991713604	0.2272509059678853	T	T	T
0.5000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.5015808907789534	0.2441774535896926	0.4005709588256963	T	T	T
0.6666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.6667478543860312	0.3333600908082843	0.3135635187229582	T	T	T
0.5832979523219564	0.4170622862049029	0.2272105543164074	T	T	T
0.7500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.7499360149658258	0.2479564808487353	0.4005232004492854	T	T	T
0.9166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.9162304071289213	0.3331878709192679	0.3136745224767736	T	T	T
0.8336327565699619	0.4173286430513059	0.2266738734803937	T	T	T
0.0000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.9994901784246224	0.4932322973957000	0.4007260376976873	T	T	T
0.1666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.1670328046980742	0.5838109177422197	0.3140012544548512	T	T	T
0.0832257840714021	0.6671639501791020	0.2272254392326971	T	T	T
0.2500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.2434182982047730	0.4984295491233937	0.4008330716893909	T	T	T
0.4166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.4174870586958548	0.5826601486438463	0.3160147301793472	T	T	T
0.3333944989534317	0.6662793572541901	0.2266684666466574	T	T	T
0.5000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.6666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.6655991837010973	0.5827995918505451	0.3164086964406678	T	T	T
0.5832979523219564	0.6662356661170392	0.2272105543164074	T	T	T
0.7500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.7496637634832979	0.4921261925362899	0.4006127038768454	T	T	T
0.9166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.9172752079342885	0.5849713339142042	0.3154961028239214	T	T	T
0.8332588356685235	0.6666294178342582	0.2275012885042642	T	T	T
0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.1666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
0.1654115850954909	0.8327052925477503	0.3157927095008404	T	T	T
0.0832257840714021	0.9160628338923118	0.2272254392326971	T	T	T
0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.2557165758309665	0.7494891952784215	0.4003990687922467	T	T	T
0.4166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
0.4160947550709011	0.8328715753973199	0.3132090773617051	T	T	T
0.3326441991862552	0.9163225995931299	0.2266780031161701	T	T	T
0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.5015808907789534	0.7574034371892608	0.4005709588256963	T	T	T
0.6666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
0.6667478543860312	0.8333867635777494	0.3135635187229582	T	T	T
0.5833948978935695	0.9164463992390921	0.2264181730540429	T	T	T
0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.7496637634832979	0.7575375709470080	0.4006127038768454	T	T	T

	0.9166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.9172752079342885	0.8323038740200843	0.3154961028239214	T	T	T
	0.8336327565699619	0.9163041135186489	0.2266738734803937	T	T	T
	0.0009159548183248	0.7504579774091553	0.4239918038861887	T	T	T
	0.4989234579863506	0.4994617289931753	0.4242921167270666	T	T	T
2Au/Ni(111)	1.0000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni	Au				
	78	2				
	Selective dynamics					
	Direct					
	0.0000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.9997155584349215	0.0063185713089098	0.4014869785995998	T	T	T
	0.1666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.1671188462942581	0.0837461840357179	0.3143064167281082	T	T	T
	0.0834562097633409	0.1666468261409548	0.2266957886291863	T	T	T
	0.2500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.2560143082637794	0.0058600210020998	0.4011743716361877	T	T	T
	0.4166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.4163091096683473	0.0833760286822312	0.3138091177027036	T	T	T
	0.3332698311519380	0.1667027267807626	0.2266970715939607	T	T	T
	0.5000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.5008500755553698	0.0004245377776826	0.4004519356915637	T	T	T
	0.6666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.6664446619535553	0.0832218309767754	0.3137248773864840	T	T	T
	0.5831530634030742	0.1668017751462187	0.2265590554115349	T	T	T
	0.7500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.7501590078636013	0.0024900110102806	0.4006306659318568	T	T	T
	0.9166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.9163045114341202	0.0831738964801971	0.3139907624835701	T	T	T
	0.8333817961853356	0.1666913980926665	0.2265072471573788	T	T	T
	0.0000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.9986764464309488	0.2493382232154744	0.4010226670662078	T	T	T
	0.1666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.1662596861517898	0.3331293430758961	0.3142060861172737	T	T	T
	0.0834562097633409	0.4168093836223861	0.2266957886291863	T	T	T
	0.2500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.2442591672626833	0.2454315300583261	0.4014946514529001	T	T	T
	0.4166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.4168136021891371	0.3334084920366678	0.3151346269582262	T	T	T
	0.3333610616211260	0.4166805308105594	0.2271444597171026	T	T	T
	0.5000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.5013447919252911	0.2443780305242100	0.4013375015067524	T	T	T
	0.6666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.6667319849304931	0.3332257677226167	0.3139222984066379	T	T	T
	0.5833204531235907	0.4169042204414524	0.2271193425360707	T	T	T
	0.7500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.7501590078636013	0.2476689968533279	0.4006306659318568	T	T	T
	0.9166669999999968	0.3333330000000032	0.0514190000000028	F	F	F

	0.9163045114341202	0.3331296149539185	0.3139907624835701	T	T	T
	0.8332365946375120	0.4169024989721493	0.2267385905220962	T	T	T
	0.0000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.9997155584349215	0.4933959871260143	0.4014869785995998	T	T	T
	0.1666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.1671188462942581	0.5833726622585331	0.3143064167281082	T	T	T
	0.0832070725371352	0.6670092016527747	0.2271636639220489	T	T	T
	0.2500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.2442591672626833	0.4988276372043572	0.4014946514529001	T	T	T
	0.4166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.4168136021891371	0.5834051101524693	0.3151346269582262	T	T	T
	0.3332698311519380	0.6665671043711683	0.2266970715939607	T	T	T
	0.5000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.6666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.6664454313539423	0.5832227156769676	0.3156326555333067	T	T	T
	0.5833204531235907	0.6664162326821383	0.2271193425360707	T	T	T
	0.7500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.7502104654678377	0.4918230827517007	0.4019822993725981	T	T	T
	0.9166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.9165600394833930	0.5834548202570460	0.3149817020545740	T	T	T
	0.8333422221463636	0.6666711110731782	0.2274083559549140	T	T	T
	0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.1666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.1666091925001822	0.8333040962500959	0.3150200679198889	T	T	T
	0.0832070725371352	0.9161988708843580	0.2271636639220489	T	T	T
	0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.2560143082637794	0.7501542872616795	0.4011743716361877	T	T	T
	0.4166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.4163091096683473	0.8329330809861162	0.3138091177027036	T	T	T
	0.3328720796631188	0.9164365398315653	0.2267594546936138	T	T	T
	0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.5013447919252911	0.7569667614010811	0.4013375015067524	T	T	T
	0.6666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.6667319849304931	0.8335052172078790	0.3139222984066379	T	T	T
	0.5831530634030742	0.9163512882568554	0.2265590554115349	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.7502104654678377	0.7583873827161369	0.4019822993725981	T	T	T
	0.9166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.9165600394833930	0.8331052192263471	0.3149817020545740	T	T	T
	0.8332365946375120	0.9163340956653698	0.2267385905220962	T	T	T
	0.0012236782479604	0.7506118391239767	0.4175555071928017	T	T	T
	0.4995048222340088	0.4997524111170009	0.4182659538189029	T	T	T
2Ni/Cu(111)	1.0000000000000000					
	8.8905944857135406	-5.1329871195825199	-0.0000000000000010			
	0.0000000000000000	10.2659742391650006	0.0000000000000010			
	0.0000000000000000	0.0000000000000000	23.3821328661704015			
	Ni	Cu				
	2	78				
	Selective dynamics					
	Direct					
	0.2507590585598507	0.5003795292799254	0.3795593606484005	T	T	T

0.7498321516565767	0.7499160758282883	0.3796062667083575	T	T	T
0.0000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.9982973732246876	0.9983296914565685	0.3833558522787541	T	T	T
0.1666666667000030	0.0833333332999970	0.0259047434999999	F	F	F
0.1665628695603374	0.0835288129068275	0.2945613206120328	T	T	T
0.0833063570312973	0.1667475800739311	0.2050644057065014	T	T	T
0.2500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.2496663567241271	0.9998331783620671	0.3832065795812625	T	T	T
0.4166666667000030	0.0833333332999970	0.0259047434999999	F	F	F
0.4166764859478249	0.0833382429239080	0.2944931866799578	T	T	T
0.3333609481516433	0.1667149166901396	0.2050586224013529	T	T	T
0.5000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.4999462873984299	0.9994130592607959	0.3831869773720058	T	T	T
0.6666666667000030	0.0833333332999970	0.0259047434999999	F	F	F
0.6668477733692626	0.0831820175577533	0.2944793521219538	T	T	T
0.5833400860527718	0.1666700430763868	0.2050585547294830	T	T	T
0.7500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.7498242454607933	0.9979199967420698	0.3832369900197889	T	T	T
0.9166666667000030	0.0833333332999970	0.0259047434999999	F	F	F
0.9166761500376168	0.0834084361978498	0.2944543214214193	T	T	T
0.8333850549935846	0.1667138949690781	0.2050497269011231	T	T	T
0.0000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.0018259109909735	0.2514789950279379	0.3832610412000506	T	T	T
0.1666666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.1668569199693337	0.3336829783917565	0.2941195060361537	T	T	T
0.0831871590489257	0.4165935795744602	0.2047119563573645	T	T	T
0.2500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.2500267281201118	0.2519987799148993	0.3832581002837827	T	T	T
0.4166666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.4167325758454794	0.3336858394455220	0.2944206624278749	T	T	T
0.3333780330648253	0.4166135259808925	0.2047318974879531	T	T	T
0.5000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.4999462873984299	0.2505332281376269	0.3831869773720058	T	T	T
0.6666666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.6668477733692626	0.3336657557114933	0.2944793521219538	T	T	T
0.5833073342869426	0.4167006316922794	0.2050534219286675	T	T	T
0.7500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.7505033010124080	0.2502516505062005	0.3830825285017525	T	T	T
0.9166666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.9168764120774568	0.3334382059887204	0.2943877458301927	T	T	T
0.8333850549935846	0.4166711601245225	0.2050497269011231	T	T	T
0.0000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.0018259109909735	0.5003469159630356	0.3832610412000506	T	T	T
0.1666666667000030	0.5833333332999970	0.0259047434999999	F	F	F
0.1668569199693337	0.5831739414775754	0.2941195060361537	T	T	T
0.0833063570312973	0.6665587770573822	0.2050644057065014	T	T	T
0.2500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.4166666667000030	0.5833333332999970	0.0259047434999999	F	F	F
0.4165977035596526	0.5832988517298148	0.2940199983254956	T	T	T
0.3333780330648253	0.6667645071839416	0.2047318974879531	T	T	T
0.5000000000000000	0.5000000000000000	0.1155258754999977	F	F	F

	0.5001677263390860	0.5019400471531199	0.3833839014141347	T	T	T
	0.666666667000030	0.583333332999970	0.0259047434999999	F	F	F
	0.6665433282791042	0.5835700127685186	0.2941386855542092	T	T	T
	0.5830955831639528	0.6665477916319844	0.2047138955697889	T	T	T
	0.7500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.7498242454607933	0.5019042487187164	0.3832369900197889	T	T	T
	0.916666667000030	0.583333332999970	0.0259047434999999	F	F	F
	0.9166761500376168	0.5832677137397582	0.2944543214214193	T	T	T
	0.8333966248261788	0.6665685135153723	0.2047400189798338	T	T	T
	0.0000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.9982973732246876	0.7499676817681262	0.3833558522787541	T	T	T
	0.166666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.1665628695603374	0.8330340565535010	0.2945613206120328	T	T	T
	0.0832867778461477	0.9166433889730783	0.2050766591386406	T	T	T
	0.2500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.2500267281201118	0.7480279482052126	0.3832581002837827	T	T	T
	0.416666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.4167325758454794	0.8330467362999485	0.2944206624278749	T	T	T
	0.3333609481516433	0.9166460315615126	0.2050586224013529	T	T	T
	0.5000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.5001677263390860	0.7482276791859661	0.3833839014141347	T	T	T
	0.666666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.6665433282791042	0.8329733154105838	0.2941386855542092	T	T	T
	0.5833073342869426	0.9166067026946720	0.2050534219286675	T	T	T
	0.7500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.916666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.9164086969752248	0.8332043484376115	0.2941449686718016	T	T	T
	0.8333966248261788	0.9168281114108154	0.2047400189798338	T	T	T
2Pd/Cu(111)	1.0000000000000000					
	8.8905944857135406	-5.1329871195825199	-0.0000000000000010			
	0.0000000000000000	10.2659742391650006	0.0000000000000010			
	0.0000000000000000	0.0000000000000000	23.3821328661704015			
	Pd	Cu				
	2	78				
	Selective dynamics					
	Direct					
	0.2495143164211910	0.4997571582105991	0.3868596702594189	T	T	T
	0.7507072329355395	0.7503536164677698	0.3867127327151820	T	T	T
	0.0000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.0034005587720500	0.0029345109008929	0.3835791143994385	T	T	T
	0.166666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.1667412596187887	0.0833535675878920	0.2940626307281491	T	T	T
	0.0833100438456000	0.1669169886672108	0.2051061865942359	T	T	T
	0.2500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.2505878550297993	0.0002939275149032	0.3830104827994560	T	T	T
	0.416666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.4166772470377822	0.0833386234688902	0.2940002196662519	T	T	T
	0.3333914321991855	0.1668373860586527	0.2048661050559204	T	T	T
	0.5000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.4999509547089858	0.0011929048844195	0.3831109913578672	T	T	T
	0.666666667000030	0.083333332999970	0.0259047434999999	F	F	F

0.6666218964625017	0.0833840747328694	0.2941371730384077	T	T	T
0.5834054295603792	0.1667027148301941	0.2047936514250637	T	T	T
0.7500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.7498214153109970	0.0035168249746249	0.3835765185018687	T	T	T
0.9166666667000030	0.083333332999970	0.0259047434999999	F	F	F
0.9164274578841756	0.0829643588831388	0.2943988141817613	T	T	T
0.8334956216256373	0.1667812457006832	0.2050601733196800	T	T	T
0.0000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.9967215277113937	0.2469791893389583	0.3836354756913849	T	T	T
0.1666666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.1663132565693957	0.3327065621588048	0.2942909927063653	T	T	T
0.0832938029479280	0.4166469015239684	0.2048535805070983	T	T	T
0.2500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.2501560584235492	0.2464349168805100	0.3835669492832352	T	T	T
0.4166666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.4165150309370205	0.3333153342555590	0.2943256811482158	T	T	T
0.3333633500184945	0.4167803243573118	0.2049519490879916	T	T	T
0.5000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.4999509547089858	0.2487580498245663	0.3831109913578672	T	T	T
0.6666666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.6666218964625017	0.3332378216296163	0.2941371730384077	T	T	T
0.5833377224327023	0.4168626743618091	0.2050790056646576	T	T	T
0.7500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.7493655298756750	0.2496827649378375	0.3830727460931698	T	T	T
0.9166666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.9169123339994982	0.3334561669497518	0.2944470690783589	T	T	T
0.8334956216256373	0.4167143760249559	0.2050601733196800	T	T	T
0.0000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.9967215277113937	0.4997423383724353	0.3836354756913849	T	T	T
0.1666666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.1663132565693957	0.5836066943105749	0.2942909927063653	T	T	T
0.0833100438456000	0.6663930552783981	0.2051061865942359	T	T	T
0.2500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.4166666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.4175784020672779	0.5837892009836310	0.2945520003658189	T	T	T
0.3333633500184945	0.6665830257611987	0.2049519490879916	T	T	T
0.5000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.5000951927901838	0.4956167471361326	0.3841458318771913	T	T	T
0.6666666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.6663643990694084	0.5827220691541868	0.2942113416797980	T	T	T
0.5829734250091434	0.6664867125545726	0.2049749776906538	T	T	T
0.7500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.7498214153109970	0.4963045903363650	0.3835765185018687	T	T	T
0.9166666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.9164274578841756	0.5834630989010279	0.2943988141817613	T	T	T
0.8333151608406126	0.6665883061074780	0.2047943076316159	T	T	T
0.0000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
0.0034005587720500	0.7504660478711500	0.3835791143994385	T	T	T
0.1666666667000030	0.833333332999970	0.0259047434999999	F	F	F
0.1667412596187887	0.8333876919308878	0.2940626307281491	T	T	T
0.0830909289922559	0.9165454645461324	0.2049409397098074	T	T	T

	0.2500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.2501560584235492	0.7537211415430463	0.3835669492832352	T	T	T
	0.4166666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.4165150309370205	0.8331996965814454	0.2943256811482158	T	T	T
	0.3333914321991855	0.9165540462405488	0.2048661050559204	T	T	T
	0.5000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.5000951927901838	0.7544784456540441	0.3841458318771913	T	T	T
	0.6666666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.6663643990694084	0.8336423298152127	0.2942113416797980	T	T	T
	0.5833377224327023	0.9164750481709021	0.2050790056646576	T	T	T
	0.7500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.9166666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.9173581286584209	0.8336790642792025	0.2940907368935726	T	T	T
	0.8333151608406126	0.9167268548331435	0.2047943076316159	T	T	T
2Pt/Cu(111)	1.0000000000000000					
	8.8905944857135406	-5.1329871195825199	-0.0000000000000010			
	0.0000000000000000	10.2659742391650006	0.0000000000000010			
	0.0000000000000000	0.0000000000000000	23.3821328661704015			
	Pt	Cu				
	2	78				
	Selective dynamics					
	Direct					
	0.2492381937355124	0.4996190968677562	0.3846624553383337	T	T	T
	0.7510506486622258	0.7505253243311129	0.3846743124807038	T	T	T
	0.0000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.0026701171206326	0.0019838822535204	0.3843627896819809	T	T	T
	0.1666666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.1668409479931666	0.0835720395074534	0.2945732196380659	T	T	T
	0.0832980669190572	0.1667492177457857	0.2050392031234033	T	T	T
	0.2500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.2508276959789111	0.0004138479894555	0.3832303774949576	T	T	T
	0.4166666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.4166889109297660	0.0833444554148785	0.2941638458139268	T	T	T
	0.3333520347285616	0.1667245090571970	0.2049954413391010	T	T	T
	0.5000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.4998854388689705	0.0008863250971199	0.3832180571035611	T	T	T
	0.6666666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.6668552272045899	0.0833203327038224	0.2944585897024414	T	T	T
	0.5834453288894090	0.1667226644947090	0.2050269687660498	T	T	T
	0.7500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.7497564377422508	0.0024234300662036	0.3843138599456166	T	T	T
	0.9166666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.9166240634284477	0.0836178549615142	0.2945891577395771	T	T	T
	0.8333761831603034	0.1667118449010586	0.2050587273019407	T	T	T
	0.0000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
	0.9975306597590331	0.2477489543868857	0.3842803010690730	T	T	T
	0.1666666667000030	0.333333332999970	0.0259047434999999	F	F	F
	0.1657762783134283	0.3315762383269344	0.2936446464083000	T	T	T
	0.0830745161218174	0.4165372581109131	0.2047520958918075	T	T	T
	0.2500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
	0.2499940655831354	0.2475367588220257	0.3843395856657097	T	T	T

0.416666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.4167500110546128	0.3331418609902871	0.2945136724442549	T	T	T
0.3334283158744752	0.4165489758928151	0.2047741024901187	T	T	T
0.5000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.4998854388689705	0.2489991137718577	0.3832180571035611	T	T	T
0.666666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.6668552272045899	0.3335348944007586	0.2944585897024414	T	T	T
0.5833288884201722	0.4167175953405020	0.2050430892983306	T	T	T
0.7500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.7494403980328550	0.2497201990164274	0.3831498341068972	T	T	T
0.916666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.9162573141122990	0.3331286570061451	0.2944427224861901	T	T	T
0.8333761831603034	0.4166643383592536	0.2050587273019407	T	T	T
0.0000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.9975306597590331	0.4997817053721474	0.3842803010690730	T	T	T
0.166666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.1657762783134283	0.5842000398864849	0.2936446464083000	T	T	T
0.0832980669190572	0.6665488492732805	0.2050392031234033	T	T	T
0.2500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.416666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.4179609225395691	0.5839804612197801	0.2937377426709671	T	T	T
0.3334283158744752	0.6668793400816689	0.2047741024901187	T	T	T
0.5000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.5001169129500602	0.4971674031395015	0.3854445151009517	T	T	T
0.666666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.6656931345840299	0.5815863745702923	0.2937479993234571	T	T	T
0.5829348334824764	0.6664674167912393	0.2047222628265073	T	T	T
0.7500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.7497564377422508	0.4973330076760471	0.3843138599456166	T	T	T
0.916666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.9166240634284477	0.5830062083669244	0.2945891577395771	T	T	T
0.8334350235097562	0.6664700723991118	0.2047220563467487	T	T	T
0.0000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
0.0026701171206326	0.7506862348671122	0.3843627896819809	T	T	T
0.166666667000030	0.833333332999970	0.0259047434999999	F	F	F
0.1668409479931666	0.8332689083857046	0.2945732196380659	T	T	T
0.0833519485866274	0.9166759743433218	0.2049958791557433	T	T	T
0.2500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
0.2499940655831354	0.7524573067611026	0.3843395856657097	T	T	T
0.416666667000030	0.833333332999970	0.0259047434999999	F	F	F
0.4167500110546128	0.8336081499643169	0.2945136724442549	T	T	T
0.3333520347285616	0.9166275257713805	0.2049954413391010	T	T	T
0.5000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
0.5001169129500602	0.7529495098105586	0.3854445151009517	T	T	T
0.666666667000030	0.833333332999970	0.0259047434999999	F	F	F
0.6656931345840299	0.8341067599137287	0.2937479993234571	T	T	T
0.5833288884201722	0.9166112931796718	0.2050430892983306	T	T	T
0.7500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
0.916666667000030	0.833333332999970	0.0259047434999999	F	F	F
0.9184945741281998	0.8342472870140955	0.2934929573351738	T	T	T
0.8334350235097562	0.9169649512106535	0.2047220563467487	T	T	T

(3) 2X-S2	
2Cu/Ni(111)	1.0000000000000000 8.6224000674449712 -4.9781450000000014 0.0000000000000000 0.0000000000000000 9.9562900000000010 0.0000000000000000 0.0000000000000000 0.0000000000000000 23.1292800000000014 Ni Cu 78 2 Selective dynamics Direct 0.0000000000000000 0.0000000000000000 0.1392870000000030 F F F 0.1666669999999968 0.0833330000000032 0.0514190000000028 F F F 0.1664709468822853 0.0832514176420984 0.3148109531381215 T T T 0.0833963786408000 0.1667472429461126 0.2270130835289483 T T T 0.2500000000000000 0.0000000000000000 0.1392870000000030 F F F 0.2520414574532656 0.9997017941208619 0.4010389243898939 T T T 0.4166669999999968 0.0833330000000032 0.0514190000000028 F F F 0.4163324103648300 0.0836822142906622 0.3143288197432568 T T T 0.3333331278612343 0.1666524728787613 0.2266631076177539 T T T 0.5000000000000000 0.0000000000000000 0.1392870000000030 F F F 0.5000247145534926 0.0000047248833557 0.4015163065349339 T T T 0.6666669999999968 0.0833330000000032 0.0514190000000028 F F F 0.6669626800284604 0.0835046168017871 0.3143929319504122 T T T 0.5833101784082908 0.1667864704432468 0.2269049789076069 T T T 0.7500000000000000 0.0000000000000000 0.1392870000000030 F F F 0.7479469389419526 0.0000502842694188 0.4011308818169348 T T T 0.9166669999999968 0.0833330000000032 0.0514190000000028 F F F 0.9169504224656025 0.0830495775343976 0.3149804179625156 T T T 0.8333317446566131 0.1666682553433868 0.2267150662849600 T T T 0.0000000000000000 0.2500000000000000 0.1392870000000030 F F F -0.0000502842694191 0.2520530610580473 0.4011308818169348 T T T 0.1666669999999968 0.3333330000000032 0.0514190000000028 F F F 0.1666963805999432 0.3333107653396231 0.3145751267439955 T T T 0.0834658862287811 0.4165418788470663 0.2268545847551247 T T T 0.2500000000000000 0.2500000000000000 0.1392870000000030 F F F 0.2497558889014308 0.2502461533818646 0.4009960362226635 T T T 0.4166669999999968 0.3333330000000032 0.0514190000000028 F F F 0.4167814790420526 0.3335526934435641 0.3148142620671902 T T T 0.3332782670348213 0.4166050413167459 0.2270161182589778 T T T 0.5000000000000000 0.2500000000000000 0.1392870000000030 F F F 0.5002936982819383 0.2479496729650969 0.4010534188042187 T T T 0.6666669999999968 0.3333330000000032 0.0514190000000028 F F F 0.6666402976265580 0.3333597023734421 0.3145102166114240 T T T 0.5833133617817357 0.4166866382182645 0.2270262397287145 T T T 0.7500000000000000 0.2500000000000000 0.1392870000000030 F F F 0.7500919599041457 0.2499080400958544 0.4011494755017564 T T T 0.9166669999999968 0.3333330000000032 0.0514190000000028 F F F 0.9164953831982128 0.3330373199715398 0.3143929319504122 T T T 0.8332135295567533 0.4166898215917093 0.2269049789076069 T T T 0.0000000000000000 0.5000000000000000 0.1392870000000030 F F F -0.0000047248833557 0.4999752854465076 0.4015163065349339 T T T 0.1666669999999968 0.5833330000000032 0.0514190000000028 F F F

	0.1669713431493058	0.5835571755362100	0.3144009026672495	T	T	T
	0.0832946129714476	0.6667583947225895	0.2268949472713599	T	T	T
	0.2500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.2479063121630758	0.5000475252279201	0.4011338055857941	T	T	T
	0.4166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.4169472497008107	0.5830527502991892	0.3149786754085754	T	T	T
	0.3333139786893413	0.6666860213106588	0.2267130171319106	T	T	T
	0.5000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.6666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.6664473065564358	0.5832185209579474	0.3148142620671902	T	T	T
	0.5833949586832536	0.6667217329651787	0.2270161182589778	T	T	T
	0.7500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.7520503270349032	0.4997063017180621	0.4010534188042187	T	T	T
	0.9166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.9163177857093376	0.5836675896351703	0.3143288197432568	T	T	T
	0.8333475271212387	0.6666668721387655	0.2266631076177539	T	T	T
	0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.0002982058791381	0.7479585425467344	0.4010389243898939	T	T	T
	0.1666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.1666107632357261	0.8333892367642739	0.3144498909675029	T	T	T
	0.0833005783942279	0.9166994216057721	0.2269981605293766	T	T	T
	0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.2500843243642336	0.7499156756357666	0.4011434189706967	T	T	T
	0.4166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.4164428244637900	0.8330286568506943	0.3144009026672495	T	T	T
	0.3332416052774102	0.9167053870285528	0.2268949472713599	T	T	T
	0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.4999524747720799	0.7520936878369242	0.4011338055857941	T	T	T
	0.6666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.6666892346603770	0.8333036194000567	0.3145751267439955	T	T	T
	0.5834581211529338	0.9165341137712190	0.2268545847551247	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.7497538466181352	0.7502441110985689	0.4009960362226635	T	T	T
	0.9166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.9167485823579014	0.8335290531177149	0.3148109531381215	T	T	T
	0.8332527570538877	0.9166036213591999	0.2270130835289483	T	T	T
	0.0001004920158921	-0.0001004920158921	0.4063337327894365	T	T	T
	0.5000867634644749	0.4999132365355249	0.4063257915108534	T	T	T
2Ag/Ni(111)	1.0000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni	Ag				
	78	2				
	Selective dynamics					
	Direct					
	0.0000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.1666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.1654919809875733	0.0824430139675662	0.3153686076425534	T	T	T
	0.0831980867279987	0.1666645866555102	0.2272615100095693	T	T	T
	0.2500000000000000	0.0000000000000000	0.1392870000000030	F	F	F

0.2557397095260371	0.9985905112257922	0.4004211523930338	T	T	T
0.4166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
0.4160739298824423	0.0838843922058497	0.3133199909574174	T	T	T
0.3329762038493901	0.1669991504205655	0.2267763125866274	T	T	T
0.5000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
0.4999829600132309	0.0000181966542522	0.4006009196549919	T	T	T
0.6666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
0.6669547702264744	0.0836603968940067	0.3137481900767684	T	T	T
0.5832965548772955	0.1668057616726980	0.2265018800067073	T	T	T
0.7500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
0.7442095936852170	0.0006590199646622	0.4009074620616023	T	T	T
0.9166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
0.9175404301633967	0.0824595698366035	0.3160870150688924	T	T	T
0.8334970818718604	0.1665029181281399	0.2267258370159359	T	T	T
0.0000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.9993409800353377	0.2557904063147829	0.4009074620616023	T	T	T
0.1666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.1666676813330445	0.3332952771307458	0.3144885809379840	T	T	T
0.0835244546754982	0.4164761910485231	0.2266578100832831	T	T	T
0.2500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.2495594313810038	0.2503890203014343	0.4000902035094024	T	T	T
0.4166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.4175149842634656	0.3344825579634750	0.3153572536739525	T	T	T
0.3333561261188935	0.4167776583352459	0.2272545800667020	T	T	T
0.5000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.5013803090205803	0.2442337934650100	0.4004225427639775	T	T	T
0.6666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.6666163126852842	0.3333836873147155	0.3138958682822745	T	T	T
0.5832149792589562	0.4167850207410440	0.2269949542782341	T	T	T
0.7500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.7503138406323845	0.2496861593676157	0.4006553224599623	T	T	T
0.9166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.9163396031059934	0.3330452297735257	0.3137481900767684	T	T	T
0.8331942383273022	0.4167034451227045	0.2265018800067073	T	T	T
0.0000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
-0.0000181966542522	0.5000170399867691	0.4006009196549919	T	T	T
0.1666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.1669699389796783	0.5836545834865353	0.3137332643707745	T	T	T
0.0832957413053564	0.6668294777944189	0.2264945149001310	T	T	T
0.2500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.2441774163266176	0.5006083442705148	0.4008977466699166	T	T	T
0.4166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.4175399003954449	0.5824600996045557	0.3160818003962807	T	T	T
0.3335106865035471	0.6664893134964526	0.2267341635359659	T	T	T
0.5000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.6666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.6655174420365250	0.5824850157365343	0.3153572536739525	T	T	T
0.5832223416647540	0.6666438738811062	0.2272545800667020	T	T	T
0.7500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.7557662065349899	0.4986196909794199	0.4004225427639775	T	T	T
0.9166669999999968	0.5833330000000032	0.0514190000000028	F	F	F

	0.9161156077941501	0.5839260701175573	0.3133199909574174	T	T	T
	0.8330008495794344	0.6670237961506097	0.2267763125866274	T	T	T
	0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.0014094887742076	0.7442602904739630	0.4004211523930338	T	T	T
	0.1666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.1666285934342654	0.8333714065657346	0.3138882445458556	T	T	T
	0.0832001540567854	0.9167998459432147	0.2269820312164036	T	T	T
	0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.2503358956421848	0.7496641043578153	0.4006534948032531	T	T	T
	0.4166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.4163454165134647	0.8330300610203218	0.3137332643707745	T	T	T
	0.3331705222055812	0.9167042586946438	0.2264945149001310	T	T	T
	0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.4993916557294852	0.7558225836733824	0.4008977466699166	T	T	T
	0.6666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.6667047228692542	0.8333323186669555	0.3144885809379840	T	T	T
	0.5835238089514772	0.9164755453245019	0.2266578100832831	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.7496109796985658	0.7504405686189962	0.4000902035094024	T	T	T
	0.9166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.9175569860324337	0.8345080190124270	0.3153686076425534	T	T	T
	0.8333354133444898	0.9168019132720011	0.2272615100095693	T	T	T
	0.0002752451639364	-0.0002752451639364	0.4246423711150816	T	T	T
	0.5002788770633647	0.4997211229366357	0.4245530210675836	T	T	T
2Au/Ni(111)	1.0000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni Au					
	78 2					
	Selective dynamics					
	Direct					
	0.0000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.1666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.1669403821752080	0.0832127078350756	0.3148844471575838	T	T	T
	0.0834008181267098	0.1666944140185209	0.2271764031969357	T	T	T
	0.2500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.2558127241207254	0.9985171836320919	0.4012656350039157	T	T	T
	0.4166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.4164689101840636	0.0835510182531769	0.3140168163673764	T	T	T
	0.3333009687899269	0.1666757404947928	0.2267708419614654	T	T	T
	0.5000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.5002430907706937	-0.0002299228748868	0.4010706807232566	T	T	T
	0.6666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.6669715778763607	0.0834663149926912	0.3141403812324963	T	T	T
	0.5833834687862200	0.1667407296271841	0.2266728919338589	T	T	T
	0.7500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.7446644311945053	0.0007074055753193	0.4016157773813670	T	T	T
	0.9166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.9169232036483460	0.0830767963516540	0.3150964070054033	T	T	T
	0.8333880408451303	0.1666119591548700	0.2267359571572957	T	T	T

0.0000000000000000	0.2500000000000000	0.1392870000000030	F F F
0.9992925944246804	0.2553355688054947	0.4016157773813670	T T T
0.1666669999999968	0.3333330000000032	0.0514190000000028	F F F
0.1666539734385929	0.3333368772379538	0.3145778703067108	T T T
0.0835556059597225	0.4164359613091703	0.2267847371913909	T T T
0.2500000000000000	0.2500000000000000	0.1392870000000030	F F F
0.2498785439090098	0.2501079245400158	0.4018655486554383	T T T
0.4166669999999968	0.3333330000000032	0.0514190000000028	F F F
0.4168073908334735	0.3330602000113936	0.3148879504401659	T T T
0.3333018330512799	0.4166112728721509	0.2271728384324307	T T T
0.5000000000000000	0.2500000000000000	0.1392870000000030	F F F
0.5015102412912175	0.2442096051518732	0.4012658984255964	T T T
0.6666669999999968	0.3333330000000032	0.0514190000000028	F F F
0.6667658348200447	0.3332341651799556	0.3141124616639524	T T T
0.5832915828476506	0.4167084171523491	0.2269975830290610	T T T
0.7500000000000000	0.2500000000000000	0.1392870000000030	F F F
0.7503334121582220	0.2496665878417780	0.4008949747306049	T T T
0.9166669999999968	0.3333330000000032	0.0514190000000028	F F F
0.9165336850073090	0.3330284221236395	0.3141403812324963	T T T
0.8332592703728163	0.4166165312137798	0.2266728919338589	T T T
0.0000000000000000	0.5000000000000000	0.1392870000000030	F F F
0.0002299228748868	0.4997569092293065	0.4010706807232566	T T T
0.1666669999999968	0.5833330000000032	0.0514190000000028	F F F
0.1669733369780717	0.5834754088527025	0.3141328451540289	T T T
0.0833798318723247	0.6667443587852477	0.2266749337338303	T T T
0.2500000000000000	0.5000000000000000	0.1392870000000030	F F F
0.2446538887488882	0.5006857628652640	0.4016127736573190	T T T
0.4166669999999968	0.5833330000000032	0.0514190000000028	F F F
0.4169250865007579	0.5830749134992418	0.3150976451848880	T T T
0.3333859251358532	0.6666140748641461	0.2267377309616490	T T T
0.5000000000000000	0.5000000000000000	0.1392870000000030	F F F
0.6666669999999968	0.5833330000000032	0.0514190000000028	F F F
0.6669397999886062	0.5831926091665268	0.3148879504401659	T T T
0.5833887271278495	0.6666981669487199	0.2271728384324307	T T T
0.7500000000000000	0.5000000000000000	0.1392870000000030	F F F
0.7557903948481264	0.4984897587087823	0.4012658984255964	T T T
0.9166669999999968	0.5833330000000032	0.0514190000000028	F F F
0.9164489817468231	0.5835310898159367	0.3140168163673764	T T T
0.8333242595052072	0.6666990312100732	0.2267708419614654	T T T
0.0000000000000000	0.7500000000000000	0.1392870000000030	F F F
0.0014828163679077	0.7441872758792750	0.4012656350039157	T T T
0.1666669999999968	0.8333330000000032	0.0514190000000028	F F F
0.1667708580768475	0.8332291419231528	0.3141198490508943	T T T
0.0832915119205771	0.9167084880794224	0.2270027137913916	T T T
0.2500000000000000	0.7500000000000000	0.1392870000000030	F F F
0.2503283455030067	0.7496716544969935	0.4008995410296275	T T T
0.4166669999999968	0.8333330000000032	0.0514190000000028	F F F
0.4165245911472976	0.8330266630219284	0.3141328451540289	T T T
0.3332556412147522	0.9166201681276754	0.2266749337338303	T T T
0.5000000000000000	0.7500000000000000	0.1392870000000030	F F F
0.4993142371347362	0.7553461112511115	0.4016127736573190	T T T

	0.6666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.6666631227620464	0.8333460265614068	0.3145778703067108	T	T	T
	0.5835640386908294	0.9164443940402773	0.2267847371913909	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.7498920754599843	0.7501214560909906	0.4018655486554383	T	T	T
	0.9166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.9167872921649247	0.8330596178247918	0.3148844471575838	T	T	T
	0.8333055859814786	0.9165991818732903	0.2271764031969357	T	T	T
	0.0003737552283686	-0.0003737552283686	0.4179993232980767	T	T	T
	0.5003639401215907	0.4996360598784096	0.4179954704798238	T	T	T
2Ni/Cu(111)	1.0000000000000000					
	8.8905944857135406	-5.1329871195825199	-0.0000000000000010			
	0.0000000000000000	10.2659742391650006	0.0000000000000010			
	0.0000000000000000	0.0000000000000000	23.3821328661704015			
	Ni	Cu				
	2	78				
	Selective dynamics					
	Direct					
	0.4997158248754447	0.2498579124377224	0.3794935656758060	T	T	T
	0.4997158248754447	0.7498579124377222	0.3794935656758060	T	T	T
	0.0000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.0001474366891749	0.0000737183445839	0.3831648703152757	T	T	T
	0.1666666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.1668645199273266	0.0834322599136589	0.2944354813639935	T	T	T
	0.0833740682576885	0.1666613379467153	0.2050793704716497	T	T	T
	0.2500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.2521535908813487	0.0017252463429921	0.3833334110549843	T	T	T
	0.4166666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.4169710424698480	0.0835336459755928	0.2941319663773826	T	T	T
	0.3332378037547559	0.1666189019273789	0.2047403535579549	T	T	T
	0.5000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.4996919788153937	0.9998459894077003	0.3833008924034275	T	T	T
	0.6666666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.6665192545300086	0.0832596272150035	0.2943001717093512	T	T	T
	0.5834858014807288	0.1665893351300133	0.2047250692214658	T	T	T
	0.7500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.7477317057288921	0.9981177068236152	0.3831822925810763	T	T	T
	0.9166666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.9163968591347306	0.0831994152120290	0.2944842436007085	T	T	T
	0.8332963146590435	0.1666481573795263	0.2050567719999362	T	T	T
	0.0000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
	-0.0000643844706047	0.2499678077646942	0.3830310379030574	T	T	T
	0.1666666667000030	0.333333332999970	0.0259047434999999	F	F	F
	0.1670329340905497	0.3335164669952740	0.2945611550484280	T	T	T
	0.0833740682576885	0.4167127304109750	0.2050793704716497	T	T	T
	0.2500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
	0.2521535908813487	0.2504283445383496	0.3833334110549843	T	T	T
	0.4166666667000030	0.333333332999970	0.0259047434999999	F	F	F
	0.4169710424698480	0.3334373963942462	0.2941319663773826	T	T	T
	0.3334908100945780	0.4167454050972899	0.2050765012984110	T	T	T
	0.5000000000000000	0.2500000000000000	0.1155258754999977	F	F	F

	0.666666667000030	0.333333332999970	0.025904743499999	F	F	F
	0.6662445806721705	0.3331222902860808	0.2940660723807266	T	T	T
	0.5834858014807288	0.4168964664507175	0.2047250692214658	T	T	T
	0.7500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
	0.7477317057288921	0.2496139989052769	0.3831822925810763	T	T	T
	0.916666667000030	0.333333332999970	0.025904743499999	F	F	F
	0.9163968591347306	0.3331974438226853	0.2944842436007085	T	T	T
	0.8332559605669173	0.4166279803334631	0.2050537993798670	T	T	T
	0.0000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.0001474366891749	0.5000737183445841	0.3831648703152757	T	T	T
	0.166666667000030	0.583333332999970	0.025904743499999	F	F	F
	0.1668645199273266	0.5834322599136588	0.2944354813639935	T	T	T
	0.0833740682576885	0.6666613379467153	0.2050793704716497	T	T	T
	0.2500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.2521535908813487	0.5017252463429921	0.3833334110549843	T	T	T
	0.416666667000030	0.583333332999970	0.025904743499999	F	F	F
	0.4169710424698480	0.5835336459755928	0.2941319663773826	T	T	T
	0.3332378037547559	0.6666189019273789	0.2047403535579549	T	T	T
	0.5000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.4996919788153937	0.4998459894077004	0.3833008924034275	T	T	T
	0.666666667000030	0.583333332999970	0.025904743499999	F	F	F
	0.6665192545300086	0.5832596272150035	0.2943001717093512	T	T	T
	0.5834858014807288	0.6665893351300133	0.2047250692214658	T	T	T
	0.7500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.7477317057288921	0.4981177068236153	0.3831822925810763	T	T	T
	0.916666667000030	0.583333332999970	0.025904743499999	F	F	F
	0.9163968591347306	0.5831994152120291	0.2944842436007085	T	T	T
	0.8332963146590435	0.6666481573795260	0.2050567719999362	T	T	T
	0.0000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	-0.0000643844706047	0.7499678077647012	0.3830310379030574	T	T	T
	0.166666667000030	0.833333332999970	0.025904743499999	F	F	F
	0.1670329340905497	0.8335164669952740	0.2945611550484280	T	T	T
	0.0833740682576885	0.9167127304109819	0.2050793704716497	T	T	T
	0.2500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.2521535908813487	0.7504283445383496	0.3833334110549843	T	T	T
	0.416666667000030	0.833333332999970	0.025904743499999	F	F	F
	0.4169710424698480	0.8334373963942461	0.2941319663773826	T	T	T
	0.3334908100945780	0.9167454050972900	0.2050765012984110	T	T	T
	0.5000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.666666667000030	0.833333332999970	0.025904743499999	F	F	F
	0.6662445806721705	0.8331222902860808	0.2940660723807266	T	T	T
	0.5834858014807288	0.9168964664507174	0.2047250692214658	T	T	T
	0.7500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.7477317057288921	0.7496139989052768	0.3831822925810763	T	T	T
	0.916666667000030	0.833333332999970	0.025904743499999	F	F	F
	0.9163968591347306	0.8331974438226855	0.2944842436007085	T	T	T
	0.8332559605669173	0.9166279803334630	0.2050537993798670	T	T	T
2Pd/Cu(111)	1.000000000000000					
	8.8905944857135406	-5.1329871195825199	-0.0000000000000010			
	0.0000000000000000	10.2659742391650006	0.0000000000000010			
	0.0000000000000000	0.0000000000000000	23.3821328661704015			

Pd Cu
2 78
Selective dynamics
Direct

0.4999183260040048	0.2499591630020059	0.3865557557270350	T	T	T
0.4999183260040048	0.7499591630020058	0.3865557557270350	T	T	T
0.0000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.0000999937193728	0.0000499968596829	0.3831449606666890	T	T	T
0.1666666667000030	0.083333332999970	0.0259047434999999	F	F	F
0.1668475510628119	0.0834237754814051	0.2942821055842286	T	T	T
0.0833503219899182	0.1666128943488833	0.2049156495439296	T	T	T
0.2500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.2460952130588883	0.9967215050624213	0.3835963132219139	T	T	T
0.4166666667000030	0.083333332999970	0.0259047434999999	F	F	F
0.4163012189095653	0.0827793707159929	0.2941947838953959	T	T	T
0.3332835632525736	0.1666417816762912	0.2047626734614772	T	T	T
0.5000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.4997595185697331	0.9998797592848631	0.3840929361182922	T	T	T
0.6666666667000030	0.083333332999970	0.0259047434999999	F	F	F
0.6665063062668154	0.0832531530834032	0.2946973702278539	T	T	T
0.5834537062992569	0.1665670811933659	0.2049205119579500	T	T	T
0.7500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.7539701134045333	0.0032530136737407	0.3836316340123037	T	T	T
0.9166666667000030	0.083333332999970	0.0259047434999999	F	F	F
0.9167565538732504	0.0833456960225736	0.2941775675669597	T	T	T
0.8330593009051577	0.1665296505025833	0.2050712495936068	T	T	T
0.0000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.0000788245200769	0.2500394122600420	0.3829907079440334	T	T	T
0.1666666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.1666447130204523	0.3333223564602217	0.2940995765189647	T	T	T
0.0833503219899182	0.4167374277410509	0.2049156495439296	T	T	T
0.2500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.2460952130588883	0.2493737079964669	0.3835963132219139	T	T	T
0.4166666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.4163012189095653	0.3335218480935635	0.2941947838953959	T	T	T
0.3336065492747330	0.4168032746873709	0.2051337164028840	T	T	T
0.5000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.6666666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.6673794048148052	0.3336897023574017	0.2942538500943039	T	T	T
0.5834537062992569	0.4168866252058998	0.2049205119579500	T	T	T
0.7500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.7539701134045333	0.2507170997307926	0.3836316340123037	T	T	T
0.9166666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.9167565538732504	0.3334108577506680	0.2941775675669597	T	T	T
0.8330407602047123	0.4165203801523570	0.2050145408003460	T	T	T
0.0000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.0000999937193728	0.5000499968596829	0.3831449606666890	T	T	T
0.1666666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.1668475510628119	0.5834237754814050	0.2942821055842286	T	T	T
0.0833503219899182	0.6666128943488835	0.2049156495439296	T	T	T
0.2500000000000000	0.5000000000000000	0.1155258754999977	F	F	F

	0.2460952130588883	0.4967215050624214	0.3835963132219139	T	T	T
	0.4166666667000030	0.5833333332999970	0.0259047434999999	F	F	F
	0.4163012189095653	0.5827793707159931	0.2941947838953959	T	T	T
	0.3332835632525736	0.6666417816762912	0.2047626734614772	T	T	T
	0.5000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.4997595185697331	0.4998797592848630	0.3840929361182922	T	T	T
	0.6666666667000030	0.5833333332999970	0.0259047434999999	F	F	F
	0.6665063062668154	0.5832531530834033	0.2946973702278539	T	T	T
	0.5834537062992569	0.6665670811933659	0.2049205119579500	T	T	T
	0.7500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.7539701134045333	0.5032530136737406	0.3836316340123037	T	T	T
	0.9166666667000030	0.5833333332999970	0.0259047434999999	F	F	F
	0.9167565538732504	0.5833456960225736	0.2941775675669597	T	T	T
	0.8330593009051577	0.6665296505025833	0.2050712495936068	T	T	T
	0.0000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.0000788245200769	0.7500394122600420	0.3829907079440334	T	T	T
	0.1666666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.1666447130204523	0.8333223564602218	0.2940995765189647	T	T	T
	0.0833503219899182	0.9167374277410509	0.2049156495439296	T	T	T
	0.2500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.2460952130588883	0.7493737079964670	0.3835963132219139	T	T	T
	0.4166666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.4163012189095653	0.8335218480935636	0.2941947838953959	T	T	T
	0.3336065492747330	0.9168032746873709	0.2051337164028840	T	T	T
	0.5000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.6666666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.6673794048148052	0.8336897023574017	0.2942538500943039	T	T	T
	0.5834537062992569	0.9168866252058998	0.2049205119579500	T	T	T
	0.7500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.7539701134045333	0.7507170997307926	0.3836316340123037	T	T	T
	0.9166666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.9167565538732504	0.8334108577506680	0.2941775675669597	T	T	T
	0.8330407602047123	0.9165203801523572	0.2050145408003460	T	T	T
2Pt/Cu(111)	1.0000000000000000					
	8.8905944857135406	-5.1329871195825199	-0.0000000000000010			
	0.0000000000000000	10.2659742391650006	0.0000000000000010			
	0.0000000000000000	0.0000000000000000	23.3821328661704015			
	Pt	Cu				
	2	78				
	Selective dynamics					
	Direct					
	0.5000931582927182	0.2500465791463591	0.3844573389170169	T	T	T
	0.5000931582927182	0.7500465791463592	0.3844573389170169	T	T	T
	0.0000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.0002918048126107	0.0001459024063018	0.3832246771642987	T	T	T
	0.1666666667000030	0.0833333332999970	0.0259047434999999	F	F	F
	0.1662889300094055	0.0831444649546948	0.2943111057105234	T	T	T
	0.0832513273935476	0.1666323432987435	0.2050248980917876	T	T	T
	0.2500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.2471918858221159	0.9977600960349190	0.3843390948757227	T	T	T
	0.4166666667000030	0.0833333332999970	0.0259047434999999	F	F	F

0.4159150421705126	0.0817177449626379	0.2936915806832167	T	T	T
0.3330411787963337	0.1665205894481713	0.2046969470161028	T	T	T
0.5000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.4996374619685569	0.9998187309842786	0.3856561435170248	T	T	T
0.666666667000030	0.083333332999970	0.0259047434999999	F	F	F
0.6669881883977408	0.0834940941488696	0.2946011990300733	T	T	T
0.5835149346652573	0.1665155939528348	0.2047578050800088	T	T	T
0.7500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.7530027483041202	0.0022881482969732	0.3842949538813686	T	T	T
0.916666667000030	0.083333332999970	0.0259047434999999	F	F	F
0.9166056724570019	0.0834546450476833	0.2944692799132238	T	T	T
0.8332488909368445	0.1666244455184266	0.2050661998836094	T	T	T
0.0000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.0000492938659915	0.2500246469329921	0.3831230581045937	T	T	T
0.166666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.1665487856963792	0.3332743927981816	0.2945601364932164	T	T	T
0.0832513273935476	0.4166189841948130	0.2050248980917876	T	T	T
0.2500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.2471918858221159	0.2494317897871969	0.3843390948757227	T	T	T
0.416666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.4159150421705126	0.3341972971078587	0.2936915806832167	T	T	T
0.3333958631123921	0.4166979316062004	0.2050034106130608	T	T	T
0.5000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.666666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.6682993108655508	0.3341496553827710	0.2935946480593849	T	T	T
0.5835149346652573	0.4169993408124315	0.2047578050800088	T	T	T
0.7500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.7530027483041202	0.2507146000071470	0.3842949538813686	T	T	T
0.916666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.9166056724570019	0.3331510273093097	0.2944692799132238	T	T	T
0.8332317785772224	0.4166158893386121	0.2050209239452597	T	T	T
0.0000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.0002918048126107	0.5001459024063019	0.3832246771642987	T	T	T
0.166666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.1662889300094055	0.5831444649546946	0.2943111057105234	T	T	T
0.0832513273935476	0.6666323432987437	0.2050248980917876	T	T	T
0.2500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.2471918858221159	0.4977600960349191	0.3843390948757227	T	T	T
0.416666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.4159150421705126	0.5817177449626378	0.2936915806832167	T	T	T
0.3330411787963337	0.6665205894481711	0.2046969470161028	T	T	T
0.5000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.4996374619685569	0.4998187309842785	0.3856561435170248	T	T	T
0.666666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.6669881883977408	0.5834940941488695	0.2946011990300733	T	T	T
0.5835149346652573	0.6665155939528349	0.2047578050800088	T	T	T
0.7500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.7530027483041202	0.5022881482969732	0.3842949538813686	T	T	T
0.916666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.9166056724570019	0.5834546450476834	0.2944692799132238	T	T	T
0.8332488909368445	0.6666244455184266	0.2050661998836094	T	T	T

	0.0000000000000000 0.7500000000000000 0.1155258754999977 F F F
	0.0000492938659915 0.7500246469329922 0.3831230581045937 T T T
	0.1666666667000030 0.8333333332999970 0.0259047434999999 F F F
	0.1665487856963792 0.8332743927981816 0.2945601364932164 T T T
	0.0832513273935476 0.9166189841948130 0.2050248980917876 T T T
	0.2500000000000000 0.7500000000000000 0.1155258754999977 F F F
	0.2471918858221159 0.7494317897871970 0.3843390948757227 T T T
	0.4166666667000030 0.8333333332999970 0.0259047434999999 F F F
	0.4159150421705126 0.8341972971078587 0.2936915806832167 T T T
	0.3333958631123921 0.9166979316062004 0.2050034106130608 T T T
	0.5000000000000000 0.7500000000000000 0.1155258754999977 F F F
	0.6666666667000030 0.8333333332999970 0.0259047434999999 F F F
	0.6682993108655508 0.8341496553827710 0.2935946480593849 T T T
	0.5835149346652573 0.9169993408124315 0.2047578050800088 T T T
	0.7500000000000000 0.7500000000000000 0.1155258754999977 F F F
	0.7530027483041202 0.7507146000071471 0.3842949538813686 T T T
	0.9166666667000030 0.8333333332999970 0.0259047434999999 F F F
	0.9166056724570019 0.8331510273093099 0.2944692799132238 T T T
	0.8332317785772224 0.9166158893386122 0.2050209239452597 T T T
(4) 3X-S1	
3Cu/Ni(111)	1.0000000000000000
	8.6224000674449712 -4.9781450000000014 0.0000000000000000
	0.0000000000000000 9.9562900000000010 0.0000000000000000
	0.0000000000000000 0.0000000000000000 23.1292800000000014
	Ni Cu
	77 3
	Selective dynamics
	Direct
	0.0000000000000000 0.0000000000000000 0.1392870000000030 F F F
	0.0002990646812577 0.0021360572210298 0.4009736936569226 T T T
	0.1666669999999968 0.0833330000000032 0.0514190000000028 F F F
	0.1671277651889511 0.0835398167691039 0.3142886299411884 T T T
	0.0833761896079608 0.1667128118852474 0.2267833485002839 T T T
	0.2500000000000000 0.0000000000000000 0.1392870000000030 F F F
	0.2517832630144241 0.0023121079131982 0.4009397958845042 T T T
	0.4166669999999968 0.0833330000000032 0.0514190000000028 F F F
	0.4165254555310582 0.0834671895552148 0.3141658594032464 T T T
	0.3333208493697271 0.1665966493772331 0.2266338087125987 T T T
	0.5000000000000000 0.0000000000000000 0.1392870000000030 F F F
	0.4976010511428939 0.9979736187703523 0.4009031381860453 T T T
	0.6666669999999968 0.0833330000000032 0.0514190000000028 F F F
	0.6667181219175191 0.0837270681005933 0.3148041519472571 T T T
	0.5836158096434190 0.1670497897915197 0.2270211297499145 T T T
	0.7500000000000000 0.0000000000000000 0.1392870000000030 F F F
	0.7504037705250184 0.9981200019996166 0.4008633675011666 T T T
	0.9166669999999968 0.0833330000000032 0.0514190000000028 F F F
	0.9162844319987755 0.0832450693135272 0.3142619258474397 T T T
	0.8333162831967584 0.1666723583647922 0.2269889376761540 T T T
	0.0000000000000000 0.2500000000000000 0.1392870000000030 F F F
	0.0018005478290561 0.2495922305950415 0.4010709815598830 T T T
	0.1666669999999968 0.3333330000000032 0.0514190000000028 F F F

0.1665978348746577	0.3334165613081979	0.3141713145308742	T	T	T
0.0834859887504038	0.4167653109319502	0.2266926925994213	T	T	T
0.2500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.2478845573661346	0.2483158123346598	0.4010706371731416	T	T	T
0.4166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.4171952968952084	0.3336455434699630	0.3146919229814102	T	T	T
0.3333220372862229	0.4166108222144871	0.2269695674455647	T	T	T
0.5000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.4985529295826723	0.2482994927369120	0.4010435264405388	T	T	T
0.6666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.6670630525878849	0.3333524157474841	0.3148866536806807	T	T	T
0.5833588260379727	0.4166940685080860	0.2269159246419150	T	T	T
0.7500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.9166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.9159551306713638	0.3331939225103895	0.3146722740003582	T	T	T
0.8330773122547654	0.4164294674065303	0.2269242557106992	T	T	T
0.0000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.0015291295874533	0.5002074549841993	0.4009603574313161	T	T	T
0.1666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.1669656253882934	0.5834607577545441	0.3141571935258369	T	T	T
0.0832838636174742	0.6668872253881091	0.2270128286640656	T	T	T
0.2500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.2476569159337814	0.4994832735341959	0.4009178170344612	T	T	T
0.4166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.4169141572537498	0.5831969802069281	0.3148519730784685	T	T	T
0.3332732380518948	0.6666673806944559	0.2267017805469180	T	T	T
0.5000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.6666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.6663883365918437	0.5829180230894480	0.3148034133773265	T	T	T
0.5834684738153584	0.6666110502475462	0.2269690032009777	T	T	T
0.7500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.7500268384512765	0.5000502516569227	0.4010710431105693	T	T	T
0.9166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.9167662539434360	0.5840399339447373	0.3147738085442313	T	T	T
0.8334291700552043	0.6666886532640319	0.2268360614048390	T	T	T
0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.1666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
0.1665941914031563	0.8332500501731275	0.3149104194148862	T	T	T
0.0834895189205440	0.9164520957317421	0.2270160675006494	T	T	T
0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.2520032597128861	0.7495428103400954	0.4009861400087189	T	T	T
0.4166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
0.4165502698471357	0.8329651450559084	0.3140161850912619	T	T	T
0.3336246144745161	0.9168584404496798	0.2267472029215227	T	T	T
0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.5003519928444575	0.7523756001615141	0.4009502254723216	T	T	T
0.6666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
0.6666859186043368	0.8333140363708864	0.3139487144800839	T	T	T
0.5833832135515848	0.9164262738545972	0.2267035929150225	T	T	T
0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.7496690570837288	0.7514622092188503	0.4009159335806274	T	T	T

	0.916666999999968	0.833333000000032	0.051419000000028	F	F	F
	0.9166836381490668	0.8326856864945569	0.3146108789565005	T	T	T
	0.8333302417872019	0.9167019345764089	0.2266577116841475	T	T	T
	0.7500319150301635	0.2492273167705150	0.4063283142521499	T	T	T
	0.0006837330670493	0.7508180554972128	0.4062818691951051	T	T	T
	0.4992449832292323	0.4999460571779366	0.4062750811383680	T	T	T
3Ag/Ni(111)	1.000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni	Ag				
	77	3				
	Selective dynamics					
	Direct					
	0.0000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.0000730000000004	0.0021509999999978	0.4009849999999986	T	T	T
	0.1666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.1671630000000022	0.0833900000000014	0.3143540000000016	T	T	T
	0.0834520000000012	0.1667670000000001	0.2268660000000011	T	T	T
	0.2500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.2520159999999976	0.0024609999999967	0.4009980000000013	T	T	T
	0.4166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.4163789999999992	0.0833769999999987	0.3142020000000016	T	T	T
	0.3333050000000028	0.1666030000000021	0.2267000000000010	T	T	T
	0.5000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.4996780000000030	0.9998390000000015	0.4012740000000008	T	T	T
	0.6666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.6665309999999991	0.0832649999999973	0.3145680000000013	T	T	T
	0.5834320000000019	0.1669020000000003	0.2268600000000021	T	T	T
	0.7500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.7500100000000032	0.0001519999999999	0.4011110000000002	T	T	T
	0.9166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.9162940000000006	0.0830559999999991	0.3143389999999968	T	T	T
	0.8333200000000005	0.1666600000000003	0.2268380000000008	T	T	T
	0.0000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.9995159999999998	0.2497579999999999	0.4012379999999993	T	T	T
	0.1666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.1666379999999990	0.3333190000000030	0.3144970000000029	T	T	T
	0.0834520000000012	0.4166850000000011	0.2268660000000011	T	T	T
	0.2500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.2477779999999967	0.2482919999999993	0.4010919999999984	T	T	T
	0.4166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.4169309999999982	0.3336850000000027	0.3149159999999966	T	T	T
	0.3333330000000032	0.4166669999999968	0.2270079999999979	T	T	T
	0.5000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.5003669999999971	0.2479829999999978	0.4011190000000013	T	T	T
	0.6666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.6667899999999989	0.3334660000000014	0.3142580000000024	T	T	T
	0.5834169999999972	0.4167449999999988	0.2269950000000023	T	T	T
	0.7500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.9166669999999968	0.3333330000000032	0.0514190000000028	F	F	F

	0.9162940000000006	0.3332369999999969	0.3143389999999968	T	T	T
	0.8332400000000035	0.4166290000000004	0.2267379999999974	T	T	T
	0.0000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.0000730000000004	0.4979209999999981	0.4009849999999986	T	T	T
	0.1666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.1671630000000022	0.5837730000000008	0.3143540000000016	T	T	T
	0.0834070000000011	0.6669770000000028	0.2270480000000035	T	T	T
	0.2500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.2477779999999967	0.4994859999999974	0.4010919999999984	T	T	T
	0.4166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.4169309999999982	0.5832460000000026	0.3149159999999966	T	T	T
	0.3333050000000028	0.6667010000000033	0.2267000000000010	T	T	T
	0.5000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.6666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.6662729999999968	0.5831370000000007	0.3150029999999973	T	T	T
	0.5834169999999972	0.6666719999999984	0.2269950000000023	T	T	T
	0.7500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.7497060000000033	0.4979340000000008	0.4009550000000033	T	T	T
	0.9166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.9168980000000033	0.5841380000000029	0.3147209999999987	T	T	T
	0.8334059999999965	0.6667029999999983	0.2268839999999983	T	T	T
	0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.1666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.1664669999999973	0.8332329999999999	0.3150260000000031	T	T	T
	0.0834070000000011	0.9164310000000029	0.2270480000000035	T	T	T
	0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.2520159999999976	0.7495550000000009	0.4009980000000013	T	T	T
	0.4166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.4163789999999992	0.8330020000000005	0.3142020000000016	T	T	T
	0.3333969999999979	0.9166990000000013	0.2268260000000026	T	T	T
	0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.5003669999999971	0.7523839999999993	0.4011190000000013	T	T	T
	0.6666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.6667899999999989	0.8333230000000000	0.3142580000000024	T	T	T
	0.5834320000000019	0.9165300000000016	0.2268600000000021	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.7497060000000033	0.7517720000000025	0.4009550000000033	T	T	T
	0.9166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.9168980000000033	0.8327600000000004	0.3147209999999987	T	T	T
	0.8332400000000035	0.9166110000000032	0.2267379999999974	T	T	T
	0.7500100000000032	0.2498580000000032	0.4011110000000002	T	T	T
	0.0003389999999968	0.7501689999999996	0.4063159999999968	T	T	T
	0.4994099999999975	0.4997049999999987	0.4063749999999970	T	T	T
3Au/Ni(111)	1.0000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni Au					
	77 3					
	Selective dynamics					
	Direct					

0.0000000000000000	0.0000000000000000	0.1392870000000030	F F F
0.0002700478478772	0.0053718334725730	0.4013600747594808	T T T
0.1666669999999968	0.0833330000000032	0.0514190000000028	F F F
0.1670383230108143	0.0837922926729604	0.3139715978785560	T T T
0.0832873509312861	0.1665770767488439	0.2265491262169093	T T T
0.2500000000000000	0.0000000000000000	0.1392870000000030	F F F
0.2539502366603799	0.0049796074902346	0.4008557833041948	T T T
0.4166669999999968	0.0833330000000032	0.0514190000000028	F F F
0.4162403762077247	0.0834745839550664	0.3137691544647367	T T T
0.3333520232701872	0.1666946071819808	0.2265759461242425	T T T
0.5000000000000000	0.0000000000000000	0.1392870000000030	F F F
0.4934345745007604	0.9943895363685868	0.4009401433579214	T T T
0.6666669999999968	0.0833330000000032	0.0514190000000028	F F F
0.6665736965274718	0.0837270102466050	0.3147605226026045	T T T
0.5838342715868023	0.1672701845134625	0.2270436638726636	T T T
0.7500000000000000	0.0000000000000000	0.1392870000000030	F F F
0.7502933782957157	0.9956176042370544	0.4007830723776635	T T T
0.9166669999999968	0.0833330000000032	0.0514190000000028	F F F
0.9163790228445308	0.0830386641742322	0.3139762934098584	T T T
0.8333264866666710	0.1667439291589048	0.2270215620879696	T T T
0.0000000000000000	0.2500000000000000	0.1392870000000030	F F F
0.0048973123432035	0.2494197813785064	0.4011854301489137	T T T
0.1666669999999968	0.3333330000000032	0.0514190000000028	F F F
0.1661923062973329	0.3332336449471285	0.3136883856703889	T T T
0.0830987524161912	0.4167144795283519	0.2265947317497066	T T T
0.2500000000000000	0.2500000000000000	0.1392870000000030	F F F
0.2444813970847122	0.2451113372805906	0.4013021625866315	T T T
0.4166669999999968	0.3333330000000032	0.0514190000000028	F F F
0.4169218463310997	0.3336034732246986	0.3148522958804207	T T T
0.3333985620136843	0.4166153376904518	0.2269664436998298	T T T
0.5000000000000000	0.2500000000000000	0.1392870000000030	F F F
0.4938191455210514	0.2439757450085267	0.4018603203936095	T T T
0.6666669999999968	0.3333330000000032	0.0514190000000028	F F F
0.6669336356480855	0.3332875892502329	0.3153052368858766	T T T
0.5834052682156070	0.4165963296213917	0.2272180394955399	T T T
0.7500000000000000	0.2500000000000000	0.1392870000000030	F F F
0.9166669999999968	0.3333330000000032	0.0514190000000028	F F F
0.9161585044375542	0.3333862027634069	0.3147903467427255	T T T
0.8327832431911091	0.4164202347046739	0.2272367684599530	T T T
0.0000000000000000	0.5000000000000000	0.1392870000000030	F F F
0.0059632687347886	0.4997593594448375	0.4017449130071071	T T T
0.1666669999999968	0.5833330000000032	0.0514190000000028	F F F
0.1670976202307557	0.5833430579346981	0.3137323981942046	T T T
0.0830550443333209	0.6668925461607671	0.2269986347383011	T T T
0.2500000000000000	0.5000000000000000	0.1392870000000030	F F F
0.2450934368994027	0.4990645218006335	0.4008138881869456	T T T
0.4166669999999968	0.5833330000000032	0.0514190000000028	F F F
0.4168736892174749	0.5835483918342845	0.3146888961920880	T T T
0.3333239123329719	0.6666069257380158	0.2264761881183972	T T T
0.5000000000000000	0.5000000000000000	0.1392870000000030	F F F
0.6666669999999968	0.5833330000000032	0.0514190000000028	F F F

	0.6660998974788512	0.5829974186018632	0.3150476095013843	T	T	T
	0.5833920542180806	0.6664593607106255	0.2269199289854456	T	T	T
	0.7500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.7499697948824320	0.5000212222649978	0.4020961932694789	T	T	T
	0.9166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.9169058885522219	0.5840767166528025	0.3150157039639652	T	T	T
	0.8333567447516685	0.6666607590702682	0.2272505723639782	T	T	T
	0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.1666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.1666155907744411	0.8332403248456046	0.3147783672423614	T	T	T
	0.0831902570170229	0.9161995750365293	0.2270254752856289	T	T	T
	0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.2550523570086582	0.7489164091350133	0.4008595971810394	T	T	T
	0.4166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.4166480412148630	0.8333155688325888	0.3133679347020504	T	T	T
	0.3332987729936150	0.9168672335438472	0.2265877376522454	T	T	T
	0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.5006334286757976	0.7560601215053495	0.4008425447423960	T	T	T
	0.6666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.6666929379429476	0.8334427082336973	0.3135474990901130	T	T	T
	0.5836547804680734	0.9169149141951110	0.2265408338621313	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.7499207740962888	0.7560638882674553	0.4017436313777338	T	T	T
	0.9166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.9164856786410098	0.8327570810940443	0.3148469678337733	T	T	T
	0.8334457105899560	0.9164937776929349	0.2266195745524868	T	T	T
	0.7496551027695233	0.2473431817794918	0.4186585257503737	T	T	T
	0.0024807269501110	0.7521961315227159	0.4186053062695549	T	T	T
	0.4976957921070664	0.5002722842597862	0.4187111914159090	T	T	T
3Ni/Cu(111)	1.0000000000000000					
	8.8905944857135406	-5.1329871195825199	-0.0000000000000010			
	0.0000000000000000	10.2659742391650006	0.0000000000000010			
	0.0000000000000000	0.0000000000000000	23.3821328661704015			
	Ni	Cu				
	3	77				
	Selective dynamics					
	Direct					
	0.2507081561463522	0.2502916714946721	0.3796405989742695	T	T	T
	0.7497083285053279	0.5004164846516801	0.3796405989742695	T	T	T
	0.4995835153483199	0.7492918438536478	0.3796405989742695	T	T	T
	0.0000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.0015403814068691	0.0013737891498735	0.3832832429070834	T	T	T
	0.1666666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.1668599377241691	0.0836082669356912	0.2942383970864881	T	T	T
	0.0831809958411753	0.1665698892741645	0.2048219767307202	T	T	T
	0.2500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.2502347630585291	0.0017325466086007	0.3832790271418105	T	T	T
	0.4166666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.4168998871534271	0.0835990318340976	0.2944834298083165	T	T	T
	0.3333742438989944	0.1665997606819758	0.2047921407905235	T	T	T
	0.5000000000000000	0.0000000000000000	0.1155258754999977	F	F	F

0.4998334077430115	0.9984596185931309	0.3832832429070834	T	T	T
0.6666666667000030	0.0833333332999970	0.0259047434999999	F	F	F
0.6668056524559418	0.0834755638677720	0.2944589767297217	T	T	T
0.5833848079247872	0.1667018486891720	0.2050841423726908	T	T	T
0.7500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.7484569181493939	0.9980912625923750	0.3831663658495188	T	T	T
0.9166666667000030	0.0833333332999970	0.0259047434999999	F	F	F
0.9165244361322280	0.0833300884881609	0.2944589767297217	T	T	T
0.8333333332999970	0.1666666667000030	0.2050822971185440	T	T	T
0.0000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.0019087374076250	0.250365655570259	0.3831663658495188	T	T	T
0.1666666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.1670396665042020	0.3334115860294062	0.2942248883745222	T	T	T
0.0833170406643760	0.4166151920752128	0.2050841423726908	T	T	T
0.2500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.4166666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.4165463606061692	0.3334306519173396	0.2940631338007051	T	T	T
0.3334335014897505	0.4168519548482053	0.2047848336814226	T	T	T
0.5000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.5001870527479397	0.2520654640267495	0.3832925995276355	T	T	T
0.6666666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.6665884139705938	0.3336280803747798	0.2942248883745222	T	T	T
0.5831480451517947	0.4165815467415541	0.2047848336814226	T	T	T
0.7500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.7496343444429741	0.2515430818506061	0.3831663658495188	T	T	T
0.9166666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.9166699115118391	0.3331943475440582	0.2944589767297217	T	T	T
0.8334301107258355	0.4166111066670197	0.2048219767307202	T	T	T
0.0000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.9986262108501265	0.5001665922569885	0.3832832429070834	T	T	T
0.1666666667000030	0.5833333332999970	0.0259047434999999	F	F	F
0.1666991447806794	0.5831001128465729	0.2944834298083165	T	T	T
0.0832849649923588	0.6665851425415568	0.2050894920580149	T	T	T
0.2500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.2518784112788097	0.4998129472520603	0.3832925995276355	T	T	T
0.4166666667000030	0.5833333332999970	0.0259047434999999	F	F	F
0.4168842914111792	0.5834536393938308	0.2940631338007051	T	T	T
0.3332255166829654	0.6666257561010056	0.2047921407905235	T	T	T
0.5000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.5000000000000000	0.5000000000000000	0.3834012785316148	T	T	T
0.6666666667000030	0.5833333332999970	0.0259047434999999	F	F	F
0.6665693480826604	0.5831157085888208	0.2940631338007051	T	T	T
0.5834184532584459	0.6665664985102495	0.2047848336814226	T	T	T
0.7500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.9166666667000030	0.5833333332999970	0.0259047434999999	F	F	F
0.9163917330643088	0.5832516706884689	0.2942383970864881	T	T	T
0.8334002393180242	0.6667744833170346	0.2047921407905235	T	T	T
0.0000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
0.9982674533913993	0.7485022164499284	0.3832790271418105	T	T	T
0.1666666667000030	0.8333333332999970	0.0259047434999999	F	F	F
0.1666666667000030	0.8333333332999970	0.2946427775492140	T	T	T

	0.0833001774491819	0.9167150350076412	0.2050894920580149	T	T	T
	0.2500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.2514977835500716	0.7497652369414709	0.3832790271418105	T	T	T
	0.4166666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.4167483293115311	0.8331400622758309	0.2942383970864881	T	T	T
	0.3334148574584432	0.9166998225508181	0.2050894920580149	T	T	T
	0.5000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.6666666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.6663719196252202	0.8329603334957980	0.2942248883745222	T	T	T
	0.5833888933329803	0.9168190041588247	0.2048219767307202	T	T	T
	0.7500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.7479345359732505	0.7481215887211903	0.3832925995276355	T	T	T
	0.9166666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.9164009681659024	0.8333008552193206	0.2944834298083165	T	T	T
	0.8332981513108280	0.9166829593356240	0.2050841423726908	T	T	T
3Pd/Cu(111)	1.0000000000000000					
	8.8905944857135406	-5.1329871195825199	-0.0000000000000010			
	0.0000000000000000	10.2659742391650006	0.0000000000000010			
	0.0000000000000000	0.0000000000000000	23.3821328661704015			
	Pd	Cu				
	3	77				
	Selective dynamics					
	Direct					
	0.2488569352431824	0.2487644906215110	0.3869242018734269	T	T	T
	0.7512355093784890	0.5000924446216715	0.3869242018734269	T	T	T
	0.4999075553783285	0.7511430647568176	0.3869242018734269	T	T	T
	0.0000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.9974968756153331	0.9973815771867933	0.3834939915773816	T	T	T
	0.1666666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.1662992187987129	0.0826670748129814	0.2940229186135923	T	T	T
	0.0833202120320138	0.1667233434898492	0.2047337648634908	T	T	T
	0.2500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.2497894292494109	0.9967520148690383	0.3834263516320462	T	T	T
	0.4166666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.4164890272946451	0.0835072017012379	0.2941856097550684	T	T	T
	0.3334094292878831	0.1668438655574178	0.2048092955238516	T	T	T
	0.5000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.4998847015714603	0.0025031243846669	0.3834939915773816	T	T	T
	0.6666666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.6665507504784074	0.0829521784290606	0.2942903052378583	T	T	T
	0.5834489942531391	0.1668010770276567	0.2051297071155176	T	T	T
	0.7500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.7530284357869164	0.0031749126003646	0.3834971104212741	T	T	T
	0.9166666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.9170478215709394	0.0835985719493451	0.2942903052378583	T	T	T
	0.833333332999970	0.1666666667000030	0.2050974763219600	T	T	T
	0.0000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
	0.9968250873996354	0.2498535231865446	0.3834971104212741	T	T	T
	0.1666666667000030	0.333333332999970	0.0259047434999999	F	F	F
	0.1663355382912357	0.3335655590277753	0.2941737520157233	T	T	T
	0.0833520826745087	0.4165510057468609	0.2051297071155176	T	T	T

0.2500000000000000	0.2500000000000000	0.1155258754999977	F F F
0.4166666667000030	0.3333333332999970	0.0259047434999999	F F F
0.4173341547606384	0.3336005263266699	0.2943723508557312	T T T
0.3335267493080138	0.4168846495189982	0.2050139078915763	T T T
0.5000000000000000	0.2500000000000000	0.1155258754999977	F F F
0.5000454869741731	0.2461385512142868	0.3840181598767316	T T T
0.6666666667000030	0.3333333332999970	0.0259047434999999	F F F
0.6664344409722247	0.3327699791634515	0.2941737520157233	T T T
0.5831153504810018	0.4166420998890246	0.2050139078915763	T T T
0.7500000000000000	0.2500000000000000	0.1155258754999977	F F F
0.7501464768134554	0.2469715642130836	0.3834971104212741	T T T
0.9166666667000030	0.3333333332999970	0.0259047434999999	F F F
0.9164014280506549	0.3334492495215926	0.2942903052378583	T T T
0.8332766565101508	0.4165968686421806	0.2047337648634908	T T T
0.0000000000000000	0.5000000000000000	0.1155258754999977	F F F
0.0026184228132067	0.5001152984285397	0.3834939915773816	T T T
0.1666666667000030	0.5833333332999970	0.0259047434999999	F F F
0.1670181745066017	0.5835109727053549	0.2941856097550684	T T T
0.0831477219951182	0.6664278946966036	0.2049491635474396	T T T
0.2500000000000000	0.5000000000000000	0.1155258754999977	F F F
0.2460930642401209	0.4999545130258269	0.3840181598767316	T T T
0.4166666667000030	0.5833333332999970	0.0259047434999999	F F F
0.4162663716660333	0.5826658452393616	0.2943723508557312	T T T
0.3334344361695258	0.6665905707121169	0.2048092955238516	T T T
0.5000000000000000	0.5000000000000000	0.1155258754999977	F F F
0.5000000000000000	0.5000000000000000	0.3844603538008187	T T T
0.6666666667000030	0.5833333332999970	0.0259047434999999	F F F
0.6663994736733301	0.5837336283339667	0.2943723508557312	T T T
0.5833579001109754	0.6664732506919862	0.2050139078915763	T T T
0.7500000000000000	0.5000000000000000	0.1155258754999977	F F F
0.9166666667000030	0.5833333332999970	0.0259047434999999	F F F
0.9173329251870186	0.5836321438857226	0.2940229186135923	T T T
0.8331561344425822	0.6665655638304742	0.2048092955238516	T T T
0.0000000000000000	0.7500000000000000	0.1155258754999977	F F F
0.0032479851309617	0.7530374143803797	0.3834263516320462	T T T
0.1666666667000030	0.8333333332999970	0.0259047434999999	F F F
0.1666666667000030	0.8333333332999970	0.2939199276550042	T T T
0.0832801726014765	0.9168522780048818	0.2049491635474396	T T T
0.2500000000000000	0.7500000000000000	0.1155258754999977	F F F
0.2469625856196203	0.7502105707505891	0.3834263516320462	T T T
0.4166666667000030	0.8333333332999970	0.0259047434999999	F F F
0.4163678561142774	0.8337007812012871	0.2940229186135923	T T T
0.3335721053033964	0.9167198273985235	0.2049491635474396	T T T
0.5000000000000000	0.7500000000000000	0.1155258754999977	F F F
0.6666666667000030	0.8333333332999970	0.0259047434999999	F F F
0.6672300208365485	0.8336644617087643	0.2941737520157233	T T T
0.5834031313578194	0.9166797879679862	0.2047337648634908	T T T
0.7500000000000000	0.7500000000000000	0.1155258754999977	F F F
0.7538614487857132	0.7539069357598791	0.3840181598767316	T T T
0.9166666667000030	0.8333333332999970	0.0259047434999999	F F F
0.9164927982987621	0.8329818254933983	0.2941856097550684	T T T

	0.8331989229723433	0.9166479173254913	0.2051297071155176	T	T	T	
3Pt/Cu(111)	1.00000000000000						
	8.8905944857135406	-5.1329871195825199	-0.0000000000000010				
	0.0000000000000000	10.2659742391650006	0.0000000000000010				
	0.0000000000000000	0.0000000000000000	23.3821328661704015				
	Pt	Cu					
	3	77					
	Selective dynamics						
	Direct						
	0.2485808714129823	0.2484672240514232	0.3847966050964930	T	T	T	
	0.7515327759485770	0.5001136473615592	0.3847966050964930	T	T	T	
	0.4998863526384410	0.7514191285870176	0.3847966050964930	T	T	T	
	0.0000000000000000	0.0000000000000000	0.1155258754999977	F	F	F	
	0.9980081471752634	0.9976858575769504	0.3842977358316493	T	T	T	
	0.1666666667000030	0.0833333332999970	0.0259047434999999	F	F	F	
	0.1655848402537705	0.0814245205741783	0.2934838688879192	T	T	T	
	0.0830560744444687	0.1666626576754068	0.2047731899533312	T	T	T	
	0.2500000000000000	0.0000000000000000	0.1155258754999977	F	F	F	
	0.2493341858885864	0.9974984028068189	0.3843283363739530	T	T	T	
	0.4166666667000030	0.0833333332999970	0.0259047434999999	F	F	F	
	0.4168767814286695	0.0834924899538035	0.2946786423358834	T	T	T	
	0.3334467153527063	0.1666510792855787	0.2048002707897832	T	T	T	
	0.5000000000000000	0.0000000000000000	0.1155258754999977	F	F	F	
	0.4996777104016871	0.0019918528247367	0.3842977358316493	T	T	T	
0.6666666667000030	0.0833333332999970	0.0259047434999999	F	F	F		
0.6670378670734078	0.0837269007349113	0.2945854608659731	T	T	T		
0.5833861565977690	0.1667000060406588	0.2051410902868618	T	T	T		
0.7500000000000000	0.0000000000000000	0.1155258754999977	F	F	F		
0.7522431193113550	0.0024273386455645	0.3842686594019611	T	T	T		
0.9166666667000030	0.0833333332999970	0.0259047434999999	F	F	F		
0.9162730992650888	0.0833109662384876	0.2945854608659731	T	T	T		
0.8333333332999970	0.1666666667000030	0.2051451822520068	T	T	T		
0.0000000000000000	0.2500000000000000	0.1155258754999977	F	F	F		
0.9975726613544353	0.2498157806657834	0.3842686594019611	T	T	T		
0.1666666667000030	0.3333333332999970	0.0259047434999999	F	F	F		
0.1658311593136631	0.3344025759669964	0.2938244142577896	T	T	T		
0.0833138493428808	0.4166138434022310	0.2051410902868618	T	T	T		
0.2500000000000000	0.2500000000000000	0.1155258754999977	F	F	F		
0.4166666667000030	0.3333333332999970	0.0259047434999999	F	F	F		
0.4179675874129940	0.3340631959186154	0.2939910441875354	T	T	T		
0.3335457645735377	0.4170691555848086	0.2048739615341442	T	T	T		
0.5000000000000000	0.2500000000000000	0.1155258754999977	F	F	F		
0.5000865940759540	0.2473538557577291	0.3856105631074070	T	T	T		
0.6666666667000030	0.3333333332999970	0.0259047434999999	F	F	F		
0.6655974240330037	0.3314285832466579	0.2938244142577896	T	T	T		
0.5829308444151844	0.4164766090887309	0.2048739615341442	T	T	T		
0.7500000000000000	0.2500000000000000	0.1155258754999977	F	F	F		
0.7501842193342165	0.2477568806886450	0.3842686594019611	T	T	T		
0.9166666667000030	0.3333333332999970	0.0259047434999999	F	F	F		
0.9166890337615122	0.3329621329265922	0.2945854608659731	T	T	T		
0.8333373423245933	0.4163934168690709	0.2047731899533312	T	T	T		

	0.0000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.0023141424230497	0.5003222895983132	0.3842977358316493	T	T	T
	0.1666666667000030	0.5833333332999970	0.0259047434999999	F	F	F
	0.1666157086251429	0.5831232185713304	0.2946786423358834	T	T	T
	0.0833536527871425	0.6665644925133090	0.2050472174287443	T	T	T
	0.2500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.2472672616817750	0.4999134059240459	0.3856105631074070	T	T	T
	0.4166666667000030	0.5833333332999970	0.0259047434999999	F	F	F
	0.4160956086056301	0.5820324125870059	0.2939910441875354	T	T	T
	0.3332043638328706	0.6665532846472938	0.2048002707897832	T	T	T
	0.5000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.5000000000000000	0.5000000000000000	0.3870546433405890	T	T	T
	0.6666666667000030	0.5833333332999970	0.0259047434999999	F	F	F
	0.6659368040813847	0.5839043913943699	0.2939910441875354	T	T	T
	0.5835233909112690	0.6664542354264622	0.2048739615341442	T	T	T
	0.7500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.9166666667000030	0.5833333332999970	0.0259047434999999	F	F	F
	0.9185754794258219	0.5841603195795833	0.2934838688879192	T	T	T
	0.8333489207144212	0.6667956361671294	0.2048002707897832	T	T	T
	0.0000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.0025015971931811	0.7518357830817672	0.3843283363739530	T	T	T
	0.1666666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.1666666667000030	0.8333333332999970	0.2946518099123288	T	T	T
	0.0832108396261647	0.9166463472128574	0.2050472174287443	T	T	T
	0.2500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.2481642169182325	0.7506658141114135	0.3843283363739530	T	T	T
	0.4166666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.4158396804204166	0.8344151597462295	0.2934838688879192	T	T	T
	0.3334355074866910	0.9167891603738353	0.2050472174287443	T	T	T
	0.5000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.6666666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.6685714167533421	0.8341688406863367	0.2938244142577896	T	T	T
	0.5836065831309289	0.9169439255555313	0.2047731899533312	T	T	T
	0.7500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.7526461442422708	0.7527327383182250	0.3856105631074070	T	T	T
	0.9166666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.9165075100461967	0.8333842913748573	0.2946786423358834	T	T	T
	0.8332999939593408	0.9166861506571192	0.2051410902868618	T	T	T
(5) 3X-S2						
3Cu/Ni(111)	1.0000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni	Cu				
	77	3				
	Selective dynamics					
	Direct					
	0.0000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.1666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.1668217419313797	0.0834013478538435	0.3146611309027919	T	T	T
	0.0834205783652514	0.1666803547026653	0.2269946148295845	T	T	T

0.2500000000000000	0.0000000000000000	0.1392870000000030	F F F
0.2497871189722577	0.9994021352583896	0.4008847092058826	T T T
0.4166669999999968	0.0833330000000032	0.0514190000000028	F F F
0.4166903483573084	0.0833622070484222	0.3146248716768822	T T T
0.3333433445743766	0.1666370072155678	0.2264834631084065	T T T
0.5000000000000000	0.0000000000000000	0.1392870000000030	F F F
0.6666669999999968	0.0833330000000032	0.0514190000000028	F F F
0.6664027207275495	0.0831981969273067	0.3147476053832554	T T T
0.5833198657524706	0.1666947298078920	0.2269780023973041	T T T
0.7500000000000000	0.0000000000000000	0.1392870000000030	F F F
0.7500045951367376	-0.0000584677838184	0.4010473444011461	T T T
0.9166669999999968	0.0833330000000032	0.0514190000000028	F F F
0.9168243871615749	0.0832050139706159	0.3147449327135403	T T T
0.8333757896106530	0.1667152937909798	0.2265849903878021	T T T
0.0000000000000000	0.2500000000000000	0.1392870000000030	F F F
0.0000057757828391	0.2520973953539450	0.4010303726770343	T T T
0.1666669999999968	0.3333330000000032	0.0514190000000028	F F F
0.1666878585862378	0.3333171888241528	0.3144596244912263	T T T
0.0834530409690382	0.4165455252540747	0.2268566026090739	T T T
0.2500000000000000	0.2500000000000000	0.1392870000000030	F F F
0.2497239462430155	0.2502808937932618	0.4009003082340099	T T T
0.4166669999999968	0.3333330000000032	0.0514190000000028	F F F
0.4166180733648107	0.3332056350827591	0.3146621337141084	T T T
0.3333184597746532	0.4165794897654936	0.2269913970201871	T T T
0.5000000000000000	0.2500000000000000	0.1392870000000030	F F F
0.500590522751063	0.2502152796010817	0.4008857420330082	T T T
0.6666669999999968	0.3333330000000032	0.0514190000000028	F F F
0.6665881030836985	0.3332942150474033	0.3144121961100342	T T T
0.5832774658678945	0.4166121711240798	0.2269916306234684	T T T
0.7500000000000000	0.2500000000000000	0.1392870000000030	F F F
0.7521236872532134	0.2520864449007533	0.4009917307323672	T T T
0.9166669999999968	0.3333330000000032	0.0514190000000028	F F F
0.9164510909857972	0.3328776906681858	0.3142356775556304	T T T
0.8331350434920402	0.4165838147412799	0.2268547211556521	T T T
0.0000000000000000	0.5000000000000000	0.1392870000000030	F F F
0.0000172224940915	0.5000036049308320	0.4015330467678458	T T T
0.1666669999999968	0.5833330000000032	0.0514190000000028	F F F
0.1671282685839985	0.5835618184249424	0.3142432967962712	T T T
0.0834225758242568	0.6668831813586606	0.2268536435551044	T T T
0.2500000000000000	0.5000000000000000	0.1392870000000030	F F F
0.2479083509622985	0.4999992617173909	0.4010328885396960	T T T
0.4166669999999968	0.5833330000000032	0.0514190000000028	F F F
0.4168067526392941	0.5831744517477163	0.3147418036046181	T T T
0.3332961273646147	0.6666430971771157	0.2265912904890878	T T T
0.5000000000000000	0.5000000000000000	0.1392870000000030	F F F
0.6666669999999968	0.5833330000000032	0.0514190000000028	F F F
0.6663884828777986	0.5831981375251134	0.3147444167098103	T T T
0.5833853915851230	0.6668287206679112	0.2270044843070282	T T T
0.7500000000000000	0.5000000000000000	0.1392870000000030	F F F
0.7520881378304944	0.4999656420397730	0.4010062843619277	T T T
0.9166669999999968	0.5833330000000032	0.0514190000000028	F F F

	0.9164624271755447	0.5835596390944611	0.3142547134351488	T	T	T
	0.8333428286543724	0.6666512620277236	0.2265916728741109	T	T	T
	0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.0000252850670859	0.7479035101279601	0.4010079158193635	T	T	T
	0.1666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.1666851631490601	0.8333727929228153	0.3144240632169244	T	T	T
	0.0833742001673004	0.9167136957085716	0.2269905919647646	T	T	T
	0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.2479058161202161	0.7478859004122566	0.4010099255990185	T	T	T
	0.4166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.4168055216477833	0.8336182277842223	0.3147439398011569	T	T	T
	0.3333092868426851	0.9166887304265269	0.2269842178000515	T	T	T
	0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.5000474465138214	0.7499868746464327	0.4010457315612752	T	T	T
	0.6666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.6666720523123674	0.8333286611544326	0.3146773060554804	T	T	T
	0.5834055870646030	0.9165916153063828	0.2270004315854389	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.7499945460745525	0.7500074947252651	0.4010471289070148	T	T	T
	0.9166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.9168015872694990	0.8335880112110162	0.3147453753921010	T	T	T
	0.8331616534195719	0.9165980255023771	0.2270075193844086	T	T	T
	0.4999955057382274	0.0000163125090950	0.4062461055606420	T	T	T
	0.0001242489793254	0.0000336028213530	0.4062482635123179	T	T	T
	0.4999669426878178	0.4998783245859544	0.4062499328004091	T	T	T
3Ag/Ni(111)	1.0000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni	Ag				
	77	3				
	Selective dynamics					
	Direct					
	0.0000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.0000146523920725	0.0000135563512981	0.4000192181866987	T	T	T
	0.1666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.1676218132406581	0.0838757211340792	0.3131096350507976	T	T	T
	0.0834937536546492	0.1669851149264677	0.2263467713253747	T	T	T
	0.2500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.2446393004388171	0.0000356116085579	0.4002116121422104	T	T	T
	0.4166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.4173858601949359	0.0822223304711715	0.3153351511921103	T	T	T
	0.3339822965569651	0.1669887522511525	0.2267585549120622	T	T	T
	0.5000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.6666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.6648747785075295	0.0822437825438415	0.3153310781385538	T	T	T
	0.5832801512617208	0.1665663730016947	0.2270970294827965	T	T	T
	0.7500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.7553999192102917	0.0000323750486488	0.4002245878507309	T	T	T
	0.9166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.9162470333985134	0.0838526359255450	0.3131125583668632	T	T	T

0.8330120128374396	0.1669896190652739	0.2267591756994049	T	T	T
0.0000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.0000678959569283	0.2447547648107305	0.4002385057393180	T	T	T
0.1666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.1667046828764319	0.3334167297614393	0.3137445412507827	T	T	T
0.0832624110785770	0.4167679272974907	0.2269155468480243	T	T	T
0.2500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.2446850082335940	0.2447654012853685	0.4002313424015727	T	T	T
0.4166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.4173950779306017	0.3352543376541037	0.3153516083579776	T	T	T
0.3335071416583287	0.4167686629039468	0.2269078001940080	T	T	T
0.5000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.4999407018840299	0.2500289273585621	0.4000352550346267	T	T	T
0.6666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.6666635602708884	0.3333336197685839	0.3142796892686102	T	T	T
0.5832905584886208	0.4166625592118610	0.2271017133498920	T	T	T
0.7500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.7500628995262416	0.2500223369598703	0.4000433222507698	T	T	T
0.9166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.9178696039899465	0.3352656139286316	0.3153568114456716	T	T	T
0.8333504987414451	0.4166489365999212	0.2271002030973797	T	T	T
0.0000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.1666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.1656564876279996	0.5828627041371487	0.3148802604756046	T	T	T
0.0832373427010532	0.6664917231402991	0.2269053715542637	T	T	T
0.2500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.2491462141077977	0.4983056737031927	0.3994688166725810	T	T	T
0.4166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.4172111298265326	0.5828481470517136	0.3148808814694094	T	T	T
0.3333403366330501	0.6666669618506970	0.2268689211980346	T	T	T
0.5000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.6666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.6648225264038634	0.5826461315554519	0.3153265029468756	T	T	T
0.5832706118938579	0.6665116647190653	0.2269065069973736	T	T	T
0.7500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.7500741189843402	0.5001507165351697	0.4000270684316133	T	T	T
0.9166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.9178153939029406	0.5826400967464962	0.3153140208453429	T	T	T
0.8330060571398075	0.6660041093971237	0.2267487969613120	T	T	T
0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.0000694482072123	0.7553540690675504	0.4001848041313003	T	T	T
0.1666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
0.1667015078718930	0.8333584699277995	0.3137098020375997	T	T	T
0.0834710014074318	0.9165659760268711	0.2263385868122939	T	T	T
0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.2491107223310575	0.7508910996071428	0.3994465905184131	T	T	T
0.4166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
0.4172079956926045	0.8343929514139011	0.3148719915581619	T	T	T
0.3334758001454126	0.9167160771541903	0.2269053416361615	T	T	T
0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.5017855283684554	0.7508585015499362	0.3994532517332305	T	T	T

	0.6666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.6666654158089346	0.8333720297323918	0.3137271079889266	T	T	T
	0.5832638071561637	0.9167324372468677	0.2269028961544338	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.7553474230430388	0.7553597387173431	0.4002090100049834	T	T	T
	0.9166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.9162374153208277	0.8324656420595374	0.3130883424383780	T	T	T
	0.8330933454777919	0.9165627976981101	0.2263444779366757	T	T	T
	0.4998652846475893	-0.0002665692591350	0.4267251935049014	T	T	T
	0.0002736343999363	0.5001804527082281	0.4268306239113252	T	T	T
	0.4998992330137358	0.5001835487263034	0.4268248762963157	T	T	T
3Au/Ni(111)	1.0000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni	Au				
	77	3				
	Selective dynamics					
	Direct					
	0.0000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.0000197489266567	0.0000305057644952	0.4005823359049455	T	T	T
	0.1666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.1670761854444973	0.0835389758016944	0.3137085719942481	T	T	T
	0.0834243064922611	0.1668479612762070	0.2265318779637573	T	T	T
	0.2500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.2441187592154424	-0.0000695690244915	0.4010796957640008	T	T	T
	0.4166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.4167523629998012	0.0832956014261790	0.3147731110907368	T	T	T
	0.3334285854025958	0.1667204149454794	0.2266997294201554	T	T	T
	0.5000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.6666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.6665467565029924	0.0833005705293995	0.3147761498466926	T	T	T
	0.5833777132259962	0.1667661811205007	0.2270767084248560	T	T	T
	0.7500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.7558061585111958	-0.0000771991854522	0.4010853115537530	T	T	T
	0.9166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.9164720455255654	0.0835291310392273	0.3137079983126178	T	T	T
	0.8332893601904289	0.1667148829147802	0.2267022507135547	T	T	T
	0.0000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.0000698782870623	0.2442024879665190	0.4010769928838187	T	T	T
	0.1666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.1666537933174226	0.3332929961410289	0.3139001793384078	T	T	T
	0.0833258813142949	0.4167059791835925	0.2269133586184098	T	T	T
	0.2500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.2441447900134086	0.2442075938905595	0.4010777787793032	T	T	T
	0.4166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.4167832140250228	0.3335172789045483	0.3147678519011747	T	T	T
	0.3334029881647536	0.4167219080613548	0.2269101496415479	T	T	T
	0.5000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.4991223129400367	0.2495679687381337	0.4019136158806959	T	T	T
	0.6666669999999968	0.3333330000000032	0.0514190000000028	F	F	F

0.6666725673858035	0.3333386807004205	0.3145635095677722	T	T	T
0.5834028649632698	0.4166042913441702	0.2270738188290141	T	T	T
0.7500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.7504333991981242	0.2495683211398871	0.4019188261499954	T	T	T
0.9166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.9167459538704470	0.3335077520746149	0.3147721994723077	T	T	T
0.8331913107435384	0.4165861414393692	0.2270779575890907	T	T	T
0.0000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.1666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.1669273467527274	0.5834734757362515	0.3145896714662174	T	T	T
0.0833062823924379	0.6666078215064416	0.2269094641373540	T	T	T
0.2500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.2491643011452312	0.4983252637737140	0.4013794915601467	T	T	T
0.4166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.4165562877249627	0.5834694351764597	0.3145887059984531	T	T	T
0.3333305426903074	0.6666770060239215	0.2267635376328562	T	T	T
0.5000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.6666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.6665276977895960	0.5832463122299850	0.3147726978021801	T	T	T
0.5833111119784411	0.6666313620375770	0.2269127742523346	T	T	T
0.7500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.7504298193071866	0.5008588156149804	0.4019084272972328	T	T	T
0.9166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.9167290559261458	0.5832350841268981	0.3147721919649597	T	T	T
0.8332833367571110	0.6665738986298061	0.2266956028067581	T	T	T
0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.0000646973686104	0.7558814609865367	0.4010789337992510	T	T	T
0.1666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
0.1666265458310016	0.8333523982201295	0.3139026434836715	T	T	T
0.0834206673172653	0.9165787211128862	0.2265269619080374	T	T	T
0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.2491527819557181	0.7508394943813294	0.4013759253727142	T	T	T
0.4166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
0.4165695130474686	0.8331407750923875	0.3146021047814454	T	T	T
0.3333668596516606	0.9166591674071086	0.2269141085635633	T	T	T
0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.5016770248976506	0.7508437535894181	0.4013759634765209	T	T	T
0.6666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
0.6667397927450809	0.8333685442648761	0.3139126892434811	T	T	T
0.5832878506697118	0.9166586701458784	0.2269173974612602	T	T	T
0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.7558253549436911	0.7558869343968073	0.4010794345339474	T	T	T
0.9166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
0.9164766704789107	0.8329426574894866	0.3137077238656317	T	T	T
0.8331508030982384	0.9165771629399613	0.2265299484583251	T	T	T
0.4999365429481073	-0.0001251791136093	0.4183904586526231	T	T	T
0.0001434643604973	0.5000746229009196	0.4183967544075756	T	T	T
0.4999422095026682	0.5000762892440255	0.4183953742957534	T	T	T
3Ni/Cu(111)	1.0000000000000000				
	8.8905944857135406	-5.1329871195825199	-0.0000000000000010		
	0.0000000000000000	10.2659742391650006	0.0000000000000010		

0.0000000000000000 0.0000000000000000 23.3821328661704015

Ni Cu

3 77

Selective dynamics

Direct

0.2503283554902788	0.2501641777451430	0.3794700586603963	T	T	T
0.7498358222548569	0.2501641777451430	0.3794700586603963	T	T	T
0.7498358222548569	0.7496716445097211	0.3794700586603963	T	T	T
0.0000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
-0.0000497843033176	0.0000497843033175	0.3831097317326189	T	T	T
0.1666666667000030	0.0833333332999970	0.0259047434999999	F	F	F
0.1667005415388891	0.0837186102355600	0.2941450338539350	T	T	T
0.0831252213114602	0.1665626107057381	0.2047456245043671	T	T	T
0.2500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.2500298855253219	0.0019311072473419	0.3831706475614562	T	T	T
0.4166666667000030	0.0833333332999970	0.0259047434999999	F	F	F
0.4167129421610440	0.0834258842220792	0.2943525974382475	T	T	T
0.3334440824856191	0.1665496762791837	0.2047800753431704	T	T	T
0.5000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.5019012217220199	0.0019311072473419	0.3831706475614562	T	T	T
0.6666666667000030	0.0833333332999970	0.0259047434999999	F	F	F
0.6670180687966727	0.0837186102355600	0.2941450338539350	T	T	T
0.5831055936935555	0.1665496762791837	0.2047800753431704	T	T	T
0.7500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.7500995686066282	0.0000497843033175	0.3831097317326189	T	T	T
0.9166666667000030	0.0833333332999970	0.0259047434999999	F	F	F
0.9166666667000030	0.0833333332999970	0.2941765175039666	T	T	T
0.8334373892942618	0.1665626107057381	0.2047456245043671	T	T	T
0.0000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
-0.0000497843033176	0.2499004313933720	0.3831097317326189	T	T	T
0.1666666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.1667005415388891	0.3329819312033273	0.2941450338539350	T	T	T
0.0833243689485500	0.4166487379971019	0.2050772422052570	T	T	T
0.2500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.4166666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.4165143429601725	0.3332571714300819	0.2942199719381587	T	T	T
0.3334440824856191	0.4168944063064443	0.2047800753431704	T	T	T
0.5000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.5002432424111972	0.2504864848223943	0.3832630645344138	T	T	T
0.6666666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.6667428285699181	0.3332571714300819	0.2942199719381587	T	T	T
0.5833333332999970	0.4166666667000030	0.2050834760805971	T	T	T
0.7500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.9166666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.9162813897644398	0.3329819312033273	0.2941450338539350	T	T	T
0.8334503237208163	0.4168944063064443	0.2047800753431704	T	T	T
0.0000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.9980688927526582	0.4980987782779800	0.3831706475614562	T	T	T
0.1666666667000030	0.5833333332999970	0.0259047434999999	F	F	F
0.1665611624000990	0.5831223247001963	0.2945300852964385	T	T	T
0.0832818227060763	0.6666409114030427	0.2051013294995641	T	T	T

	0.2500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.2500298855253219	0.4980987782779800	0.3831706475614562	T	T	T
	0.4166666667000030	0.5833333332999970	0.0259047434999999	F	F	F
	0.4167129421610440	0.5832870578389561	0.2943525974382475	T	T	T
	0.3333590885969573	0.6666409114030427	0.2051013294995641	T	T	T
	0.5000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.5002432424111972	0.4997567575888029	0.3832630645344138	T	T	T
	0.6666666667000030	0.5833333332999970	0.0259047434999999	F	F	F
	0.6667428285699181	0.5834856570398274	0.2942199719381587	T	T	T
	0.5831055936935555	0.6665559175143807	0.2047800753431704	T	T	T
	0.7500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.7495135151776059	0.4997567575888029	0.3832630645344138	T	T	T
	0.9166666667000030	0.5833333332999970	0.0259047434999999	F	F	F
	0.9165741157779209	0.5832870578389561	0.2943525974382475	T	T	T
	0.8334503237208163	0.6665559175143807	0.2047800753431704	T	T	T
	0.0000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.9980688927526582	0.7499701144746781	0.3831706475614562	T	T	T
	0.1666666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.1665611624000990	0.8334388375999010	0.2945300852964385	T	T	T
	0.0833243689485500	0.9166756310514501	0.2050772422052570	T	T	T
	0.2500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.2500000000000000	0.7500000000000000	0.3829148699938958	T	T	T
	0.4166666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.4168776752998038	0.8334388375999010	0.2945300852964385	T	T	T
	0.3333590885969573	0.9167181772939236	0.2051013294995641	T	T	T
	0.5000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.5019012217220199	0.7499701144746781	0.3831706475614562	T	T	T
	0.6666666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.6670180687966727	0.8332994584611108	0.2941450338539350	T	T	T
	0.5833512620028981	0.9166756310514501	0.2050772422052570	T	T	T
	0.7500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.9166666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.9162813897644398	0.8332994584611108	0.2941450338539350	T	T	T
	0.8334373892942618	0.9168747786885398	0.2047456245043671	T	T	T
3Pd/Cu(111)	1.0000000000000000					
	8.8905944857135406	-5.1329871195825199	-0.0000000000000010			
	0.0000000000000000	10.2659742391650006	0.0000000000000010			
	0.0000000000000000	0.0000000000000000	23.3821328661704015			
	Pd Cu					
	3 77					
	Selective dynamics					
	Direct					
	0.2500724824808321	0.2500362412404196	0.3864559310398177	T	T	T
	0.7499637587595804	0.2500362412404196	0.3864559310398177	T	T	T
	0.7499637587595804	0.7499275175191680	0.3864559310398177	T	T	T
	0.0000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.0004682453022572	0.9995317546977428	0.3839580119271725	T	T	T
	0.1666666667000030	0.0833333332999970	0.0259047434999999	F	F	F
	0.1665253008303561	0.0828290451355722	0.2940909959369945	T	T	T
	0.0830293743728773	0.1665146872364467	0.2049641242528912	T	T	T
	0.2500000000000000	0.0000000000000000	0.1155258754999977	F	F	F

0.2500316318545875	0.9965851348429671	0.3835390856607719	T	T	T
0.4166666667000030	0.083333332999970	0.0259047434999999	F	F	F
0.4167305599137760	0.0834611197275502	0.2944042250772039	T	T	T
0.3334056307467254	0.1665858787483858	0.2047922535410796	T	T	T
0.5000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.4965535029883724	0.9965851348429671	0.3835390856607719	T	T	T
0.6666666667000030	0.083333332999970	0.0259047434999999	F	F	F
0.6663037444052249	0.0828290451355722	0.2940909959369945	T	T	T
0.5831802479016517	0.1665858787483858	0.2047922535410796	T	T	T
0.7500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.7490635093954854	0.9995317546977428	0.3839580119271725	T	T	T
0.9166666667000030	0.083333332999970	0.0259047434999999	F	F	F
0.9166666667000030	0.083333332999970	0.2947459163947945	T	T	T
0.8334853127635534	0.1665146872364467	0.2049641242528912	T	T	T
0.0000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.0004682453022572	0.2509364906045145	0.3839580119271725	T	T	T
0.1666666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.1665253008303561	0.3336962555947751	0.2940909959369945	T	T	T
0.0831667634068415	0.4163335269136991	0.2050822283295567	T	T	T
0.2500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.4166666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.4170965516143063	0.3335482757571523	0.2940558366786583	T	T	T
0.3334056307467254	0.4168197520983484	0.2047922535410796	T	T	T
0.5000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.4997046538996950	0.2494093077993901	0.3839599979096304	T	T	T
0.6666666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.6664517242428477	0.3335482757571523	0.2940558366786583	T	T	T
0.583333332999970	0.4166666667000030	0.2052006196880597	T	T	T
0.7500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.9166666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.9171709548644279	0.3336962555947751	0.2940909959369945	T	T	T
0.8334141212516140	0.4168197520983484	0.2047922535410796	T	T	T
0.0000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.0034148651570331	0.5034464970116277	0.3835390856607719	T	T	T
0.1666666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.1667295101521390	0.5834590202042620	0.2940936357149928	T	T	T
0.0831095343558255	0.6665547672279136	0.2049730037922567	T	T	T
0.2500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.2500316318545875	0.5034464970116277	0.3835390856607719	T	T	T
0.4166666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.4167305599137760	0.5832694400862242	0.2944042250772039	T	T	T
0.3334452327720864	0.6665547672279136	0.2049730037922567	T	T	T
0.5000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.4997046538996950	0.5002953461003050	0.3839599979096304	T	T	T
0.6666666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.6664517242428477	0.5829034483856936	0.2940558366786583	T	T	T
0.5831802479016517	0.6665943692532746	0.2047922535410796	T	T	T
0.7500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.7505906922006100	0.5002953461003050	0.3839599979096304	T	T	T
0.9166666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.9165388802724498	0.5832694400862242	0.2944042250772039	T	T	T

	0.8334141212516140 0.6665943692532746 0.2047922535410796 T T T
	0.0000000000000000 0.7500000000000000 0.1155258754999977 F F F
	0.0034148651570331 0.7499683681454126 0.3835390856607719 T T T
	0.1666666667000030 0.8333333332999970 0.0259047434999999 F F F
	0.1667295101521390 0.8332704898478610 0.2940936357149928 T T T
	0.0831667634068415 0.9168332365931585 0.2050822283295567 T T T
	0.2500000000000000 0.7500000000000000 0.1155258754999977 F F F
	0.2500000000000000 0.7500000000000000 0.3828897891205418 T T T
	0.4166666667000030 0.8333333332999970 0.0259047434999999 F F F
	0.4165409797957380 0.8332704898478610 0.2940936357149928 T T T
	0.3334452327720864 0.9168904656441745 0.2049730037922567 T T T
	0.5000000000000000 0.7500000000000000 0.1155258754999977 F F F
	0.4965535029883724 0.7499683681454126 0.3835390856607719 T T T
	0.6666666667000030 0.8333333332999970 0.0259047434999999 F F F
	0.6663037444052249 0.8334746991696438 0.2940909959369945 T T T
	0.5836664730863009 0.9168332365931585 0.2050822283295567 T T T
	0.7500000000000000 0.7500000000000000 0.1155258754999977 F F F
	0.9166666667000030 0.8333333332999970 0.0259047434999999 F F F
	0.9171709548644279 0.8334746991696438 0.2940909959369945 T T T
	0.8334853127635534 0.9169706256271227 0.2049641242528912 T T T
3Pt/Cu(111)	1.0000000000000000
	8.8905944857135406 -5.1329871195825199 -0.0000000000000010
	0.0000000000000000 10.2659742391650006 0.0000000000000010
	0.0000000000000000 0.0000000000000000 23.3821328661704015
	Pt Cu
	3 77
	Selective dynamics
	Direct
	0.2499493776084591 0.2499746888042296 0.3844447678874801 T T T
	0.7500253111957704 0.2499746888042296 0.3844447678874801 T T T
	0.7500253111957704 0.7500506223915409 0.3844447678874801 T T T
	0.0000000000000000 0.0000000000000000 0.1155258754999977 F F F
	0.0005437977761744 0.9994562022238256 0.3857867268065931 T T T
	0.1666666667000030 0.0833333332999970 0.0259047434999999 F F F
	0.1657504645061181 0.0817238472942776 0.2937477518614955 T T T
	0.0829058056255860 0.1664529028628010 0.2048818171890119 T T T
	0.2500000000000000 0.0000000000000000 0.1155258754999977 F F F
	0.2500900272260935 0.9973974540751485 0.3842429596475228 T T T
	0.4166666667000030 0.0833333332999970 0.0259047434999999 F F F
	0.4165011782186809 0.0830023563373459 0.2944778631106715 T T T
	0.3334323781655897 0.1664992381424426 0.2047900505805913 T T T
	0.5000000000000000 0.0000000000000000 0.1155258754999977 F F F
	0.4973074268490549 0.9973974540751485 0.3842429596475228 T T T
	0.6666666667000030 0.0833333332999970 0.0259047434999999 F F F
	0.6659733828881542 0.0817238472942776 0.2937477518614955 T T T
	0.5830668598768440 0.1664992381424426 0.2047900505805913 T T T
	0.7500000000000000 0.0000000000000000 0.1155258754999977 F F F
	0.7489124044476512 0.9994562022238256 0.3857867268065931 T T T
	0.9166666667000030 0.0833333332999970 0.0259047434999999 F F F
	0.9166666667000030 0.0833333332999970 0.2949529930385282 T T T
	0.8335470971371990 0.1664529028628010 0.2048818171890119 T T T

0.0000000000000000	0.2500000000000000	0.1155258754999977	F F F
0.0005437977761744	0.2510875955523488	0.3857867268065931	T T T
0.166666667000030	0.333333332999970	0.0259047434999999	F F F
0.1657504645061181	0.3340266171118458	0.2937477518614955	T T T
0.0832564242966285	0.4165128486932659	0.2050424094222763	T T T
0.2500000000000000	0.2500000000000000	0.1155258754999977	F F F
0.416666667000030	0.333333332999970	0.0259047434999999	F F F
0.4182678723777258	0.3341339361388620	0.2938461052600729	T T T
0.3334323781655897	0.4169331401231560	0.2047900505805913	T T T
0.5000000000000000	0.2500000000000000	0.1155258754999977	F F F
0.4997734268354250	0.2495468536708501	0.3857637875647768	T T T
0.666666667000030	0.333333332999970	0.0259047434999999	F F F
0.6658660638611380	0.3341339361388620	0.2938461052600729	T T T
0.583333332999970	0.416666667000030	0.2051152254755593	T T T
0.7500000000000000	0.2500000000000000	0.1155258754999977	F F F
0.916666667000030	0.333333332999970	0.0259047434999999	F F F
0.9182761527057224	0.3340266171118458	0.2937477518614955	T T T
0.8335007618575574	0.4169331401231560	0.2047900505805913	T T T
0.0000000000000000	0.5000000000000000	0.1155258754999977	F F F
0.0026025459248515	0.5026925731509451	0.3842429596475228	T T T
0.166666667000030	0.583333332999970	0.0259047434999999	F F F
0.1667132723476996	0.5834265445953974	0.2945095332787346	T T T
0.0833206486057350	0.6666603243528684	0.2050795807957400	T T T
0.2500000000000000	0.5000000000000000	0.1155258754999977	F F F
0.2500900272260935	0.5026925731509451	0.3842429596475228	T T T
0.416666667000030	0.583333332999970	0.0259047434999999	F F F
0.4165011782186809	0.5834988217813191	0.2944778631106715	T T T
0.3333396756471316	0.6666603243528684	0.2050795807957400	T T T
0.5000000000000000	0.5000000000000000	0.1155258754999977	F F F
0.4997734268354250	0.5002265731645750	0.3857637875647768	T T T
0.666666667000030	0.583333332999970	0.0259047434999999	F F F
0.6658660638611380	0.5817321276222742	0.2938461052600729	T T T
0.5830668598768440	0.6665676218344103	0.2047900505805913	T T T
0.7500000000000000	0.5000000000000000	0.1155258754999977	F F F
0.7504531463291499	0.5002265731645750	0.3857637875647768	T T T
0.916666667000030	0.583333332999970	0.0259047434999999	F F F
0.9169976436626541	0.5834988217813191	0.2944778631106715	T T T
0.8335007618575574	0.6665676218344103	0.2047900505805913	T T T
0.0000000000000000	0.7500000000000000	0.1155258754999977	F F F
0.0026025459248515	0.7499099727739065	0.3842429596475228	T T T
0.166666667000030	0.833333332999970	0.0259047434999999	F F F
0.1667132723476996	0.8332867276522933	0.2945095332787346	T T T
0.0832564242966285	0.9167435757033715	0.2050424094222763	T T T
0.2500000000000000	0.7500000000000000	0.1155258754999977	F F F
0.2500000000000000	0.7500000000000000	0.3828496532656160	T T T
0.416666667000030	0.833333332999970	0.0259047434999999	F F F
0.4165734554046026	0.8332867276522933	0.2945095332787346	T T T
0.3333396756471316	0.9166793513942650	0.2050795807957400	T T T
0.5000000000000000	0.7500000000000000	0.1155258754999977	F F F
0.4973074268490549	0.7499099727739065	0.3842429596475228	T T T
0.666666667000030	0.833333332999970	0.0259047434999999	F F F

	0.6659733828881542	0.8342495354938819	0.2937477518614955	T	T	T
	0.5834871513067341	0.9167435757033715	0.2050424094222763	T	T	T
	0.7500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.9166666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.9182761527057224	0.8342495354938819	0.2937477518614955	T	T	T
	0.8335470971371990	0.9170941943744140	0.2048818171890119	T	T	T
(6) 3X-PC						
3Cu/Ni(111)	1.0000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni	Cu				
	77	3				
	Selective dynamics					
	Direct					
	0.0000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.0001021284029221	0.0001339421440321	0.4012091539824141	T	T	T
	0.1666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.1670526650752606	0.0836768196742028	0.3142238214666762	T	T	T
	0.0833614327521346	0.1666127649798455	0.2267663458005842	T	T	T
	0.2500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.2500409907192207	0.9999817835630935	0.4010612580711665	T	T	T
	0.4166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.4162962702235546	0.0833439851545208	0.3141764469058188	T	T	T
	0.3332843432736112	0.1666366759365587	0.2267013345240798	T	T	T
	0.5000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.5004351362332571	0.0023881065427815	0.4009091817151997	T	T	T
	0.6666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.6669376233367004	0.0831723423541320	0.3144179160763159	T	T	T
	0.5833318261357405	0.1666522534894881	0.2268090728620109	T	T	T
	0.7500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.7520176810384100	0.0024985854513204	0.4010478307373333	T	T	T
	0.9166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.9167894943155517	0.0832423705872500	0.3142056596018108	T	T	T
	0.8333612880204058	0.1666245767947601	0.2267217663380023	T	T	T
	0.0000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.9977118134431819	0.2481009679254385	0.4010845456782022	T	T	T
	0.1666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.1671592305872238	0.3338027664981595	0.3148673246145179	T	T	T
	0.0836408631501016	0.4165928715499163	0.2270158411631371	T	T	T
	0.2500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.2479894983890318	0.2455144220508956	0.4009684934026581	T	T	T
	0.4166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.4166795348594476	0.3338377069519680	0.3148167748557285	T	T	T
	0.3330893850421575	0.4165544421796383	0.2271195163297222	T	T	T
	0.5000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.5004470650204951	0.2480904813742768	0.4010359649828672	T	T	T
	0.6666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.6665848791581439	0.3334107948611233	0.3144035708079898	T	T	T
	0.5832533570892053	0.4166759071380142	0.2269920579556484	T	T	T
	0.7500000000000000	0.2500000000000000	0.1392870000000030	F	F	F

	0.7500220188514533	0.2500605106873621	0.4012146703105088	T	T	T
	0.9166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.9170651211825458	0.3332510403366982	0.3144647464859531	T	T	T
	0.8332293625115028	0.4165594208027272	0.2268368149943782	T	T	T
	0.0000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.9977494899451429	0.4997191924906446	0.4009430354616157	T	T	T
	0.1666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.1672986356733546	0.5832926229572877	0.3146821920112259	T	T	T
	0.0832373310335868	0.6666875720121510	0.2266835501471007	T	T	T
	0.2500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.4166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.4166366955244527	0.5833743889917855	0.3153389509145583	T	T	T
	0.3333325573875570	0.6666554298472391	0.2270992548471753	T	T	T
	0.5000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.6666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.6662523269247274	0.5834245944453187	0.3147743716334546	T	T	T
	0.5833971513754932	0.6668322023467823	0.2270693000120687	T	T	T
	0.7500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.7520758232373339	0.4997056235511010	0.4010227383744365	T	T	T
	0.9166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.9167419980884119	0.5838006269360960	0.3141965262214086	T	T	T
	0.8333587071766928	0.6667087647968941	0.2266858590605096	T	T	T
	0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.0000728174911444	0.7500936155297921	0.4010544200734358	T	T	T
	0.1666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.1667706339963502	0.8333097887231986	0.3139258105128135	T	T	T
	0.0833594831914226	0.9166546846284618	0.2268785912584264	T	T	T
	0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.2476317246815114	0.7524068134994337	0.4007086638128428	T	T	T
	0.4166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.4167824096133401	0.8327649631651397	0.3147004473588311	T	T	T
	0.3331592768064482	0.9166017080609876	0.2266828970694874	T	T	T
	0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.6666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.6662984521625006	0.8329907484261128	0.3148578387334879	T	T	T
	0.5832317984781170	0.9162254148959121	0.2269800229280392	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.7546864890380078	0.7522767054088462	0.4009225548194379	T	T	T
	0.9166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.9164349288222056	0.8330751084867600	0.3141832053022284	T	T	T
	0.8333423773652413	0.9166121964128919	0.2267388876750047	T	T	T
	0.5011313871617915	0.7523092512681160	0.4059009225751780	T	T	T
	0.2477917723538567	0.4990041148585362	0.4058925128798165	T	T	T
	0.5012367004088318	0.4989867650444779	0.4058877664980187	T	T	T
3Ag/Ni(111)	1.0000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni	Ag				
	77	3				
	Selective dynamics					

Direct			
0.0000000000000000	0.0000000000000000	0.1392870000000030	F F F
0.0002565524006428	0.9997547098189230	0.3998455714181830	T T T
0.1666669999999968	0.0833330000000032	0.0514190000000028	F F F
0.1671483929933828	0.0840987705681187	0.3130149361319141	T T T
0.0839478046837883	0.1676459836433821	0.2264666392503472	T T T
0.2500000000000000	0.0000000000000000	0.1392870000000030	F F F
0.2491192221077725	0.9997073276087534	0.3998375323839127	T T T
0.4166669999999968	0.0833330000000032	0.0514190000000028	F F F
0.4154040145805666	0.0832883075494308	0.3127252497208346	T T T
0.3335910153711623	0.1675157584191496	0.2263793026167278	T T T
0.5000000000000000	0.0000000000000000	0.1392870000000030	F F F
0.5005113270023287	0.0077614219692421	0.3997910615753213	T T T
0.6666669999999968	0.0833330000000032	0.0514190000000028	F F F
0.6668379606791248	0.0831171313909636	0.3139162215236411	T T T
0.5834573096611280	0.1666745860187859	0.2263731740453281	T T T
0.7500000000000000	0.0000000000000000	0.1392870000000030	F F F
0.7570650053101531	0.0076917978963991	0.3998975125808002	T T T
0.9166669999999968	0.0833330000000032	0.0514190000000028	F F F
0.9169987166938753	0.0829953612244481	0.3127361147014369	T T T
0.8333073818722383	0.1667186401373755	0.2262348934568763	T T T
0.0000000000000000	0.2500000000000000	0.1392870000000030	F F F
0.9923760185835917	0.2430697184232642	0.3998932430429605	T T T
0.1666669999999968	0.3333330000000032	0.0514190000000028	F F F
0.1679387903838361	0.3349123952425188	0.3158803926430949	T T T
0.0842116011168201	0.4169001767568403	0.2272460274074604	T T T
0.2500000000000000	0.2500000000000000	0.1392870000000030	F F F
0.2440027989433560	0.2379776791080417	0.4009581772355233	T T T
0.4166669999999968	0.3333330000000032	0.0514190000000028	F F F
0.4171539793199486	0.3353454899420925	0.3158497479450944	T T T
0.3336092498585614	0.4176335221096821	0.2279796099423805	T T T
0.5000000000000000	0.2500000000000000	0.1392870000000030	F F F
0.5007986834300624	0.2429171383698190	0.3998100508049163	T T T
0.6666669999999968	0.3333330000000032	0.0514190000000028	F F F
0.6665870101628713	0.3334162867386112	0.3136250525624504	T T T
0.5830520319371288	0.4169489359393808	0.2271681854645564	T T T
0.7500000000000000	0.2500000000000000	0.1392870000000030	F F F
0.7499974676584245	0.2500083482721323	0.4010813393722330	T T T
0.9166669999999968	0.3333330000000032	0.0514190000000028	F F F
0.9168996798758542	0.3332053558711081	0.3139055363464820	T T T
0.8333171680448359	0.4165604634161895	0.2263599471862747	T T T
0.0000000000000000	0.5000000000000000	0.1392870000000030	F F F
0.9922709948908164	0.4995091649045946	0.3997968567344117	T T T
0.1666669999999968	0.5833330000000032	0.0514190000000028	F F F
0.1677655984058433	0.5830662191725295	0.3157627893706874	T T T
0.0837877910224805	0.6663793957234176	0.2264655209436128	T T T
0.2500000000000000	0.5000000000000000	0.1392870000000030	F F F
0.4166669999999968	0.5833330000000032	0.0514190000000028	F F F
0.4163941693554634	0.5836544850415564	0.3184713091093201	T T T
0.3336043157918809	0.6664176487401434	0.2280848225719510	T T T
0.5000000000000000	0.5000000000000000	0.1392870000000030	F F F

	0.6666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.6647776128110863	0.5829422956342825	0.3158304239463021	T	T	T
	0.5824122253433828	0.6664063842472601	0.2279712661058042	T	T	T
	0.7500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.7570946827703295	0.4992263097289893	0.3998006455216441	T	T	T
	0.9166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.9167488931764680	0.5845886867212684	0.3127275772009028	T	T	T
	0.8325009640346295	0.6663804221668954	0.2263838476939171	T	T	T
	0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.0003356564190966	0.7509464047033987	0.3998385906752304	T	T	T
	0.1666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.1667978205595730	0.8332638662624845	0.3128609487643814	T	T	T
	0.0833314968496026	0.9166811624756903	0.2262832412711830	T	T	T
	0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.2439701004381973	0.7560722318800543	0.4008432276498226	T	T	T
	0.4166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.4169729208118511	0.8322498914021281	0.3157566302972654	T	T	T
	0.3336564749178592	0.9162470168923349	0.2264529138134250	T	T	T
	0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.6666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.6650860505987382	0.8320543457210334	0.3158673569243362	T	T	T
	0.5831255998192688	0.9157964625109969	0.2272453265617642	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.7620498399367648	0.7560004218312102	0.4009474141892682	T	T	T
	0.9166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.9159837991397808	0.8329015679250560	0.3130153706218977	T	T	T
	0.8323489286639258	0.9160782782758758	0.2264657066060138	T	T	T
	0.5068730321223498	0.7637155172933561	0.4245757148262754	T	T	T
	0.2363439795440030	0.4931930266605065	0.4245800954795840	T	T	T
	0.5069005813194067	0.4931266147208078	0.4247171373825225	T	T	T
3Au/Ni(111)	1.0000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni	Au				
	77	3				
	Selective dynamics					
	Direct					
	0.0000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.0003985341731507	0.9995978565921746	0.4000383488199688	T	T	T
	0.1666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.1669922961274537	0.0839723465770561	0.3135504239445623	T	T	T
	0.0836559220091075	0.1672173864301172	0.2266635176775438	T	T	T
	0.2500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.2486894501871930	0.9995385911100243	0.4001231375443055	T	T	T
	0.4166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.4155937687685025	0.0831219237215493	0.3131945749481915	T	T	T
	0.3334558630564075	0.1670107581091429	0.2263715919764309	T	T	T
	0.5000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.5003230866621067	0.0079790181396504	0.4007415162169679	T	T	T
	0.6666669999999968	0.0833330000000032	0.0514190000000028	F	F	F

0.6669253519832026	0.0836255382202395	0.3140370592101718	T	T	T
0.5834272663821096	0.1666178174584871	0.2264267698756157	T	T	T
0.7500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
0.7573402592875667	0.0080257183599244	0.4008736864474116	T	T	T
0.9166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
0.9167513378030705	0.0832638277635667	0.3133347934306059	T	T	T
0.8333154275469710	0.1667091480865182	0.2263071459680432	T	T	T
0.0000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.9919970041119655	0.2426757345171850	0.4008723447576443	T	T	T
0.1666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.1668070158398365	0.3335583930653812	0.3154242323333420	T	T	T
0.0840229237980807	0.4168230348142146	0.2272320461027917	T	T	T
0.2500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.2446470379984973	0.2391127043977690	0.4019956522417516	T	T	T
0.4166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.4167032149966019	0.3337282621560433	0.3150751710541897	T	T	T
0.3332494116678859	0.4170867851047646	0.2276737588372200	T	T	T
0.5000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.5004941417720943	0.2426786299277950	0.4006086128480177	T	T	T
0.6666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.6666254506292262	0.3333229152865158	0.3136584713331629	T	T	T
0.5831529554774875	0.4168347687414169	0.2269800046116686	T	T	T
0.7500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.7498187305673767	0.2502135784708841	0.4009367273037796	T	T	T
0.9166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.9163292564975407	0.3330489223995698	0.3140538610423391	T	T	T
0.8333821032111572	0.4165649387812635	0.2264423844737138	T	T	T
0.0000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.9920503878573896	0.4997208228576966	0.4007368392876529	T	T	T
0.1666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.1669609569714439	0.5833646314164724	0.3152938762059421	T	T	T
0.0837711463883153	0.6665661351955450	0.2265794417584033	T	T	T
0.2500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.4166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.4166850796675519	0.5833637031212859	0.3168639016715176	T	T	T
0.3336295785478427	0.6664101826231388	0.2279144851369921	T	T	T
0.5000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.6666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.6662333822563582	0.5833182826808638	0.3150900973984960	T	T	T
0.5829676294853812	0.6667699308474369	0.2276836183496798	T	T	T
0.7500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.7573595114930214	0.4995655546507507	0.4006100601325571	T	T	T
0.9166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.9168677381180075	0.5843598143321529	0.3131986543506287	T	T	T
0.8329924783531126	0.6665407091388147	0.2263747451978233	T	T	T
0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.0004568517588410	0.7513417710071693	0.4001245040998711	T	T	T
0.1666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
0.1667947608026310	0.8332161647234955	0.3135147478618805	T	T	T
0.0833882568381981	0.9166266665536256	0.2264886537224911	T	T	T
0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F

	0.2443693944398433	0.7555947127907885	0.4020834220356164	T	T	T
	0.4166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.4166365064367739	0.8330682547884720	0.3153026422402121	T	T	T
	0.3334462487051653	0.9162423115388805	0.2265847949314264	T	T	T
	0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.6666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.6664570515700845	0.8332376187589645	0.3154192693537681	T	T	T
	0.5831668474404310	0.9159571571831435	0.2272295580918566	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.7608567589636621	0.7553863708108466	0.4019807067720222	T	T	T
	0.9166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.9160012766585410	0.8329827108877907	0.3135447421708903	T	T	T
	0.8328212535550747	0.9163622129854190	0.2266611977890065	T	T	T
	0.5073201210312632	0.7648657746178813	0.4208942738573640	T	T	T
	0.2351530216454236	0.4926824628714854	0.4208968888781470	T	T	T
	0.5072719740639968	0.4927469627614300	0.4207229095687453	T	T	T
3Ni/Cu(111)	1.0000000000000000					
	8.8905944857135406	-5.1329871195825199	-0.0000000000000010			
	0.0000000000000000	10.2659742391650006	0.0000000000000010			
	0.0000000000000000	0.0000000000000000	23.3821328661704015			
	Ni	Cu				
	3	77				
	Selective dynamics					
	Direct					
	0.2547086412390556	0.5023543206195313	0.3795340836406638	T	T	T
	0.4976456793804687	0.5023543206195313	0.3795340836406638	T	T	T
	0.4976456793804687	0.7452913587609444	0.3795340836406638	T	T	T
	0.0000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.9998056775174291	0.0001943224825709	0.3832283182817449	T	T	T
	0.1666666667000030	0.0833333332999970	0.0259047434999999	F	F	F
	0.1669594655295583	0.0839189309591077	0.2946386798133034	T	T	T
	0.0833047848561819	0.1667087366007536	0.2050932915893142	T	T	T
	0.2500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.2503886449651418	0.0001943224825709	0.3832283182817449	T	T	T
	0.4166666667000030	0.0833333332999970	0.0259047434999999	F	F	F
	0.4169887568994426	0.0834943783997133	0.2946419963990152	T	T	T
	0.3334039516445628	0.1667087366007536	0.2050932915893142	T	T	T
	0.5000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.4996280501835741	0.9971969552411224	0.3831885774262673	T	T	T
	0.6666666667000030	0.0833333332999970	0.0259047434999999	F	F	F
	0.6666066183437138	0.0832132365874187	0.2943544265351292	T	T	T
	0.5833316760498803	0.1666658380749482	0.2050476995477624	T	T	T
	0.7500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.7475689050575482	0.9971969552411224	0.3831885774262673	T	T	T
	0.9166666667000030	0.0833333332999970	0.0259047434999999	F	F	F
	0.9165056216002867	0.0834943783997133	0.2946419963990152	T	T	T
	0.8333341619250518	0.1666658380749482	0.2050476995477624	T	T	T
	0.0000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
	0.0028030447588776	0.2524310949424518	0.3831885774262673	T	T	T
	0.1666666667000030	0.3333333332999970	0.0259047434999999	F	F	F
	0.1671535093871626	0.3340404958535501	0.2940871745757576	T	T	T

0.0831574057273485	0.4165787029136752	0.2047174909737564	T	T	T
0.2500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.2520501626822806	0.2541003253645542	0.3834293441024528	T	T	T
0.4166666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.4168869865663964	0.3340404958535501	0.2940871745757576	T	T	T
0.3331897443945095	0.4163794888890138	0.2043502906290300	T	T	T
0.5000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.4996280501835741	0.2524310949424518	0.3831885774262673	T	T	T
0.6666666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.6666066183437138	0.3333933816562862	0.2943544265351292	T	T	T
0.5834212970863248	0.4165787029136752	0.2047174909737564	T	T	T
0.7500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.7500000000000000	0.2500000000000000	0.3829465008137447	T	T	T
0.9166666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.9167867634125813	0.3333933816562862	0.2943544265351292	T	T	T
0.8333341619250518	0.4166683239501197	0.2050476995477624	T	T	T
0.0000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.0028030447588776	0.5003719498164259	0.3831885774262673	T	T	T
0.1666666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.1671535093871626	0.5831130134336036	0.2940871745757576	T	T	T
0.0833047848561819	0.6665960483554372	0.2050932915893142	T	T	T
0.2500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.4166666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.4166666667000030	0.583333332999970	0.2930874609559808	T	T	T
0.3331897443945095	0.6668102556054905	0.2043502906290300	T	T	T
0.5000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.6666666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.6659595041464499	0.5831130134336036	0.2940871745757576	T	T	T
0.5836205111109862	0.6668102556054905	0.2043502906290300	T	T	T
0.7500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.7475689050575482	0.5003719498164259	0.3831885774262673	T	T	T
0.9166666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.9165056216002867	0.5830112431005574	0.2946419963990152	T	T	T
0.8332912633992464	0.6665960483554372	0.2050932915893142	T	T	T
0.0000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
0.9998056775174291	0.7496113550348582	0.3832283182817449	T	T	T
0.1666666667000030	0.833333332999970	0.0259047434999999	F	F	F
0.1669594655295583	0.8330405344704417	0.2946386798133034	T	T	T
0.083333332999970	0.9166666667000030	0.2051115948682209	T	T	T
0.2500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
0.2520501626822806	0.7479498373177194	0.3834293441024528	T	T	T
0.4166666667000030	0.833333332999970	0.0259047434999999	F	F	F
0.4168869865663964	0.8328464906128374	0.2940871745757576	T	T	T
0.3334039516445628	0.9166952151438181	0.2050932915893142	T	T	T
0.5000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
0.6666666667000030	0.833333332999970	0.0259047434999999	F	F	F
0.6659595041464499	0.8328464906128374	0.2940871745757576	T	T	T
0.5834212970863248	0.9168425942726586	0.2047174909737564	T	T	T
0.7500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
0.7458996746354458	0.7479498373177194	0.3834293441024528	T	T	T
0.9166666667000030	0.833333332999970	0.0259047434999999	F	F	F

	0.9160810690408923 0.8330405344704417 0.2946386798133034 T T T
	0.8332912633992464 0.9166952151438181 0.2050932915893142 T T T
3Pd/Cu(111)	1.0000000000000000
	8.8905944857135406 -5.1329871195825199 -0.0000000000000010
	0.0000000000000000 10.2659742391650006 0.0000000000000010
	0.0000000000000000 0.0000000000000000 23.3821328661704015
	Pd Cu
	3 77
	Selective dynamics
	Direct
	0.2408236731265418 0.4954118365632709 0.3876173292063569 T T T
	0.5045881634367291 0.4954118365632709 0.3876173292063569 T T T
	0.5045881634367291 0.7591763268734582 0.3876173292063569 T T T
	0.0000000000000000 0.0000000000000000 0.1155258754999977 F F F
	0.0004455892534452 0.9995544107465548 0.3827079028632170 T T T
	0.1666666667000030 0.083333332999970 0.0259047434999999 F F F
	0.1666341130159523 0.0832682259318958 0.2937155609596189 T T T
	0.0835558426157732 0.1672491600934904 0.2048794491479242 T T T
	0.2500000000000000 0.0000000000000000 0.1155258754999977 F F F
	0.2491088214931096 0.9995544107465548 0.3827079028632170 T T T
	0.4166666667000030 0.083333332999970 0.0259047434999999 F F F
	0.4167280579492072 0.0833640289246063 0.2938331878279996 T T T
	0.3336933173777084 0.1672491600934904 0.2048794491479242 T T T
	0.5000000000000000 0.0000000000000000 0.1155258754999977 F F F
	0.5000363227467943 0.0045863447487093 0.3834692659667027 T T T
	0.6666666667000030 0.083333332999970 0.0259047434999999 F F F
	0.6665809781888612 0.0831619562777064 0.2942502560997795 T T T
	0.5835664324181380 0.1667832162590770 0.2049122763829132 T T T
	0.7500000000000000 0.0000000000000000 0.1155258754999977 F F F
	0.7545500220019150 0.0045863447487093 0.3834692659667027 T T T
	0.9166666667000030 0.083333332999970 0.0259047434999999 F F F
	0.9166359710753937 0.0833640289246063 0.2938331878279996 T T T
	0.8332167837409230 0.1667832162590770 0.2049122763829132 T T T
	0.0000000000000000 0.2500000000000000 0.1155258754999977 F F F
	0.9954136552512907 0.2454499779980850 0.3834692659667027 T T T
	0.1666666667000030 0.333333332999970 0.0259047434999999 F F F
	0.1665198565902770 0.3327972715407910 0.2942805336160816 T T T
	0.0833804491925605 0.4166902246462882 0.2048845706749418 T T T
	0.2500000000000000 0.2500000000000000 0.1155258754999977 F F F
	0.2467217706387359 0.2434435412774718 0.3839515087819692 T T T
	0.4166666667000030 0.333333332999970 0.0259047434999999 F F F
	0.4162774150505157 0.3327972715407910 0.2942805336160816 T T T
	0.3335608330772644 0.4171216662545234 0.2049705977125100 T T T
	0.5000000000000000 0.2500000000000000 0.1155258754999977 F F F
	0.5000363227467943 0.2454499779980850 0.3834692659667027 T T T
	0.6666666667000030 0.333333332999970 0.0259047434999999 F F F
	0.6665809781888612 0.3334190218111388 0.2942502560997795 T T T
	0.5833097753537118 0.4166902246462882 0.2048845706749418 T T T
	0.7500000000000000 0.2500000000000000 0.1155258754999977 F F F
	0.7500000000000000 0.2500000000000000 0.3829186554056321 T T T
	0.9166666667000030 0.333333332999970 0.0259047434999999 F F F

	0.9168380437222936	0.3334190218111388	0.2942502560997795	T	T	T
	0.8332167837409230	0.4164335675818620	0.2049122763829132	T	T	T
	0.0000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.9954136552512907	0.4999636772532057	0.3834692659667027	T	T	T
	0.1666666667000030	0.583333332999970	0.0259047434999999	F	F	F
	0.1665198565902770	0.5837225849494843	0.2942805336160816	T	T	T
	0.0835558426157732	0.6663066826222916	0.2048794491479242	T	T	T
	0.2500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.4166666667000030	0.583333332999970	0.0259047434999999	F	F	F
	0.4166666667000030	0.583333332999970	0.2953080993956192	T	T	T
	0.3335608330772644	0.6664391669227356	0.2049705977125100	T	T	T
	0.5000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.6666666667000030	0.583333332999970	0.0259047434999999	F	F	F
	0.6672027284592090	0.5837225849494843	0.2942805336160816	T	T	T
	0.5828783337454766	0.6664391669227356	0.2049705977125100	T	T	T
	0.7500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.7545500220019150	0.4999636772532057	0.3834692659667027	T	T	T
	0.9166666667000030	0.583333332999970	0.0259047434999999	F	F	F
	0.9166359710753937	0.5832719420507928	0.2938331878279996	T	T	T
	0.8327508399065096	0.6663066826222916	0.2048794491479242	T	T	T
	0.0000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.0004455892534452	0.7508911785068904	0.3827079028632170	T	T	T
	0.1666666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.1666341130159523	0.8333658869840477	0.2937155609596189	T	T	T
	0.083333332999970	0.9166666667000030	0.2044883805471116	T	T	T
	0.2500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.2467217706387359	0.7532782293612641	0.3839515087819692	T	T	T
	0.4166666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.4162774150505157	0.8334801434097230	0.2942805336160816	T	T	T
	0.3336933173777084	0.9164441573842268	0.2048794491479242	T	T	T
	0.5000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.6666666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.6672027284592090	0.8334801434097230	0.2942805336160816	T	T	T
	0.5833097753537118	0.9166195508074395	0.2048845706749418	T	T	T
	0.7500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.7565564587225282	0.7532782293612641	0.3839515087819692	T	T	T
	0.9166666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.9167317740681042	0.8333658869840477	0.2937155609596189	T	T	T
	0.8327508399065096	0.9164441573842268	0.2048794491479242	T	T	T
3Pt/Cu(111)	1.0000000000000000					
	8.8905944857135406	-5.1329871195825199	-0.0000000000000010			
	0.0000000000000000	10.2659742391650006	0.0000000000000010			
	0.0000000000000000	0.0000000000000000	23.3821328661704015			
	Pt	Cu				
	3	77				
	Selective dynamics					
	Direct					
	0.2417084444191815	0.4958542222095943	0.3858836208477143	T	T	T
	0.5041457777904057	0.4958542222095943	0.3858836208477143	T	T	T
	0.5041457777904057	0.7582915555808185	0.3858836208477143	T	T	T
	0.0000000000000000	0.0000000000000000	0.1155258754999977	F	F	F

0.0003495950638595	0.9996504049361405	0.3831805313465537	T	T	T
0.1666666667000030	0.0833333332999970	0.0259047434999999	F	F	F
0.1666385349424431	0.0832770697848773	0.2942366176721833	T	T	T
0.0833395526197904	0.1668817479324289	0.2049762493755978	T	T	T
0.2500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.2493008098722882	0.9996504049361405	0.3831805313465537	T	T	T
0.4166666667000030	0.0833333332999970	0.0259047434999999	F	F	F
0.4169078476654278	0.0834539237827059	0.2944965166100886	T	T	T
0.3335421952126296	0.1668817479324289	0.2049762493755978	T	T	T
0.5000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.5001198478445588	0.0039050545474595	0.3843591354639386	T	T	T
0.6666666667000030	0.0833333332999970	0.0259047434999999	F	F	F
0.6668590905497993	0.0837181809995897	0.2944215313647405	T	T	T
0.5833866678536310	0.1666933339768164	0.2050883303033402	T	T	T
0.7500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.7537852067029007	0.0039050545474595	0.3843591354639386	T	T	T
0.9166666667000030	0.0833333332999970	0.0259047434999999	F	F	F
0.9165460762172941	0.0834539237827059	0.2944965166100886	T	T	T
0.8333066660231836	0.1666933339768164	0.2050883303033402	T	T	T
0.0000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.9960949454525405	0.2462147932970993	0.3843591354639386	T	T	T
0.1666666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.1652417242045630	0.3314256911644335	0.2937008265998102	T	T	T
0.0829495039923529	0.4164747520461844	0.2046996572192299	T	T	T
0.2500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.2473446260228513	0.2446892520457027	0.3850726408319218	T	T	T
0.4166666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.4161839670598724	0.3314256911644335	0.2937008265998102	T	T	T
0.3333755560057341	0.4167511121114771	0.2046363889470584	T	T	T
0.5000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.5001198478445588	0.2462147932970993	0.3843591354639386	T	T	T
0.6666666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.6668590905497993	0.3331409094502007	0.2944215313647405	T	T	T
0.5835252479538156	0.4164747520461844	0.2046996572192299	T	T	T
0.7500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.7500000000000000	0.2500000000000000	0.3830040866563067	T	T	T
0.9166666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.9162818190004103	0.3331409094502007	0.2944215313647405	T	T	T
0.8333066660231836	0.4166133321463690	0.2050883303033402	T	T	T
0.0000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.9960949454525405	0.4998801521554412	0.3843591354639386	T	T	T
0.1666666667000030	0.5833333332999970	0.0259047434999999	F	F	F
0.1652417242045630	0.5838160329401276	0.2937008265998102	T	T	T
0.0833395526197904	0.6664578047873704	0.2049762493755978	T	T	T
0.2500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.4166666667000030	0.5833333332999970	0.0259047434999999	F	F	F
0.4166666667000030	0.5833333332999970	0.2935718713073499	T	T	T
0.3333755560057341	0.6666244439942659	0.2046363889470584	T	T	T
0.5000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.6666666667000030	0.5833333332999970	0.0259047434999999	F	F	F
0.6685743088355665	0.5838160329401276	0.2937008265998102	T	T	T

	0.5832488878885229	0.6666244439942659	0.2046363889470584	T	T	T
	0.7500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.7537852067029007	0.4998801521554412	0.3843591354639386	T	T	T
	0.9166666667000030	0.5833333332999970	0.0259047434999999	F	F	F
	0.9165460762172941	0.5830921523345722	0.2944965166100886	T	T	T
	0.8331182520675711	0.6664578047873704	0.2049762493755978	T	T	T
	0.0000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.0003495950638595	0.7506991901277118	0.3831805313465537	T	T	T
	0.1666666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.1666385349424431	0.8333614650575569	0.2942366176721833	T	T	T
	0.0833333332999970	0.9166666667000030	0.2048415932289558	T	T	T
	0.2500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.2473446260228513	0.7526553739771487	0.3850726408319218	T	T	T
	0.4166666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.4161839670598724	0.8347582757954370	0.2937008265998102	T	T	T
	0.3335421952126296	0.9166604473802096	0.2049762493755978	T	T	T
	0.5000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.6666666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.6685743088355665	0.8347582757954370	0.2937008265998102	T	T	T
	0.5835252479538156	0.9170504960076471	0.2046996572192299	T	T	T
	0.7500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.7553107479542973	0.7526553739771487	0.3850726408319218	T	T	T
	0.9166666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.9167229302151227	0.8333614650575569	0.2942366176721833	T	T	T
	0.8331182520675711	0.9166604473802096	0.2049762493755978	T	T	T
(7) 3X-PL						
3Cu/Ni(111)	1.0000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni	Cu				
	77	3				
	Selective dynamics					
	Direct					
	0.0000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.1666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.1669470494017489	0.0833005257258392	0.3150406065789042	T	T	T
	0.0836542898631265	0.1669910747296299	0.2272063652793648	T	T	T
	0.2500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.2525263189304709	0.9973359874165624	0.4008219316366848	T	T	T
	0.4166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.4163789078194426	0.0836246285408322	0.3142647559328680	T	T	T
	0.3332981060482894	0.1666803681179445	0.2267817498104918	T	T	T
	0.5000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.5003815483314042	0.9996061492058672	0.4012743648806065	T	T	T
	0.6666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.6671207711658624	0.0836239806997341	0.3143228545337635	T	T	T
	0.5833363779864840	0.1669206101616254	0.2268339584201726	T	T	T
	0.7500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.7480535786793041	0.9998910956595140	0.4010839439468867	T	T	T
	0.9166669999999968	0.0833330000000032	0.0514190000000028	F	F	F

0.9173531387902969	0.0833253048271345	0.3149216935675767	T	T	T
0.8333573172403845	0.1667126790312921	0.2266719289736372	T	T	T
0.0000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.9973388901811049	0.2520901354197349	0.4010072291914284	T	T	T
0.1666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.1670788411643898	0.3329641262578917	0.3150839811026316	T	T	T
0.0834507784474994	0.4165472399337773	0.2267767766947841	T	T	T
0.2500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.4166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.4167190595815171	0.3330754729267653	0.3150410650817790	T	T	T
0.3330112738525983	0.4163692640361631	0.2272047516100599	T	T	T
0.5000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.5026491205305703	0.2474815132558774	0.4008098087470984	T	T	T
0.6666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.6665885703485372	0.3336628002306128	0.3141898613385194	T	T	T
0.5835003434710586	0.4169605253235318	0.2268795767219487	T	T	T
0.7500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.7500903406128856	0.2499795630501822	0.4011309839582964	T	T	T
0.9166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.9166567427739309	0.3330824143362534	0.3141926165642914	T	T	T
0.8332799745924362	0.4166584138882001	0.2268582551986569	T	T	T
0.0000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.9997566916991829	0.5002851784039493	0.4012096116164301	T	T	T
0.1666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.1668890141312716	0.5833721087642516	0.3141829721719560	T	T	T
0.0833004235576027	0.6666873694916475	0.2268546601099786	T	T	T
0.2500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.2479604803162587	0.5027142279751899	0.4010078350545356	T	T	T
0.4166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.4166924238911704	0.5826625352226031	0.3149237423257460	T	T	T
0.3332613503429585	0.6666057930764850	0.2266721054740160	T	T	T
0.5000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.6666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.6663527378895964	0.5832767887807293	0.3147094028725022	T	T	T
0.5832226439791910	0.6667315984218547	0.2269877043605106	T	T	T
0.7500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.7518482777396613	0.4997709335270173	0.4008627840822214	T	T	T
0.9166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.9162173758101133	0.5837922633627315	0.3142173471340044	T	T	T
0.8333298292387852	0.6666993508156480	0.2266126662792800	T	T	T
0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.0002508696804924	0.7481818922411847	0.4008527699334294	T	T	T
0.1666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
0.1663281371374765	0.8333978816919583	0.3141820207587713	T	T	T
0.0830538181358023	0.9165097576979306	0.2268803070698766	T	T	T
0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.2500454276353139	0.7499365667768672	0.4011239737155989	T	T	T
0.4166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
0.4163613448397072	0.8328296844914220	0.3143069870510757	T	T	T
0.3330886364555781	0.9166699431636900	0.2268347066561702	T	T	T
0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F

	0.5001260507730052	0.7519857698129044	0.4010859570134855	T	T	T
	0.6666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.6666867721670826	0.8332904368909766	0.3145241115039212	T	T	T
	0.5833598971823193	0.9166439733474192	0.2268028856930542	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.7497673126992268	0.7501979086055499	0.4009513454502454	T	T	T
	0.9166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.9166919326189813	0.8336360447026863	0.3147184086042287	T	T	T
	0.8332876578045898	0.9167984630721051	0.2269931960472391	T	T	T
	0.2500068368782493	0.2499936984317657	0.4059240416525398	T	T	T
	0.9995772277059558	0.9994578823222966	0.4060832335357389	T	T	T
	0.5005535376547101	0.5004210833144853	0.4060852391338017	T	T	T
3Ag/Ni(111)	1.0000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni	Ag				
	77	3				
	Selective dynamics					
	Direct					
	0.0000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.9999882925412749	0.9999735462739565	0.4000206543036740	T	T	T
	0.1666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.1667937327693068	0.0834228731419486	0.3133579136052234	T	T	T
	0.0836664640248586	0.1673364362388909	0.2266768825287500	T	T	T
	0.2500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.2503074746569283	0.0007614362579531	0.4005698693307309	T	T	T
	0.4166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.4162149308036902	0.0831587167784704	0.3135352600728609	T	T	T
	0.3334737354919071	0.1672504434073758	0.2266812803713449	T	T	T
	0.5000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.5005299620508268	0.0010626090732373	0.4007649205623522	T	T	T
	0.6666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.6668694599083196	0.0831711184445467	0.3135438981203151	T	T	T
	0.5833325843404396	0.1666815769421888	0.2263617599698762	T	T	T
	0.7500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.7504674452524611	0.0007638674089776	0.4005758324693005	T	T	T
	0.9166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.9165727240880486	0.0834422171308660	0.3133561494638499	T	T	T
	0.8337350822405796	0.1672364859351916	0.2266815961784587	T	T	T
	0.0000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.9925401865377523	0.2387069579415666	0.4013188841863311	T	T	T
	0.1666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.1668946887018876	0.3337786887530072	0.3158479134811074	T	T	T
	0.0836679253737742	0.4166540658004791	0.2277996232416726	T	T	T
	0.2500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.2461763107218928	0.2387038829813051	0.4013108869943522	T	T	T
	0.4166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.4175929808079104	0.3355712974552958	0.3163346664447175	T	T	T
	0.3329984872906309	0.4166828028561511	0.2277976658466585	T	T	T
	0.5000000000000000	0.2500000000000000	0.1392870000000030	F	F	F

0.5000591716505127	0.2433304028368894	0.4005343075297745	T	T	T
0.6666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.6666035489290607	0.3332058328881615	0.3135551530706664	T	T	T
0.5825966106740736	0.4163750686586170	0.2270247159442462	T	T	T
0.7500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.7432715032878505	0.2432982073180980	0.4005477231681169	T	T	T
0.9166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.9179617578742949	0.3355618403398353	0.3163466534968364	T	T	T
0.8337956937934479	0.4163831993572558	0.2270185827321569	T	T	T
0.0000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.1666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.1657941700018100	0.5829682016008704	0.3167387497431662	T	T	T
0.0836162790305011	0.6661595741372395	0.2269909342532799	T	T	T
0.2500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.4166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.4171848419095241	0.5829867085314149	0.3167316620231375	T	T	T
0.3327802217026345	0.6655608280172132	0.2275810153614799	T	T	T
0.5000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.6666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.6648076181049802	0.5832090819244442	0.3148327406911520	T	T	T
0.5825441326075378	0.6661760803565784	0.2269883242316055	T	T	T
0.7500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.7495448647707477	0.4990739550976215	0.3978519537335004	T	T	T
0.9166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.9183576590761078	0.5832089861603507	0.3148197991816986	T	T	T
0.8328244551757535	0.6656649544984177	0.2264772800544890	T	T	T
0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.0013295724724927	0.7578977948490859	0.3997614616960945	T	T	T
0.1666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
0.1666161225296037	0.8331937878674935	0.3135447781191800	T	T	T
0.0835030812018402	0.9165858337168800	0.2263469640238256	T	T	T
0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.2547704176036092	0.7629139072152284	0.4009889234288764	T	T	T
0.4166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
0.4159050592199591	0.8318300951534638	0.3140266881435849	T	T	T
0.3333142842733281	0.9163234208353117	0.2265229578247769	T	T	T
0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.5081485447229213	0.7628857190546654	0.4009815027081771	T	T	T
0.6666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
0.6665928716816936	0.8331870090156954	0.3135494421480018	T	T	T
0.5829696732727001	0.9162953220778363	0.2265201074174428	T	T	T
0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.7565479227334819	0.7578862550565972	0.3997693777635973	T	T	T
0.9166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
0.9158894710486294	0.8318450890131786	0.3127831954351734	T	T	T
0.8330616672490549	0.9165822266344108	0.2263399568533018	T	T	T
0.2502489278718656	0.5004523502237035	0.4184693933481185	T	T	T
0.9900553736045694	0.5008492150854451	0.4281699060698116	T	T	T
0.5107804402649663	0.5008418274577409	0.4281909119299883	T	T	T
3Au/Ni(111)	1.0000000000000000				
	8.6224000674449712	-4.9781450000000014	0.0000000000000000		

0.0000000000000000	9.9562900000000010	0.0000000000000000		
0.0000000000000000	0.0000000000000000	23.1292800000000014		
Ni	Au			
77	3			
Selective dynamics				
Direct				
0.0000000000000000	0.0000000000000000	0.1392870000000030	F	F
0.0004614609798210	0.0009207847393142	0.4003066285075434	T	T
0.1666669999999968	0.0833330000000032	0.0514190000000028	F	F
0.1672647342935605	0.0840201799917963	0.3138036264878465	T	T
0.0835651664173866	0.1671697129130933	0.2267378367637320	T	T
0.2500000000000000	0.0000000000000000	0.1392870000000030	F	F
0.2502501970761770	0.0005516728348027	0.4005575049528218	T	T
0.4166669999999968	0.0833330000000032	0.0514190000000028	F	F
0.4162878497204616	0.0827909853572777	0.3136679394056756	T	T
0.3333834674482574	0.1667650682765256	0.2266013084065222	T	T
0.5000000000000000	0.0000000000000000	0.1392870000000030	F	F
0.4998783075163900	0.9997390223573319	0.4007832970382950	T	T
0.6666669999999968	0.0833330000000032	0.0514190000000028	F	F
0.6665042808738093	0.0827751180498311	0.3136665680292552	T	T
0.5833185848141582	0.1666399575198483	0.2264224072683518	T	T
0.7500000000000000	0.0000000000000000	0.1392870000000030	F	F
0.7503341077905219	0.0005566175582814	0.4005666680048563	T	T
0.9166669999999968	0.0833330000000032	0.0514190000000028	F	F
0.9167532614827039	0.0840115439754001	0.3138207884960238	T	T
0.8333742482349535	0.1667746321979848	0.2266092220447220	T	T
0.0000000000000000	0.2500000000000000	0.1392870000000030	F	F
0.9935308235101417	0.2402719338194714	0.4021892638900653	T	T
0.1666669999999968	0.3333330000000032	0.0514190000000028	F	F
0.1666001740624736	0.3332350303546505	0.3154650708297950	T	T
0.0835637300757526	0.4164836221669930	0.2275432642933808	T	T
0.2500000000000000	0.2500000000000000	0.1392870000000030	F	F
0.2467785616247014	0.2402695891341295	0.4021784414916638	T	T
0.4166669999999968	0.3333330000000032	0.0514190000000028	F	F
0.4172364061899358	0.3337449993245585	0.3151050053180953	T	T
0.3329222979825275	0.4164820941645289	0.2275472711978423	T	T
0.5000000000000000	0.2500000000000000	0.1392870000000030	F	F
0.4993811715115157	0.2419024630936661	0.4010010323110151	T	T
0.6666669999999968	0.3333330000000032	0.0514190000000028	F	F
0.6664099989330339	0.3328223986519703	0.3135698400541784	T	T
0.5830417205826564	0.4166243606664040	0.2268907679190022	T	T
0.7500000000000000	0.2500000000000000	0.1392870000000030	F	F
0.7425044658113720	0.2418907483634953	0.4009993520988573	T	T
0.9166669999999968	0.3333330000000032	0.0514190000000028	F	F
0.9165122329221518	0.3337327445191960	0.3151081478071589	T	T
0.8335746052459712	0.4166128280425525	0.2268949225546706	T	T
0.0000000000000000	0.5000000000000000	0.1392870000000030	F	F
0.1666669999999968	0.5833330000000032	0.0514190000000028	F	F
0.1662413638266003	0.5830971320118152	0.3159172600576809	T	T
0.0836664050290139	0.6663968040339796	0.2269584110161276	T	T
0.2500000000000000	0.5000000000000000	0.1392870000000030	F	F

	0.416666999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.4168616900124320	0.5830776482445259	0.3159122777295806	T	T	T
	0.3329060022494872	0.6658465983416022	0.2274861470932876	T	T	T
	0.5000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.666666999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.6669302096830094	0.5841394749635356	0.3142756589048190	T	T	T
	0.5826950497719494	0.6663758569739855	0.2269652123857426	T	T	T
	0.7500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.7493155321019174	0.4985932077372865	0.3994121074912158	T	T	T
	0.916666999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.9172013094242359	0.5841420407414262	0.3142688459503233	T	T	T
	0.8333121199290758	0.6666446536414981	0.2264021200023834	T	T	T
	0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.0013339306219962	0.7587072245597213	0.4006909240096661	T	T	T
	0.166666999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.1667678149954739	0.8333184766370749	0.3136513305960449	T	T	T
	0.0836095560768086	0.9167952146286495	0.2264962083453952	T	T	T
	0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.2539394915150908	0.7610357230832534	0.4019833647242592	T	T	T
	0.416666999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.4160078856504938	0.8319917917988136	0.3143275062842719	T	T	T
	0.3333497017138995	0.9162292773304443	0.2265705207964075	T	T	T
	0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.5071460499222482	0.7610556769393213	0.4019907109529868	T	T	T
	0.666666999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.6665626513098744	0.8333042585581438	0.3136484603389391	T	T	T
	0.5828673117810368	0.9162188131525681	0.2265669175666005	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.7573773092513463	0.7587426069377443	0.4006969682787584	T	T	T
	0.916666999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.9167030788568695	0.8333739237747722	0.3133476830988897	T	T	T
	0.8331701446811834	0.9167946532171527	0.2264927407618416	T	T	T
	0.2503042339384862	0.5005830801409203	0.4196954305705134	T	T	T
	0.9898332733547832	0.5004542763837065	0.4198154208214788	T	T	T
	0.5106687530103713	0.5004674145524461	0.4198198656836283	T	T	T
3Ni/Cu(111)	1.0000000000000000					
	8.8905944857135406	-5.1329871195825199	-0.0000000000000010			
	0.0000000000000000	10.2659742391650006	0.0000000000000010			
	0.0000000000000000	0.0000000000000000	23.3821328661704015			
	Ni	Cu				
	3	77				
	Selective dynamics					
	Direct					
	0.4994666361713982	0.2519844260339497	0.3794257279903661	T	T	T
	0.4990876965987212	0.4995438482993606	0.3795565029478212	T	T	T
	0.4994666361713982	0.7474822101374485	0.3794257279903661	T	T	T
	0.0000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.0000598016835767	0.9999654481029836	0.3830112364813871	T	T	T
	0.1666666667000030	0.0833333332999970	0.0259047434999999	F	F	F
	0.1670374753980113	0.0836642649718371	0.2944710843703433	T	T	T
	0.0834368378265467	0.1667138153155889	0.2050975988933104	T	T	T

0.2500000000000000	0.0000000000000000	0.1155258754999977	F F F
0.2525612344283914	0.0023385169601724	0.3833440556172931	T T T
0.4166666667000030	0.083333332999970	0.0259047434999999	F F F
0.4172653995466789	0.0839948798511045	0.2942649875906298	T T T
0.3333035673202360	0.1666283813280813	0.2047534245414084	T T T
0.5000000000000000	0.0000000000000000	0.1155258754999977	F F F
0.4997475374280640	0.9998737687140320	0.3832851826824353	T T T
0.6666666667000030	0.083333332999970	0.0259047434999999	F F F
0.6664789656945871	0.0832394827972891	0.2942929580291320	T T T
0.5835447512743670	0.1666252645224517	0.2047253129397646	T T T
0.7500000000000000	0.0000000000000000	0.1155258754999977	F F F
0.7471809561151659	0.9972735514852289	0.3830558000396422	T T T
0.9166666667000030	0.083333332999970	0.0259047434999999	F F F
0.9164251239736032	0.0832187412750187	0.2944665831008493	T T T
0.8333547122920777	0.1666773561960468	0.2050606479769641	T T T
0.0000000000000000	0.2500000000000000	0.1155258754999977	F F F
0.0001006639473147	0.2500503319736538	0.3828912734313761	T T T
0.1666666667000030	0.333333332999970	0.0259047434999999	F F F
0.1671031965870924	0.3335515982435382	0.2944381890558745	T T T
0.0834368378265467	0.4167230226109666	0.2050975988933104	T T T
0.2500000000000000	0.2500000000000000	0.1155258754999977	F F F
0.2536724918078903	0.2522190359279790	0.3833270767019386	T T T
0.4166666667000030	0.333333332999970	0.0259047434999999	F F F
0.4169836050922768	0.3338238475628685	0.2937079972776573	T T T
0.3333214477751980	0.4166607239376034	0.2046899428274926	T T T
0.5000000000000000	0.2500000000000000	0.1155258754999977	F F F
0.6666666667000030	0.333333332999970	0.0259047434999999	F F F
0.6662928705241171	0.3332479272578794	0.2939426762040611	T T T
0.5836007942138579	0.4168138532104564	0.2043633780121965	T T T
0.7500000000000000	0.2500000000000000	0.1155258754999977	F F F
0.7471809561151659	0.2499074046299370	0.3830558000396422	T T T
0.9166666667000030	0.333333332999970	0.0259047434999999	F F F
0.9164251239736032	0.3332063825985756	0.2944665831008493	T T T
0.8333424402250600	0.4166358930249672	0.2050397107390864	T T T
0.0000000000000000	0.5000000000000000	0.1155258754999977	F F F
0.0000598016835767	0.5000943535805860	0.3830112364813871	T T T
0.1666666667000030	0.583333332999970	0.0259047434999999	F F F
0.1670374753980113	0.5833732103261582	0.2944710843703433	T T T
0.0834471502652008	0.6667104152802921	0.2051045537212062	T T T
0.2500000000000000	0.5000000000000000	0.1155258754999977	F F F
0.2536724918078903	0.5014534558799042	0.3833270767019386	T T T
0.4166666667000030	0.583333332999970	0.0259047434999999	F F F
0.4169836050922768	0.5831597574293923	0.2937079972776573	T T T
0.3333035673202360	0.6666751860921636	0.2047534245414084	T T T
0.5000000000000000	0.5000000000000000	0.1155258754999977	F F F
0.6666666667000030	0.583333332999970	0.0259047434999999	F F F
0.6663475303895581	0.5831737651447710	0.2938702118896046	T T T
0.5836007942138579	0.6667869411034104	0.2043633780121965	T T T
0.7500000000000000	0.5000000000000000	0.1155258754999977	F F F
0.7458770998935478	0.4984733899794520	0.3831685599484516	T T T
0.9166666667000030	0.583333332999970	0.0259047434999999	F F F

	0.9162856553086911	0.5831795178335284	0.2944868022552214	T	T	T
	0.8333387974984916	0.6666693987992502	0.2050379629482890	T	T	T
	0.0000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.9998324066534536	0.7499162033267339	0.3830115777137948	T	T	T
	0.1666666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.1671568552031673	0.8335784275515792	0.2946427647342276	T	T	T
	0.0834471502652008	0.9167367350849247	0.2051045537212062	T	T	T
	0.2500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.2525612344283914	0.7502227174682261	0.3833440556172931	T	T	T
	0.4166666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.4172653995466789	0.8332705195955654	0.2942649875906298	T	T	T
	0.3335528763555828	0.9167764382277994	0.2051264646336577	T	T	T
	0.5000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.6666666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.6662928705241171	0.8330449431662288	0.2939426762040611	T	T	T
	0.5835447512743670	0.9169194868519241	0.2047253129397646	T	T	T
	0.7500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.7458770998935478	0.7474037099141029	0.3831685599484516	T	T	T
	0.9166666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.9162856553086911	0.8331061373751467	0.2944868022552214	T	T	T
	0.8333424402250600	0.9167065473001017	0.2050397107390864	T	T	T
3Pd/Cu(111)	1.0000000000000000					
	8.8905944857135406	-5.1329871195825199	-0.0000000000000010			
	0.0000000000000000	10.2659742391650006	0.0000000000000010			
	0.0000000000000000	0.0000000000000000	23.3821328661704015			
	Pd	Cu				
	3	77				
	Selective dynamics					
	Direct					
	0.4998467064730292	0.2435672159657472	0.3871224100401065	T	T	T
	0.4997443548824378	0.4998721774412118	0.3876673539287196	T	T	T
	0.4998467064730292	0.7562794905072749	0.3871224100401065	T	T	T
	0.0000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.9999917708620742	0.9999890507948876	0.3828769681622788	T	T	T
	0.1666666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.1667796906333834	0.0834728447013333	0.2940906045863372	T	T	T
	0.0836600928792137	0.1670031038340838	0.2049218584187216	T	T	T
	0.2500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.2449132749833538	0.9954835794969767	0.3832939574966829	T	T	T
	0.4166666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.4160410355112063	0.0824914212610253	0.2939782218412077	T	T	T
	0.3336984851015146	0.1672018463622180	0.2048543601779258	T	T	T
	0.5000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.4996756728976024	0.9998378364487976	0.3840719861363482	T	T	T
	0.6666666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.6663168418070455	0.0831584208535219	0.2945635403231179	T	T	T
	0.5836007082240755	0.1667444398410254	0.2048881436192147	T	T	T
	0.7500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.7549003654058026	0.0043056987665580	0.3836378287689755	T	T	T
	0.9166666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.9168452744333848	0.0836608798921574	0.2940295879465680	T	T	T

0.8331190433470965	0.1665595217235492	0.2049485383827232	T	T	T
0.0000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.0005343031271963	0.2502671515635981	0.3828942686564005	T	T	T
0.1666666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.1674303305810128	0.3337151652405055	0.2943118781745895	T	T	T
0.0836600928792137	0.4166569891451388	0.2049218584187216	T	T	T
0.2500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.2443199888402319	0.2463091167046798	0.3840536411749227	T	T	T
0.4166666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.4166411522244857	0.3330213303714942	0.2945342711018242	T	T	T
0.3340640879600443	0.4170320440300301	0.2051473659567975	T	T	T
0.5000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.6666666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.6671253860473527	0.3333742068072851	0.2943916444885630	T	T	T
0.5837113002336736	0.4169298674039794	0.2048763293551588	T	T	T
0.7500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.7549003654058026	0.2505946666392447	0.3836378287689755	T	T	T
0.9166666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.9168452744333848	0.3331843944412114	0.2940295879465680	T	T	T
0.8329879770094166	0.4163482561107941	0.2049866936650844	T	T	T
0.0000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.9999917708620742	0.5000027200671866	0.3828769681622788	T	T	T
0.1666666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.1667796906333834	0.5833068458320483	0.2940906045863372	T	T	T
0.0833973152220224	0.6664279534845363	0.2047019166284301	T	T	T
0.2500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.2443199888402319	0.4980108721355450	0.3840536411749227	T	T	T
0.4166666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.4166411522244857	0.5836198217529898	0.2945342711018242	T	T	T
0.3336984851015146	0.6664966388393054	0.2048543601779258	T	T	T
0.5000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.6666666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.6672285355693504	0.5836142677346672	0.2945950003094637	T	T	T
0.5837113002336736	0.6667814329297101	0.2048763293551588	T	T	T
0.7500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.7555336179965835	0.5019949922372717	0.3840975432002054	T	T	T
0.9166666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.9164697238138118	0.5830207146583959	0.2939545576156419	T	T	T
0.8329498474440911	0.6664749237720500	0.2050636039087976	T	T	T
0.0000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
0.9994445597490085	0.7497222798745042	0.3826963776035086	T	T	T
0.1666666667000030	0.833333332999970	0.0259047434999999	F	F	F
0.1659430414063010	0.8329715206531461	0.2937062044052183	T	T	T
0.0833973152220224	0.9169693618375021	0.2047019166284301	T	T	T
0.2500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
0.2449132749833538	0.7494296954863771	0.3832939574966829	T	T	T
0.4166666667000030	0.833333332999970	0.0259047434999999	F	F	F
0.4160410355112063	0.8335496141501721	0.2939782218412077	T	T	T
0.3336799806826392	0.9168399903913169	0.2049416274558169	T	T	T
0.5000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
0.6666666667000030	0.833333332999970	0.0259047434999999	F	F	F

	0.6671253860473527 0.8337511791400658 0.2943916444885630 T T T
	0.5836007082240755 0.9168562684830519 0.2048881436192147 T T T
	0.7500000000000000 0.7500000000000000 0.1155258754999977 F F F
	0.7555336179965835 0.7535386257593046 0.3840975432002054 T T T
	0.9166666667000030 0.833333332999970 0.0259047434999999 F F F
	0.9164697238138118 0.8334490090553999 0.2939545576156419 T T T
	0.8329879770094166 0.9166397209986314 0.2049866936650844 T T T
3Pt/Cu(111)	1.0000000000000000
	8.8905944857135406 -5.1329871195825199 -0.0000000000000010
	0.0000000000000000 10.2659742391650006 0.0000000000000010
	0.0000000000000000 0.0000000000000000 23.3821328661704015
	Pt Cu
	3 77
	Selective dynamics
	Direct
	0.5001681756599226 0.2441665544992873 0.3851284869244154 T T T
	0.4994653506329882 0.4997326753165012 0.3865921714348772 T T T
	0.5001681756599226 0.7560016211606353 0.3851284869244154 T T T
	0.0000000000000000 0.0000000000000000 0.1155258754999977 F F F
	0.0002123844926345 0.0000788218131902 0.3830773876375204 T T T
	0.1666666667000030 0.083333332999970 0.0259047434999999 F F F
	0.1662340451700359 0.0833130181053079 0.2943400506892786 T T T
	0.0833685096274905 0.1668478403787219 0.2051086363251358 T T T
	0.2500000000000000 0.0000000000000000 0.1155258754999977 F F F
	0.2462162617534744 0.9964658395789314 0.3842553189123805 T T T
	0.4166666667000030 0.083333332999970 0.0259047434999999 F F F
	0.4155580149469458 0.0812522694349127 0.2937161862399975 T T T
	0.3333121068939846 0.1668818450087741 0.2048204974971313 T T T
	0.5000000000000000 0.0000000000000000 0.1155258754999977 F F F
	0.4994520061414960 0.9997260030707409 0.3860603195537138 T T T
	0.6666666667000030 0.083333332999970 0.0259047434999999 F F F
	0.6665586014066136 0.0832793006533024 0.2948867855778090 T T T
	0.5835703102846779 0.1664829613366479 0.2048364317563980 T T T
	0.7500000000000000 0.0000000000000000 0.1155258754999977 F F F
	0.7539430600388854 0.0034205451974216 0.3845303315570447 T T T
	0.9166666667000030 0.083333332999970 0.0259047434999999 F F F
	0.9166633028261941 0.0836684023380982 0.2944720130802025 T T T
	0.8331162173734512 0.1665581087367300 0.2052021261825843 T T T
	0.0000000000000000 0.2500000000000000 0.1155258754999977 F F F
	0.0004969203543226 0.2502484601771542 0.3830717478557446 T T T
	0.1666666667000030 0.333333332999970 0.0259047434999999 F F F
	0.1667909562785681 0.3333954780892796 0.2946432053683168 T T T
	0.0833685096274905 0.4165206693487775 0.2051086363251358 T T T
	0.2500000000000000 0.2500000000000000 0.1155258754999977 F F F
	0.2455831794146803 0.2469237102178639 0.3852996419794010 T T T
	0.4166666667000030 0.333333332999970 0.0259047434999999 F F F
	0.4159175129642350 0.3328436683436991 0.2936439434226088 T T T
	0.3335802406604387 0.4167901203802202 0.2050006059785332 T T T
	0.5000000000000000 0.2500000000000000 0.1155258754999977 F F F
	0.6666666667000030 0.333333332999970 0.0259047434999999 F F F
	0.6686365906021834 0.3335691148224029 0.2937410426451876 T T T

	0.5837734123459697	0.4169063685093448	0.2046350552082004	T	T	T
	0.7500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
	0.7539430600388854	0.2505225148414638	0.3845303315570447	T	T	T
	0.9166666667000030	0.333333332999970	0.0259047434999999	F	F	F
	0.9166633028261941	0.3329949003880941	0.2944720130802025	T	T	T
	0.8332780822658279	0.4164935015886968	0.2050558598678904	T	T	T
	0.0000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.0002123844926345	0.5001335626794372	0.3830773876375204	T	T	T
	0.1666666667000030	0.583333332999970	0.0259047434999999	F	F	F
	0.1662340451700359	0.5829210269647191	0.2943400506892786	T	T	T
	0.0832761840107636	0.6664653232826439	0.2049581988533689	T	T	T
	0.2500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.2455831794146803	0.4986594691968165	0.3852996419794010	T	T	T
	0.4166666667000030	0.583333332999970	0.0259047434999999	F	F	F
	0.4159175129642350	0.5830738445205341	0.2936439434226088	T	T	T
	0.3333121068939846	0.6664302619852123	0.2048204974971313	T	T	T
	0.5000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.6666666667000030	0.583333332999970	0.0259047434999999	F	F	F
	0.6687892773762698	0.5843946386381305	0.2940401797694392	T	T	T
	0.5837734123459697	0.6668670439366338	0.2046350552082004	T	T	T
	0.7500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.7544248089857462	0.5016016191524386	0.3852020324927281	T	T	T
	0.9166666667000030	0.583333332999970	0.0259047434999999	F	F	F
	0.9163787007716380	0.5830149851566304	0.2944230710612885	T	T	T
	0.8332183309783900	0.6666091655391995	0.2051110669183771	T	T	T
	0.0000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.9997073235290657	0.7498536617645399	0.3829702582441428	T	T	T
	0.1666666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.1658163309862530	0.8329081654431221	0.2942060162417732	T	T	T
	0.0832761840107636	0.9168108608281287	0.2049581988533689	T	T	T
	0.2500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.2462162617534744	0.7497504221745359	0.3842553189123805	T	T	T
	0.4166666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.4155580149469458	0.8343057454120242	0.2937161862399975	T	T	T
	0.3333472737105012	0.9166736369052515	0.2048877141488390	T	T	T
	0.5000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.6666666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.6686365906021834	0.8350674756797716	0.2937410426451876	T	T	T
	0.5835703102846779	0.9170873490480389	0.2048364317563980	T	T	T
	0.7500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.7544248089857462	0.7528231898333146	0.3852020324927281	T	T	T
	0.9166666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.9163787007716380	0.8333637155149987	0.2944230710612885	T	T	T
	0.8332780822658279	0.9167845807771329	0.2050558598678904	T	T	T
(8) 4X-S1						
4Cu/Ni(111)	1.0000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni	Cu				
	76	4				

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
0.1666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
0.1666286820150802	0.0832977958227019	0.3144794338295043	T	T	T
0.0833497196269519	0.1667332751447645	0.2269407884954475	T	T	T
0.2500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
0.2515561617714894	0.0014067365074126	0.4009077277413340	T	T	T
0.4166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
0.4163755791234252	0.0836045140976722	0.3141851360150838	T	T	T
0.3333907313656894	0.1666061527990195	0.2264572310888511	T	T	T
0.5000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
0.4997419860711858	0.0002452901378120	0.4009621571566129	T	T	T
0.6666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
0.6671462049301056	0.0838984138078160	0.3144748911052844	T	T	T
0.5834328136100879	0.1668298839102604	0.2269754365093348	T	T	T
0.7500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
0.7485660389325872	0.9984068424208559	0.4007894121626236	T	T	T
0.9166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
0.9169008311965925	0.0830991688034075	0.3148811740731574	T	T	T
0.8333038909681036	0.1666961090318964	0.2268417620171874	T	T	T
0.0000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.0015931575791441	0.2514339610674128	0.4007894121626236	T	T	T
0.1666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.1664125882341310	0.3336177671851104	0.3140358838709290	T	T	T
0.0834350239908019	0.4166449338908649	0.2265261552159714	T	T	T
0.2500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.2497157263112157	0.2503073409626211	0.4009210061168105	T	T	T
0.4166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.4166853106980568	0.3333756179852969	0.3144676303175444	T	T	T
0.3332250206878129	0.4165915369234696	0.2269246515403154	T	T	T
0.5000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.4985788209075110	0.2484830880257647	0.4008438372232348	T	T	T
0.6666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.6668511740312795	0.3331488259687205	0.3148768407577833	T	T	T
0.5833035786228038	0.4166964213771962	0.2268804062726701	T	T	T
0.7500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.9166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.9161015861921840	0.3328537950698944	0.3144748911052844	T	T	T
0.8331701160897396	0.4165671863899121	0.2269754365093348	T	T	T
0.0000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.9997547098621880	0.5002580139288142	0.4009621571566129	T	T	T
0.1666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.1671357008890979	0.5839628942811288	0.3144615648762894	T	T	T
0.0833917146961483	0.6668823870388678	0.2270079661000466	T	T	T
0.2500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.2485953619135373	0.4984709332310828	0.4007693473550447	T	T	T
0.4166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.4168332181056584	0.5831667818943416	0.3148037334272189	T	T	T
0.3332727941441291	0.6667272058558709	0.2268330143297561	T	T	T
0.5000000000000000	0.5000000000000000	0.1392870000000030	F	F	F

	0.666666999999968	0.583333000000032	0.051419000000028	F	F	F
	0.6666243820147031	0.5833146893019432	0.3144676303175444	T	T	T
	0.5834084630765304	0.6667749793121871	0.2269246515403154	T	T	T
	0.7500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.7515169119742353	0.5014211790924890	0.4008438372232348	T	T	T
	0.916666999999968	0.583333000000032	0.051419000000028	F	F	F
	0.9163954859023278	0.5836244208765748	0.3141851360150838	T	T	T
	0.8333938472009805	0.6666092686343106	0.2264572310888511	T	T	T
	0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.9985932634925874	0.7484438382285106	0.4009077277413340	T	T	T
	0.166666999999968	0.833333000000032	0.051419000000028	F	F	F
	0.1668320472626874	0.8331679527373126	0.3149329519405413	T	T	T
	0.0833210631435293	0.9166789368564707	0.2268984007875616	T	T	T
	0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.416666999999968	0.833333000000032	0.051419000000028	F	F	F
	0.4160371057188712	0.8328642991109021	0.3144615648762894	T	T	T
	0.3331176129611251	0.9166082853038517	0.2270079661000466	T	T	T
	0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.5015290667689172	0.7514046380864627	0.4007693473550447	T	T	T
	0.666666999999968	0.833333000000032	0.051419000000028	F	F	F
	0.6663822328148896	0.8335874117658690	0.3140358838709290	T	T	T
	0.5833550661091351	0.9165649760091981	0.2265261552159714	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.7496926590373789	0.7502842736887843	0.4009210061168105	T	T	T
	0.916666999999968	0.833333000000032	0.051419000000028	F	F	F
	0.9167022041772981	0.8333713179849198	0.3144794338295043	T	T	T
	0.8332667248552355	0.9166502803730481	0.2269407884954475	T	T	T
	0.0001263311951760	0.9998736688048240	0.4062226938345930	T	T	T
	0.7501148705749543	0.2498851294250457	0.4062515215249434	T	T	T
	0.2501265219437556	0.7498734780562444	0.4062846147402865	T	T	T
	0.5001195981986157	0.4998804018013843	0.4061251966318906	T	T	T
4Ag/Ni(111)	1.0000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni	Ag				
	76	4				
	Selective dynamics					
	Direct					
	0.0000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.166666999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.1650047321982839	0.0822293067151776	0.3146510546491896	T	T	T
	0.0831759225586381	0.1662538294659512	0.2267553113052969	T	T	T
	0.2500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.2538852520753352	0.0042760777356676	0.3998217511192124	T	T	T
	0.416666999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.4161681240335540	0.0837769717065697	0.3132714352925348	T	T	T
	0.3333163209186054	0.1667425014331343	0.2264756095050942	T	T	T
	0.5000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.4993609714560918	0.0006507647077427	0.3994985858273239	T	T	T
	0.666666999999968	0.0833330000000032	0.0514190000000028	F	F	F

0.6678496236851501	0.0849828657010079	0.3145987793954177	T	T	T
0.5838344626062764	0.1670033403788409	0.2269115659404619	T	T	T
0.7500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
0.7459740755381645	0.9960363932953982	0.3995933211951126	T	T	T
0.9166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
0.9178669777463924	0.0821330222536005	0.3155220622205732	T	T	T
0.8334697696061539	0.1665302303938461	0.2270546178645247	T	T	T
0.0000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.0039636067046018	0.2540259244618355	0.3995933211951126	T	T	T
0.1666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.1665176394832457	0.3334838326545722	0.3129875377869169	T	T	T
0.0832336014956567	0.4167885279541537	0.2265441705909907	T	T	T
0.2500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.2492174660318511	0.2507242112110859	0.3994102092104654	T	T	T
0.4166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.4177142146846720	0.3349264071999229	0.3146536282211656	T	T	T
0.3337337320551725	0.4168441856040772	0.2267813541265511	T	T	T
0.5000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.4957596085267255	0.2460671337995635	0.3998487530718364	T	T	T
0.6666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.6676613973001579	0.3323386026998421	0.3157638233237066	T	T	T
0.5836482781514221	0.4163517218485779	0.2271075754237373	T	T	T
0.7500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.9166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.9150171342989921	0.3321503763148499	0.3145987793954177	T	T	T
0.8329966596211520	0.4161655373937236	0.2269115659404619	T	T	T
0.0000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.9993492352922573	0.5006390285439082	0.3994985858273239	T	T	T
0.1666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.1678401858216745	0.5849874235553614	0.3145980159541395	T	T	T
0.0838254275601145	0.6669999141928074	0.2269110991021321	T	T	T
0.2500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.2458651605059714	0.4959784839228760	0.3996160269987428	T	T	T
0.4166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.4178614480986340	0.5821385519013660	0.3155848995877975	T	T	T
0.3334680273596788	0.6665319726403212	0.2270667662017232	T	T	T
0.5000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.6666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.6650735928000771	0.5822857853153280	0.3146536282211656	T	T	T
0.5831558143959228	0.6662662679448275	0.2267813541265511	T	T	T
0.7500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.7539328662004365	0.5042403914732674	0.3998487530718364	T	T	T
0.9166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.9162230282934303	0.5838318759664460	0.3132714352925348	T	T	T
0.8332574985668657	0.6666836790813946	0.2264756095050942	T	T	T
0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.9957239222643324	0.7461147479246648	0.3998217511192124	T	T	T
0.1666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
0.1676636015747235	0.8323363984252765	0.3157569716024398	T	T	T
0.0836647527943626	0.9163352472056374	0.2270910468094698	T	T	T
0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F

	0.416666999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.4150125764446386	0.8321598141783255	0.3145980159541395	T	T	T
	0.3330000858071926	0.9161745724398855	0.2269110991021321	T	T	T
	0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.5040215160771240	0.7541348394940286	0.3996160269987428	T	T	T
	0.666666999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.6665161673454278	0.8334823605167543	0.3129875377869169	T	T	T
	0.5832114720458463	0.9167663985043433	0.2265441705909907	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.7492757887889141	0.7507825339681489	0.3994102092104654	T	T	T
	0.916666999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.9177706932848224	0.8349952678017161	0.3146510546491896	T	T	T
	0.8337461705340488	0.9168240774413619	0.2267553113052969	T	T	T
	0.9999006242338027	0.0000993757661973	0.4282511974960812	T	T	T
	0.7500159400637330	0.2499840599362670	0.4281024740610420	T	T	T
	0.2499433729824361	0.7500566270175710	0.4280606075950502	T	T	T
	0.4999008354952252	0.5000991645047748	0.4281737303171909	T	T	T
4Au/Ni(111)	1.0000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni	Au				
	76	4				
	Selective dynamics					
	Direct					
	0.0000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.166666999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.1667189885903611	0.0833557321580614	0.3144187897021880	T	T	T
	0.0832836172036622	0.1664522925282412	0.2268440800902027	T	T	T
	0.2500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.2546589171413984	0.0050055777792721	0.4011935791720802	T	T	T
	0.416666999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.4163774830218259	0.0836229975663159	0.3137023347224854	T	T	T
	0.3333356491653774	0.1666194621598933	0.2265080662534587	T	T	T
	0.5000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.4996241486014554	0.0003413916320767	0.4013566558675379	T	T	T
	0.666666999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.6671134413504376	0.0836891612534245	0.3144335537021377	T	T	T
	0.5837110083502211	0.1667926437203064	0.2268984367843458	T	T	T
	0.7500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.7451493239349176	0.9951989916112467	0.4011792754571459	T	T	T
	0.916666999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.9171755174944280	0.0828244825055720	0.3148775767730569	T	T	T
	0.8333711287214101	0.1666288712785899	0.2269914735863736	T	T	T
	0.0000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.0048010083887533	0.2548506760650824	0.4011792754571459	T	T	T
	0.166666999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.1665200513299112	0.3334922617034266	0.3135226940832965	T	T	T
	0.0833932723553730	0.4165007501109059	0.2266203460567624	T	T	T
	0.2500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.2494416353338451	0.2505423832415943	0.4014106765165479	T	T	T

0.416666999999968	0.333333000000032	0.051419000000028	F	F	F
0.4166531713415864	0.3332840071620922	0.3144212062716321	T	T	T
0.3335361060937601	0.4166872991031738	0.2268369614047430	T	T	T
0.500000000000000	0.250000000000000	0.1392870000000030	F	F	F
0.4949237335887986	0.2453179114549471	0.4012102525951278	T	T	T
0.666666999999968	0.333333000000032	0.051419000000028	F	F	F
0.6670355266568961	0.3329644733431039	0.3148777552949156	T	T	T
0.5835002608455468	0.4164997391544532	0.2269790309634914	T	T	T
0.750000000000000	0.250000000000000	0.1392870000000030	F	F	F
0.916666999999968	0.333333000000032	0.051419000000028	F	F	F
0.9163108387465755	0.3328865586495624	0.3144335537021377	T	T	T
0.8332073562796936	0.4162889916497789	0.2268984367843458	T	T	T
0.000000000000000	0.500000000000000	0.1392870000000030	F	F	F
0.9996586083679233	0.5003758513985446	0.4013566558675379	T	T	T
0.166666999999968	0.583333000000032	0.051419000000028	F	F	F
0.1670724856865817	0.5836397173627788	0.3144178106284485	T	T	T
0.0836666386539591	0.6667344014255079	0.2269032061727501	T	T	T
0.250000000000000	0.500000000000000	0.1392870000000030	F	F	F
0.2451449882775947	0.4951951380568644	0.4011561565971107	T	T	T
0.416666999999968	0.583333000000032	0.051419000000028	F	F	F
0.4171965087844143	0.5828034912155857	0.3148023449227253	T	T	T
0.3333911458349306	0.6666088541650694	0.2269723857093879	T	T	T
0.500000000000000	0.500000000000000	0.1392870000000030	F	F	F
0.666666999999968	0.583333000000032	0.051419000000028	F	F	F
0.6667159928379078	0.5833468286584136	0.3144212062716321	T	T	T
0.5833127008968262	0.6664638939062399	0.2268369614047430	T	T	T
0.750000000000000	0.500000000000000	0.1392870000000030	F	F	F
0.7546820885450529	0.5050762664112014	0.4012102525951278	T	T	T
0.916666999999968	0.583333000000032	0.051419000000028	F	F	F
0.9163770024336841	0.5836225169781741	0.3137023347224854	T	T	T
0.8333805378401067	0.6666643508346226	0.2265080662534587	T	T	T
0.000000000000000	0.750000000000000	0.1392870000000030	F	F	F
0.9949944222207279	0.7453410828586016	0.4011935791720802	T	T	T
0.166666999999968	0.833333000000032	0.051419000000028	F	F	F
0.1670233082098846	0.8329766917901154	0.3148749424223425	T	T	T
0.0835039665577497	0.9164960334422503	0.2269998627955374	T	T	T
0.250000000000000	0.750000000000000	0.1392870000000030	F	F	F
0.416666999999968	0.833333000000032	0.051419000000028	F	F	F
0.4163602826372212	0.8329275143134183	0.3144178106284485	T	T	T
0.3332655985744921	0.9163333613460409	0.2269032061727501	T	T	T
0.500000000000000	0.750000000000000	0.1392870000000030	F	F	F
0.5048048619431356	0.7548550117224053	0.4011561565971107	T	T	T
0.666666999999968	0.833333000000032	0.051419000000028	F	F	F
0.6665077382965734	0.8334799486700888	0.3135226940832965	T	T	T
0.5834992498890941	0.9166067276446270	0.2266203460567624	T	T	T
0.750000000000000	0.750000000000000	0.1392870000000030	F	F	F
0.7494576167584057	0.7505583646661549	0.4014106765165479	T	T	T
0.916666999999968	0.833333000000032	0.051419000000028	F	F	F
0.9166442678419386	0.8332810114096389	0.3144187897021880	T	T	T
0.8335477074717588	0.9167163827963378	0.2268440800902027	T	T	T
0.9999782906577011	0.0000217093422989	0.4190230366340515	T	T	T

	0.7499139035680358	0.2500860964319642	0.4188262411717005	T	T	T
	0.2499471273562079	0.7500528726437921	0.4187947056206909	T	T	T
	0.4999454572851292	0.5000545427148708	0.4189647369989942	T	T	T
4Ni/Cu(111)	1.0000000000000000					
	8.8905944857135406	-5.1329871195825199	-0.0000000000000010			
	0.0000000000000000	10.2659742391650006	0.0000000000000010			
	0.0000000000000000	0.0000000000000000	23.3821328661704015			
	Ni	Cu				
	4	76				
	Selective dynamics					
	Direct					
	0.9997784609196998	0.0002215390803002	0.3796538981583595	T	T	T
	0.7497784609196998	0.2502215390803002	0.3796538981583595	T	T	T
	0.4997784609196998	0.5002215390803002	0.3796538981583595	T	T	T
	0.2497784609196998	0.7502215390803002	0.3796538981583595	T	T	T
	0.0000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.1666666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.1665429991606615	0.0832957124631903	0.2943411542649201	T	T	T
	0.0834126960975752	0.1668188223540596	0.2048231934532794	T	T	T
	0.2500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.2484768480079964	0.9987276777489669	0.3833428573880013	T	T	T
	0.4166666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.4165940614030106	0.0834059385969894	0.2944900216098532	T	T	T
	0.3333331422537498	0.1666668577462502	0.2051729617688096	T	T	T
	0.5000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.4999758365288827	0.0000241634711173	0.3832443332109534	T	T	T
	0.6666666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.6667042875368097	0.0834570008393314	0.2943411542649201	T	T	T
	0.5831811776459404	0.1665873039024248	0.2048231934532794	T	T	T
	0.7500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.7512723222510331	0.0015231519920036	0.3833428573880013	T	T	T
	0.9166666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.9167102089571202	0.0832897910428798	0.2941644844119011	T	T	T
	0.8334346749443284	0.1665653250556716	0.2048505140800714	T	T	T
	0.0000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
	0.9984768480079964	0.2487276777489669	0.3833428573880013	T	T	T
	0.1666666667000030	0.333333332999970	0.0259047434999999	F	F	F
	0.1665940614030106	0.3334059385969894	0.2944900216098532	T	T	T
	0.0833331422537498	0.4166668577462502	0.2051729617688096	T	T	T
	0.2500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
	0.2499758365288827	0.2500241634711173	0.3832443332109534	T	T	T
	0.4166666667000030	0.333333332999970	0.0259047434999999	F	F	F
	0.4167042875368097	0.3334570008393314	0.2943411542649201	T	T	T
	0.3331811776459404	0.4165873039024248	0.2048231934532794	T	T	T
	0.5000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
	0.5012723222510331	0.2515231519920036	0.3833428573880013	T	T	T
	0.6666666667000030	0.333333332999970	0.0259047434999999	F	F	F
	0.6667102089571202	0.3332897910428798	0.2941644844119011	T	T	T
	0.5834346749443284	0.4165653250556716	0.2048505140800714	T	T	T
	0.7500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
	0.9166666667000030	0.333333332999970	0.0259047434999999	F	F	F

	0.9165429991606686	0.3332957124631903	0.2943411542649201	T	T	T
	0.8334126960975752	0.4168188223540596	0.2048231934532794	T	T	T
	0.0000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.9999758365288827	0.5000241634711173	0.3832443332109534	T	T	T
	0.1666666667000030	0.5833333332999970	0.0259047434999999	F	F	F
	0.1667042875368097	0.5834570008393314	0.2943411542649201	T	T	T
	0.0831811776459404	0.6665873039024248	0.2048231934532794	T	T	T
	0.2500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.2512723222510331	0.5015231519920036	0.3833428573880013	T	T	T
	0.4166666667000030	0.5833333332999970	0.0259047434999999	F	F	F
	0.4167102089571202	0.5832897910428798	0.2941644844119011	T	T	T
	0.3334346749443284	0.6665653250556716	0.2048505140800714	T	T	T
	0.5000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.6666666667000030	0.5833333332999970	0.0259047434999999	F	F	F
	0.6665429991606686	0.5832957124631903	0.2943411542649201	T	T	T
	0.5834126960975752	0.6668188223540596	0.2048231934532794	T	T	T
	0.7500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.7484768480079964	0.4987276777489669	0.3833428573880013	T	T	T
	0.9166666667000030	0.5833333332999970	0.0259047434999999	F	F	F
	0.9165940614030106	0.5834059385969894	0.2944900216098532	T	T	T
	0.8333331422537498	0.6666668577462502	0.2051729617688096	T	T	T
	0.0000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.0012723222510331	0.7515231519920036	0.3833428573880013	T	T	T
	0.1666666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.1667102089571202	0.8332897910428798	0.2941644844119011	T	T	T
	0.0834346749443284	0.9165653250556716	0.2048505140800714	T	T	T
	0.2500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.4166666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.4165429991606686	0.8332957124631903	0.2943411542649201	T	T	T
	0.3334126960975752	0.9168188223540596	0.2048231934532794	T	T	T
	0.5000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.4984768480079964	0.7487276777489669	0.3833428573880013	T	T	T
	0.6666666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.6665940614030106	0.8334059385969894	0.2944900216098532	T	T	T
	0.5833331422537498	0.9166668577462502	0.2051729617688096	T	T	T
	0.7500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.7499758365288827	0.7500241634711173	0.3832443332109534	T	T	T
	0.9166666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.9167042875368097	0.8334570008393314	0.2943411542649201	T	T	T
	0.8331811776459404	0.9165873039024248	0.2048231934532794	T	T	T
4Pd/Cu(111)	1.0000000000000000					
	8.8905944857135406	-5.1329871195825199	-0.0000000000000010			
	0.0000000000000000	10.2659742391650006	0.0000000000000010			
	0.0000000000000000	0.0000000000000000	23.3821328661704015			
	Pd	Cu				
	4	76				
	Selective dynamics					
	Direct					
	0.9999428349105983	0.0000571650894017	0.3864796773750641	T	T	T
	0.7499428349105983	0.2500571650894017	0.3864796773750641	T	T	T
	0.4999428349105983	0.5000571650894017	0.3864796773750641	T	T	T

0.2499428349105983	0.7500571650894017	0.3864796773750641	T	T	T
0.0000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.1666666667000030	0.0833333332999970	0.0259047434999999	F	F	F
0.1671974507504004	0.0835731418903052	0.2939606943169792	T	T	T
0.0832900187667889	0.1667383384902266	0.2048177204012092	T	T	T
0.2500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.2528436892315682	0.0029478738780853	0.3838847218772656	T	T	T
0.4166666667000030	0.0833333332999970	0.0259047434999999	F	F	F
0.4169117138029748	0.0830882861970252	0.2943084339339634	T	T	T
0.3333478616688836	0.1666521383311164	0.2051799936430641	T	T	T
0.5000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.5000203254208131	0.9999796745791869	0.3838861105165137	T	T	T
0.6666666667000030	0.0833333332999970	0.0259047434999999	F	F	F
0.6664268581096948	0.0828025492495996	0.2939606943169792	T	T	T
0.5832616615097734	0.1667099812332111	0.2048177204012092	T	T	T
0.7500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.7470521261219147	0.9971563107684318	0.3838847218772656	T	T	T
0.9166666667000030	0.0833333332999970	0.0259047434999999	F	F	F
0.9162134810054354	0.0837865189945646	0.2940768239791680	T	T	T
0.8334570887505919	0.1665429112494081	0.2047307243721690	T	T	T
0.0000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.0028436892315682	0.2529478738780782	0.3838847218772656	T	T	T
0.1666666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.1669117138029748	0.3330882861970252	0.2943084339339634	T	T	T
0.0833478616688836	0.4166521383311164	0.2051799936430641	T	T	T
0.2500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.2500203254208131	0.2499796745791869	0.3838861105165137	T	T	T
0.4166666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.4164268581096948	0.3328025492495996	0.2939606943169792	T	T	T
0.3332616615097734	0.4167099812332111	0.2048177204012092	T	T	T
0.5000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.4970521261219218	0.2471563107684318	0.3838847218772656	T	T	T
0.6666666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.6662134810054354	0.3337865189945646	0.2940768239791680	T	T	T
0.5834570887505919	0.4165429112494081	0.2047307243721690	T	T	T
0.7500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.9166666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.9171974507504004	0.3335731418903052	0.2939606943169792	T	T	T
0.8332900187667889	0.4167383384902266	0.2048177204012092	T	T	T
0.0000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.0000203254208131	0.4999796745791869	0.3838861105165137	T	T	T
0.1666666667000030	0.5833333332999970	0.0259047434999999	F	F	F
0.1664268581096948	0.5828025492495996	0.2939606943169792	T	T	T
0.0832616615097734	0.6667099812332111	0.2048177204012092	T	T	T
0.2500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.2470521261219147	0.4971563107684318	0.3838847218772656	T	T	T
0.4166666667000030	0.5833333332999970	0.0259047434999999	F	F	F
0.4162134810054354	0.5837865189945646	0.2940768239791680	T	T	T
0.3334570887505919	0.6665429112494081	0.2047307243721690	T	T	T
0.5000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.6666666667000030	0.5833333332999970	0.0259047434999999	F	F	F

	0.6671974507504004 0.5835731418903052 0.2939606943169792 T T T
	0.5832900187667889 0.6667383384902266 0.2048177204012092 T T T
	0.7500000000000000 0.5000000000000000 0.1155258754999977 F F F
	0.7528436892315682 0.5029478738780853 0.3838847218772656 T T T
	0.9166666667000030 0.5833333332999970 0.0259047434999999 F F F
	0.9169117138029748 0.5830882861970252 0.2943084339339634 T T T
	0.8333478616688836 0.6666521383311164 0.2051799936430641 T T T
	0.0000000000000000 0.7500000000000000 0.1155258754999977 F F F
	0.9970521261219147 0.7471563107684318 0.3838847218772656 T T T
	0.1666666667000030 0.8333333332999970 0.0259047434999999 F F F
	0.1662134810054354 0.8337865189945646 0.2940768239791680 T T T
	0.0834570887505919 0.9165429112494081 0.2047307243721690 T T T
	0.2500000000000000 0.7500000000000000 0.1155258754999977 F F F
	0.4166666667000030 0.8333333332999970 0.0259047434999999 F F F
	0.4171974507504004 0.8335731418903052 0.2939606943169792 T T T
	0.3332900187667889 0.9167383384902266 0.2048177204012092 T T T
	0.5000000000000000 0.7500000000000000 0.1155258754999977 F F F
	0.5028436892315682 0.7529478738780853 0.3838847218772656 T T T
	0.6666666667000030 0.8333333332999970 0.0259047434999999 F F F
	0.6669117138029748 0.8330882861970252 0.2943084339339634 T T T
	0.5833478616688836 0.9166521383311164 0.2051799936430641 T T T
	0.7500000000000000 0.7500000000000000 0.1155258754999977 F F F
	0.7500203254208131 0.7499796745791869 0.3838861105165137 T T T
	0.9166666667000030 0.8333333332999970 0.0259047434999999 F F F
	0.9164268581096948 0.8328025492495996 0.2939606943169792 T T T
	0.8332616615097734 0.9167099812332111 0.2048177204012092 T T T
4Pt/Cu(111)	1.0000000000000000
	8.8905944857135406 -5.1329871195825199 -0.0000000000000010
	0.0000000000000000 10.2659742391650006 0.0000000000000010
	0.0000000000000000 0.0000000000000000 23.3821328661704015
	Pt Cu
	4 76
	Selective dynamics
	Direct
	0.9998012187100187 0.0001987812899742 0.3845995289849142 T T T
	0.7498012187100187 0.2501987812899742 0.3845995289849142 T T T
	0.4998012187100258 0.5001987812899813 0.3845995289849142 T T T
	0.2498012187100258 0.7501987812899813 0.3845995289849142 T T T
	0.0000000000000000 0.0000000000000000 0.1155258754999977 F F F
	0.1666666667000030 0.0833333332999970 0.0259047434999999 F F F
	0.1685701865874734 0.0843017626493605 0.2939868437635340 T T T
	0.0834789157136910 0.1669523485021571 0.2049003424728895 T T T
	0.2500000000000000 0.0000000000000000 0.1155258754999977 F F F
	0.2516906982302416 0.0020071517158371 0.3857520004441071 T T T
	0.4166666667000030 0.0833333332999970 0.0259047434999999 F F F
	0.4167850539350795 0.0832149460649205 0.2949792047641822 T T T
	0.3333926215165022 0.1666073784834978 0.2052496119301424 T T T
	0.5000000000000000 0.0000000000000000 0.1155258754999977 F F F
	0.5000326404443527 0.9999673595556473 0.3860594481758497 T T T
	0.6666666667000030 0.0833333332999970 0.0259047434999999 F F F
	0.6656982373506395 0.0814298134125266 0.2939868437635340 T T T

0.5830476514978429	0.1665210842863090	0.2049003424728895	T	T	T
0.7500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.7479928482841629	0.9983093017697584	0.3857520004441071	T	T	T
0.9166666667000030	0.0833333332999970	0.0259047434999999	F	F	F
0.9159519092998067	0.0840480907001933	0.2936897353728085	T	T	T
0.8334585541487911	0.1665414458512089	0.2048210630103284	T	T	T
0.0000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.0016906982302416	0.2520071517158371	0.3857520004441071	T	T	T
0.1666666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.1667850539350795	0.3332149460649205	0.2949792047641822	T	T	T
0.0833926215165022	0.4166073784834978	0.2052496119301424	T	T	T
0.2500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.2500326404443527	0.2499673595556473	0.3860594481758497	T	T	T
0.4166666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.4156982373506395	0.3314298134125266	0.2939868437635340	T	T	T
0.3330476514978429	0.4165210842863090	0.2049003424728895	T	T	T
0.5000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.4979928482841629	0.2483093017697584	0.3857520004441071	T	T	T
0.6666666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.6659519092998067	0.3340480907001933	0.2936897353728085	T	T	T
0.5834585541487911	0.4165414458512089	0.2048210630103284	T	T	T
0.7500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.9166666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.9185701865874734	0.3343017626493605	0.2939868437635340	T	T	T
0.8334789157136910	0.4169523485021571	0.2049003424728895	T	T	T
0.0000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.0000326404443527	0.4999673595556473	0.3860594481758497	T	T	T
0.1666666667000030	0.5833333332999970	0.0259047434999999	F	F	F
0.1656982373506395	0.5814298134125266	0.2939868437635340	T	T	T
0.0830476514978429	0.6665210842863090	0.2049003424728895	T	T	T
0.2500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.2479928482841629	0.4983093017697584	0.3857520004441071	T	T	T
0.4166666667000030	0.5833333332999970	0.0259047434999999	F	F	F
0.4159519092998067	0.5840480907001933	0.2936897353728085	T	T	T
0.3334585541487911	0.6665414458512089	0.2048210630103284	T	T	T
0.5000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.6666666667000030	0.5833333332999970	0.0259047434999999	F	F	F
0.6685701865874734	0.5843017626493605	0.2939868437635340	T	T	T
0.5834789157136910	0.6669523485021571	0.2049003424728895	T	T	T
0.7500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.7516906982302416	0.5020071517158371	0.3857520004441071	T	T	T
0.9166666667000030	0.5833333332999970	0.0259047434999999	F	F	F
0.9167850539350795	0.5832149460649205	0.2949792047641822	T	T	T
0.8333926215165022	0.6666073784834978	0.2052496119301424	T	T	T
0.0000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
0.9979928482841629	0.7483093017697584	0.3857520004441071	T	T	T
0.1666666667000030	0.8333333332999970	0.0259047434999999	F	F	F
0.1659519092998067	0.8340480907001933	0.2936897353728085	T	T	T
0.0834585541487911	0.9165414458512089	0.2048210630103284	T	T	T
0.2500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
0.4166666667000030	0.8333333332999970	0.0259047434999999	F	F	F

	0.4185701865874734	0.8343017626493605	0.2939868437635340	T	T	T
	0.3334789157136910	0.9169523485021571	0.2049003424728895	T	T	T
	0.5000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.5016906982302416	0.7520071517158371	0.3857520004441071	T	T	T
	0.6666666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.6667850539350795	0.8332149460649205	0.2949792047641822	T	T	T
	0.5833926215165022	0.9166073784834978	0.2052496119301424	T	T	T
	0.7500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.7500326404443527	0.7499673595556473	0.3860594481758497	T	T	T
	0.9166666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.9156982373506395	0.8314298134125266	0.2939868437635340	T	T	T
	0.8330476514978429	0.9165210842863090	0.2049003424728895	T	T	T
(9) 4X-S2						
4Cu/Ni(111)	1.0000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni	Cu				
	76	4				
	Selective dynamics					
	Direct					
	0.0000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.1666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.1666053440092368	0.0833288158301194	0.3145626757148723	T	T	T
	0.0833710957228083	0.1667354728908353	0.2269475638352529	T	T	T
	0.2500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.2498984294770110	0.9997399193043417	0.4007941645034256	T	T	T
	0.4166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.4166892162498055	0.0833117333997646	0.3145253024191982	T	T	T
	0.3333220608885719	0.1666877624956553	0.2264188471239018	T	T	T
	0.5000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.6666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.6666329207867698	0.0833164677452168	0.3144971288657586	T	T	T
	0.5833663054967477	0.1667455906551569	0.2269431814872879	T	T	T
	0.7500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.7499095682552692	-0.0002374992826327	0.4007668762257069	T	T	T
	0.9166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.9166794563197885	0.0833205436802114	0.3144906761941451	T	T	T
	0.8333312417372712	0.1666687582627285	0.2263666313954749	T	T	T
	0.0000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.0002374992826328	0.2500904317447305	0.4007668762257069	T	T	T
	0.1666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.1666669567217709	0.3333325037147362	0.3143684690037975	T	T	T
	0.0833759088800525	0.4166249263297391	0.2269412312039739	T	T	T
	0.2500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.2498924288043506	0.2501004359608606	0.4008536182373181	T	T	T
	0.4166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.4166762198751384	0.3333971265053363	0.3145689858182567	T	T	T
	0.3332648847552748	0.4166322987113827	0.2269485408613772	T	T	T
	0.5000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.5002446252108186	0.2500864136577286	0.4008026489567150	T	T	T

0.666666999999968	0.333333000000032	0.051419000000028	F	F	F
0.6666667953878583	0.3333332046121411	0.3143639679839920	T	T	T
0.5833671617902183	0.4166328382097816	0.2269486401789896	T	T	T
0.7500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.7499156352136335	0.2500843647863663	0.4007768160578571	T	T	T
0.916666999999968	0.333333000000032	0.051419000000028	F	F	F
0.9166835322547833	0.3333670792132299	0.3144971288657586	T	T	T
0.8332544093448430	0.4166336945032528	0.2269431814872879	T	T	T
0.0000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.166666999999968	0.583333000000032	0.051419000000028	F	F	F
0.1666305383265166	0.5833106260937060	0.3145054272553150	T	T	T
0.0833623774481307	0.6667405466112514	0.2269440969192871	T	T	T
0.2500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.2499163060433183	0.4997574723081372	0.4007855494418689	T	T	T
0.416666999999968	0.583333000000032	0.051419000000028	F	F	F
0.4166874557479552	0.5833125442520445	0.3145160209594569	T	T	T
0.3333334629799770	0.6666665370200240	0.2263807075301084	T	T	T
0.5000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.666666999999968	0.583333000000032	0.051419000000028	F	F	F
0.6666028734946640	0.5833237801248625	0.3145689858182567	T	T	T
0.5833677012886176	0.6667351152447261	0.2269485408613772	T	T	T
0.7500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.7499135863422715	0.4997553747891816	0.4008026489567150	T	T	T
0.916666999999968	0.583333000000032	0.051419000000028	F	F	F
0.9166882666002351	0.5833107837501946	0.3145253024191982	T	T	T
0.8333112375043474	0.6666779391114279	0.2264188471239018	T	T	T
0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.0002600806956580	0.7501015705229885	0.4007941645034256	T	T	T
0.166666999999968	0.833333000000032	0.051419000000028	F	F	F
0.1666665051064956	0.8333334948935045	0.3143548573033017	T	T	T
0.0833676674952222	0.9166323325047775	0.2269486250015743	T	T	T
0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.2499135113605152	0.7500864886394846	0.4007682291363339	T	T	T
0.416666999999968	0.833333000000032	0.051419000000028	F	F	F
0.4166893739062945	0.8333694616734832	0.3145054272553150	T	T	T
0.3332594533887487	0.9166376225518690	0.2269440969192871	T	T	T
0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.5002425276918632	0.7500836939566820	0.4007855494418689	T	T	T
0.666666999999968	0.833333000000032	0.051419000000028	F	F	F
0.6666674962852637	0.8333330432782290	0.3143684690037975	T	T	T
0.5833750736702604	0.9166240911199474	0.2269412312039739	T	T	T
0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.7498995640391403	0.7501075711956497	0.4008536182373181	T	T	T
0.916666999999968	0.833333000000032	0.051419000000028	F	F	F
0.9166711841698806	0.8333946559907638	0.3145626757148723	T	T	T
0.8332645271091643	0.9166289042771912	0.2269475638352529	T	T	T
0.5000220932487905	-0.0000228450215780	0.4061454886823070	T	T	T
0.0000228450215781	0.4999779067512094	0.4061454886823070	T	T	T
0.0000004667423116	-0.0000004667423117	0.4061685692224705	T	T	T
0.5000110531430846	0.4999889468569158	0.4061802800070165	T	T	T
4Ag/Ni(111)	1.0000000000000000				

8.6224000674449712 -4.9781450000000014 0.0000000000000000
0.0000000000000000 9.9562900000000010 0.0000000000000000
0.0000000000000000 0.0000000000000000 23.1292800000000014

Ni Ag
76 4

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
0.1666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
0.1650922227792192	0.0825760049209020	0.3147699435707177	T	T	T
0.0832437959578311	0.1664970997026590	0.2267777903613214	T	T	T
0.2500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
0.2497603269090017	-0.0005986858426110	0.3993619496145941	T	T	T
0.4166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
0.4174560177280822	0.0825285719983808	0.3147520348792480	T	T	T
0.3333212362457676	0.1666935408446753	0.2268355772082212	T	T	T
0.5000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
0.6666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
0.6651286798952548	0.0825555196287609	0.3147353137801807	T	T	T
0.5832380070993007	0.1664905611956038	0.2267650388790088	T	T	T
0.7500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
0.7497491102527343	-0.0006141171003813	0.3993537108326319	T	T	T
0.9166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
0.9174461637223585	0.0825538362776415	0.3147545564493196	T	T	T
0.8333166218485946	0.1666833781514055	0.2268443390574786	T	T	T
0.0000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.0006141171003814	0.2502508897472654	0.3993537108326319	T	T	T
0.1666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.1667143957442338	0.3333732612326774	0.3135571173651894	T	T	T
0.0832472920317885	0.4167791552606687	0.2267703182395885	T	T	T
0.2500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.2497403198721528	0.2502899787952634	0.3993733274332004	T	T	T
0.4166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.4174696522612102	0.3348961742816840	0.3147685897883851	T	T	T
0.3335285410526291	0.4167567850851464	0.2267772130957182	T	T	T
0.5000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.5006424690646938	0.2502639640652231	0.3993647421513298	T	T	T
0.6666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.6666427214102467	0.3333572785897529	0.3135561587387411	T	T	T
0.5832608778975958	0.4167391221024042	0.2267648828647943	T	T	T
0.7500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.7497864094368624	0.2502135905631375	0.3993497451074032	T	T	T
0.9166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.9174444803712390	0.3348713201047452	0.3147353137801807	T	T	T
0.8335094388043961	0.4167619929006994	0.2267650388790088	T	T	T
0.0000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.1666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.1651171888901330	0.5825804761897848	0.3147228747272332	T	T	T
0.0832505285951465	0.6665344483374753	0.2267639418506989	T	T	T
0.2500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.2497505742079135	0.4994324380808648	0.3993546636889791	T	T	T

	0.416666999999968	0.583333000000032	0.051419000000028	F	F	F
	0.4174364505657352	0.5825635494342646	0.3147368497994212	T	T	T
	0.3333314292634470	0.6666685707365529	0.2268443610399225	T	T	T
	0.5000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.666666999999968	0.583333000000032	0.051419000000028	F	F	F
	0.6651038257183157	0.5825303477387899	0.3147685897883851	T	T	T
	0.5832432149148534	0.6664714589473710	0.2267772130957182	T	T	T
	0.7500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.7497360359347767	0.4993575309353063	0.3993647421513298	T	T	T
	0.916666999999968	0.583333000000032	0.051419000000028	F	F	F
	0.9174714280016191	0.5825439822719175	0.3147520348792480	T	T	T
	0.8333054591553275	0.6666787637542325	0.2268355772082212	T	T	T
	0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.0005986858426110	0.7502396730909979	0.3993619496145941	T	T	T
	0.166666999999968	0.833333000000032	0.051419000000028	F	F	F
	0.1666533553949935	0.8333466446050064	0.3135545337090472	T	T	T
	0.0832288798040106	0.9167711201959894	0.2267657002997380	T	T	T
	0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.2497598421710367	0.7502401578289636	0.3993429406856035	T	T	T
	0.416666999999968	0.833333000000032	0.051419000000028	F	F	F
	0.4174195238102152	0.8348828111098673	0.3147228747272332	T	T	T
	0.3334655516625246	0.9167494714048532	0.2267639418506989	T	T	T
	0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.5005675619191352	0.7502494257920865	0.3993546636889791	T	T	T
	0.666666999999968	0.833333000000032	0.051419000000028	F	F	F
	0.6666267387673228	0.8332856042557661	0.3135571173651894	T	T	T
	0.5832208447393312	0.9167527079682117	0.2267703182395885	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.7497100212047365	0.7502596801278471	0.3993733274332004	T	T	T
	0.916666999999968	0.833333000000032	0.051419000000028	F	F	F
	0.9174239950790981	0.8349077772207812	0.3147699435707177	T	T	T
	0.8335029002973410	0.9167562040421690	0.2267777903613214	T	T	T
	0.5000453731847712	-0.0000403371694351	0.4277136880505878	T	T	T
	0.0000403371694351	0.4999546268152286	0.4277136880505878	T	T	T
	0.0000450175655325	-0.0000450175655326	0.4277212682169123	T	T	T
	0.5000336001767616	0.4999663998232382	0.4277136557002825	T	T	T
4Au/Ni(111)	1.0000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni	Au				
	76	4				
	Selective dynamics					
	Direct					
	0.0000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.166666999999968	0.083333000000032	0.051419000000028	F	F	F
	0.1666455302710704	0.0833261110978930	0.3144408154246774	T	T	T
	0.0833269340481183	0.1666526704588396	0.2268270308016792	T	T	T
	0.2500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.2498082535405067	-0.0003969336593036	0.4012140994015393	T	T	T
	0.416666999999968	0.083333000000032	0.051419000000028	F	F	F

0.4166968113921796	0.0832977249087248	0.3144493590930128	T	T	T
0.3333118940206261	0.1666821199447598	0.2266968242437568	T	T	T
0.5000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
0.6666699999999968	0.0833330000000032	0.0514190000000028	F	F	F
0.6666963748724070	0.0833090534619552	0.3144183360551845	T	T	T
0.5833172854852872	0.1666274857359856	0.2268378455060945	T	T	T
0.7500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
0.7498490901837558	-0.0003370718837224	0.4011986638927426	T	T	T
0.9166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
0.9166788295748498	0.0833211704251503	0.3144399129440562	T	T	T
0.8333377699188055	0.1666622300811946	0.2266967637381134	T	T	T
0.0000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.0003370718837224	0.2501509098162444	0.4011986638927426	T	T	T
0.1666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.1666875245398455	0.3333768234643084	0.3137326379683569	T	T	T
0.0833331197320243	0.4167151243230083	0.2268182793605054	T	T	T
0.2500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.2497948274387110	0.2502055934500504	0.4012193188902752	T	T	T
0.4166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.4167018040519916	0.3333731002988706	0.3144358641897457	T	T	T
0.3333774400611513	0.4166688583926453	0.2268251119202899	T	T	T
0.5000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.5003710233219385	0.2501732620993483	0.4012021298101659	T	T	T
0.6666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.6666881921731346	0.3333118078268652	0.3137759745995639	T	T	T
0.5833368758644747	0.4166631241355251	0.2268501702162302	T	T	T
0.7500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.7498779475663052	0.2501220524336947	0.4012022089095542	T	T	T
0.9166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.9166909465380448	0.3333036251275932	0.3144183360551845	T	T	T
0.8333725142640143	0.4166827145147129	0.2268378455060945	T	T	T
0.0000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.1666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.1666772796539853	0.5833286178593936	0.3144216303755809	T	T	T
0.0833154166009778	0.6666602628601194	0.2268457502846213	T	T	T
0.2500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.2498535484703928	0.4996692187170196	0.4012123144616448	T	T	T
0.4166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.4166751758087243	0.5833248241912757	0.3144306164756205	T	T	T
0.3333646370219243	0.6666353629780757	0.2266886029647836	T	T	T
0.5000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.6666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.6666268997011295	0.5832981959480082	0.3144358641897457	T	T	T
0.5833311416073548	0.6666225599388484	0.2268251119202899	T	T	T
0.7500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.7498267379006517	0.4996289766780615	0.4012021298101659	T	T	T
0.9166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.9167022750912753	0.5833031886078203	0.3144493590930128	T	T	T
0.8333168800552430	0.6666881059793737	0.2266968242437568	T	T	T
0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.0003969336593034	0.7501917464594934	0.4012140994015393	T	T	T

	0.166666999999968	0.833333000000032	0.051419000000028	F	F	F
	0.1666818069775100	0.8333181930224900	0.3137739706152233	T	T	T
	0.0833210420681603	0.9166789579318395	0.2268403416331341	T	T	T
	0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.2498817283166208	0.7501182716833790	0.4011930927548349	T	T	T
	0.416666999999968	0.833333000000032	0.051419000000028	F	F	F
	0.4166713821406067	0.8333227203460148	0.3144216303755809	T	T	T
	0.3333397371398805	0.9166845833990223	0.2268457502846213	T	T	T
	0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.5003307812829808	0.7501464515296075	0.4012123144616448	T	T	T
	0.666666999999968	0.833333000000032	0.051419000000028	F	F	F
	0.6666231765356917	0.8333124754601543	0.3137326379683569	T	T	T
	0.5832848756769914	0.9166668802679758	0.2268182793605054	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.7497944065499496	0.7502051725612888	0.4012193188902752	T	T	T
	0.916666999999968	0.833333000000032	0.051419000000028	F	F	F
	0.9166738889021071	0.8333544697289296	0.3144408154246774	T	T	T
	0.8333473295411604	0.9166730659518819	0.2268270308016792	T	T	T
	0.5000358777631149	-0.0000342705224806	0.4187107615890787	T	T	T
	0.0000342705224805	0.4999641222368851	0.4187107615890787	T	T	T
	0.0000216202431733	-0.0000216202431733	0.4186926925151964	T	T	T
	0.5000305990420963	0.4999694009579037	0.4187015132901665	T	T	T
4Ni/Cu(111)	1.000000000000000					
	8.8905944857135406	-5.1329871195825199	-0.0000000000000010			
	0.0000000000000000	10.2659742391650006	0.0000000000000010			
	0.0000000000000000	0.0000000000000000	23.3821328661704015			
	Ni	Cu				
	4	76				
	Selective dynamics					
	Direct					
	0.2500000000000000	0.2500000000000000	0.3794282380951148	T	T	T
	0.7500000000000000	0.2500000000000000	0.3794282380951148	T	T	T
	0.2500000000000000	0.7500000000000000	0.3794282380951148	T	T	T
	0.7500000000000000	0.7500000000000000	0.3794282380951148	T	T	T
	0.0000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.0000337838244931	0.9999662161755067	0.3831201201280184	T	T	T
	0.1666666667000030	0.0833333332999970	0.0259047434999999	F	F	F
	0.1667563000874544	0.0835126000748928	0.2942108532406455	T	T	T
	0.0831361327000785	0.1665680664000437	0.2047965466772881	T	T	T
	0.2500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.2499324323510068	0.9999662161755067	0.3831201201280184	T	T	T
	0.4166666667000030	0.0833333332999970	0.0259047434999999	F	F	F
	0.4166666667000030	0.0833333332999970	0.2942371358926947	T	T	T
	0.33334319335999564	0.1665680664000437	0.2047965466772881	T	T	T
	0.5000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.5000337838244933	0.9999662161755067	0.3831201201280184	T	T	T
	0.6666666667000030	0.0833333332999970	0.0259047434999999	F	F	F
	0.6667563000874542	0.0835126000748928	0.2942108532406455	T	T	T
	0.5831361327000784	0.1665680664000437	0.2047965466772881	T	T	T
	0.7500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.7499324323510068	0.9999662161755067	0.3831201201280184	T	T	T

0.9166666667000030	0.0833333332999970	0.0259047434999999	F	F	F
0.9166666667000030	0.0833333332999970	0.2942371358926947	T	T	T
0.8334319335999563	0.1665680664000437	0.2047965466772881	T	T	T
0.0000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.0000337838244931	0.2500675676489932	0.3831201201280184	T	T	T
0.1666666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.1667563000874544	0.3332436999125455	0.2942108532406455	T	T	T
0.0833333332999970	0.4166666667000030	0.2051388865688787	T	T	T
0.2500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.4166666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.4164873999251072	0.3332436999125455	0.2942108532406455	T	T	T
0.3334319335999564	0.4168638672999215	0.2047965466772881	T	T	T
0.5000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.5000337838244933	0.2500675676489932	0.3831201201280184	T	T	T
0.6666666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.6667563000874542	0.3332436999125455	0.2942108532406455	T	T	T
0.5833333332999970	0.4166666667000030	0.2051388865688787	T	T	T
0.7500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.9166666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.9164873999251070	0.3332436999125455	0.2942108532406455	T	T	T
0.8334319335999563	0.4168638672999215	0.2047965466772881	T	T	T
0.0000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.0000337838244931	0.4999662161755070	0.3831201201280184	T	T	T
0.1666666667000030	0.5833333332999970	0.0259047434999999	F	F	F
0.1667563000874544	0.5835126000748930	0.2942108532406455	T	T	T
0.0831361327000785	0.6665680664000437	0.2047965466772881	T	T	T
0.2500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.2499324323510068	0.4999662161755070	0.3831201201280184	T	T	T
0.4166666667000030	0.5833333332999970	0.0259047434999999	F	F	F
0.4166666667000030	0.5833333332999970	0.2942371358926947	T	T	T
0.3334319335999564	0.6665680664000437	0.2047965466772881	T	T	T
0.5000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.5000337838244933	0.4999662161755070	0.3831201201280184	T	T	T
0.6666666667000030	0.5833333332999970	0.0259047434999999	F	F	F
0.6667563000874542	0.5835126000748930	0.2942108532406455	T	T	T
0.5831361327000784	0.6665680664000437	0.2047965466772881	T	T	T
0.7500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.7499324323510068	0.4999662161755070	0.3831201201280184	T	T	T
0.9166666667000030	0.5833333332999970	0.0259047434999999	F	F	F
0.9166666667000030	0.5833333332999970	0.2942371358926947	T	T	T
0.8334319335999563	0.6665680664000437	0.2047965466772881	T	T	T
0.0000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
0.0000337838244931	0.7500675676489932	0.3831201201280184	T	T	T
0.1666666667000030	0.8333333332999970	0.0259047434999999	F	F	F
0.1667563000874544	0.8332436999125458	0.2942108532406455	T	T	T
0.0833333332999970	0.9166666667000030	0.2051388865688787	T	T	T
0.2500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
0.4166666667000030	0.8333333332999970	0.0259047434999999	F	F	F
0.4164873999251072	0.8332436999125458	0.2942108532406455	T	T	T
0.3334319335999564	0.9168638672999216	0.2047965466772881	T	T	T
0.5000000000000000	0.7500000000000000	0.1155258754999977	F	F	F

	0.5000337838244933	0.7500675676489932	0.3831201201280184	T	T	T
	0.666666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.6667563000874542	0.8332436999125458	0.2942108532406455	T	T	T
	0.583333332999970	0.916666667000030	0.2051388865688787	T	T	T
	0.7500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.916666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.9164873999251070	0.8332436999125458	0.2942108532406455	T	T	T
	0.8334319335999563	0.9168638672999216	0.2047965466772881	T	T	T
4Pd/Cu(111)	1.0000000000000000					
	8.8905944857135406	-5.1329871195825199	-0.0000000000000010			
	0.0000000000000000	10.2659742391650006	0.0000000000000010			
	0.0000000000000000	0.0000000000000000	23.3821328661704015			
	Pd	Cu				
	4	76				
	Selective dynamics					
	Direct					
	0.2500000000000000	0.2500000000000000	0.3863801337777262	T	T	T
	0.7500000000000000	0.2500000000000000	0.3863801337777262	T	T	T
	0.2500000000000000	0.7500000000000000	0.3863801337777262	T	T	T
	0.7500000000000000	0.7500000000000000	0.3863801337777262	T	T	T
	0.0000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.0000831240897351	0.9999168759102650	0.3841130202925175	T	T	T
	0.166666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.1664386653971338	0.0828773306942587	0.2940153782514090	T	T	T
	0.0830101168102454	0.1665050584551271	0.2048560836128362	T	T	T
	0.2500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.2498337518205298	0.9999168759102650	0.3841130202925175	T	T	T
	0.416666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.416666667000030	0.083333332999970	0.2946628260939351	T	T	T
	0.3334949415448728	0.1665050584551271	0.2048560836128362	T	T	T
	0.5000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.5000831240897350	0.9999168759102650	0.3841130202925175	T	T	T
	0.666666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.6664386653971338	0.0828773306942587	0.2940153782514090	T	T	T
	0.5830101168102455	0.1665050584551271	0.2048560836128362	T	T	T
	0.7500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.7498337518205297	0.9999168759102650	0.3841130202925175	T	T	T
	0.916666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.916666667000030	0.083333332999970	0.2946628260939351	T	T	T
	0.8334949415448729	0.1665050584551271	0.2048560836128362	T	T	T
	0.0000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
	0.0000831240897351	0.2501662481794703	0.3841130202925175	T	T	T
	0.166666667000030	0.333333332999970	0.0259047434999999	F	F	F
	0.1664386653971338	0.3335613346028662	0.2940153782514090	T	T	T
	0.083333332999970	0.416666667000030	0.2051324365609134	T	T	T
	0.2500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
	0.416666667000030	0.333333332999970	0.0259047434999999	F	F	F
	0.4171226693057413	0.3335613346028662	0.2940153782514090	T	T	T
	0.3334949415448728	0.4169898831897476	0.2048560836128362	T	T	T
	0.5000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
	0.5000831240897350	0.2501662481794703	0.3841130202925175	T	T	T

	0.666666667000030	0.333333332999970	0.0259047434999999	F	F	F
	0.6664386653971338	0.3335613346028662	0.2940153782514090	T	T	T
	0.583333332999970	0.4166666667000030	0.2051324365609134	T	T	T
	0.7500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
	0.9166666667000030	0.333333332999970	0.0259047434999999	F	F	F
	0.9171226693057414	0.3335613346028662	0.2940153782514090	T	T	T
	0.8334949415448729	0.4169898831897476	0.2048560836128362	T	T	T
	0.0000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.0000831240897351	0.4999168759102648	0.3841130202925175	T	T	T
	0.1666666667000030	0.583333332999970	0.0259047434999999	F	F	F
	0.1664386653971338	0.5828773306942586	0.2940153782514090	T	T	T
	0.0830101168102454	0.6665050584551271	0.2048560836128362	T	T	T
	0.2500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.2498337518205298	0.4999168759102648	0.3841130202925175	T	T	T
	0.4166666667000030	0.583333332999970	0.0259047434999999	F	F	F
	0.4166666667000030	0.583333332999970	0.2946628260939351	T	T	T
	0.3334949415448728	0.6665050584551271	0.2048560836128362	T	T	T
	0.5000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.5000831240897350	0.4999168759102648	0.3841130202925175	T	T	T
	0.6666666667000030	0.583333332999970	0.0259047434999999	F	F	F
	0.6664386653971338	0.5828773306942586	0.2940153782514090	T	T	T
	0.5830101168102455	0.6665050584551271	0.2048560836128362	T	T	T
	0.7500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.7498337518205297	0.4999168759102648	0.3841130202925175	T	T	T
	0.9166666667000030	0.583333332999970	0.0259047434999999	F	F	F
	0.9166666667000030	0.583333332999970	0.2946628260939351	T	T	T
	0.8334949415448729	0.6665050584551271	0.2048560836128362	T	T	T
	0.0000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.0000831240897351	0.7501662481794703	0.3841130202925175	T	T	T
	0.1666666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.1664386653971338	0.8335613346028662	0.2940153782514090	T	T	T
	0.083333332999970	0.9166666667000030	0.2051324365609134	T	T	T
	0.2500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.4166666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.4171226693057413	0.8335613346028662	0.2940153782514090	T	T	T
	0.3334949415448728	0.9169898831897545	0.2048560836128362	T	T	T
	0.5000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.5000831240897350	0.7501662481794703	0.3841130202925175	T	T	T
	0.6666666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.6664386653971338	0.8335613346028662	0.2940153782514090	T	T	T
	0.583333332999970	0.9166666667000030	0.2051324365609134	T	T	T
	0.7500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.9166666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.9171226693057414	0.8335613346028662	0.2940153782514090	T	T	T
	0.8334949415448729	0.9169898831897545	0.2048560836128362	T	T	T
4Pt/Cu(111)	1.0000000000000000					
	8.8905944857135406	-5.1329871195825199	-0.0000000000000010			
	0.0000000000000000	10.2659742391650006	0.0000000000000010			
	0.0000000000000000	0.0000000000000000	23.3821328661704015			
	Pt	Cu				
	4	76				

Selective dynamics

Direct

0.2500000000000000	0.2500000000000000	0.3838822250741245	T	T	T
0.7500000000000000	0.2500000000000000	0.3838822250741245	T	T	T
0.2500000000000000	0.7500000000000000	0.3838822250741245	T	T	T
0.7500000000000000	0.7500000000000000	0.3838822250741245	T	T	T
0.0000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.0000380050948792	0.9999619949051208	0.3854381412099173	T	T	T
0.1666666667000030	0.083333332999970	0.0259047434999999	F	F	F
0.1659308222105480	0.0818616443210800	0.2935273412201198	T	T	T
0.0830457953074486	0.1665228977037287	0.2044338048420400	T	T	T
0.2500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.2499239898102417	0.9999619949051208	0.3854381412099173	T	T	T
0.4166666667000030	0.083333332999970	0.0259047434999999	F	F	F
0.4166666667000030	0.083333332999970	0.2942497797655079	T	T	T
0.3334771022962713	0.1665228977037287	0.2044338048420400	T	T	T
0.5000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.5000380050948792	0.9999619949051208	0.3854381412099173	T	T	T
0.6666666667000030	0.083333332999970	0.0259047434999999	F	F	F
0.6659308222105480	0.0818616443210800	0.2935273412201198	T	T	T
0.5830457953074486	0.1665228977037287	0.2044338048420400	T	T	T
0.7500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.7499239898102417	0.9999619949051208	0.3854381412099173	T	T	T
0.9166666667000030	0.083333332999970	0.0259047434999999	F	F	F
0.9166666667000030	0.083333332999970	0.2942497797655079	T	T	T
0.8334771022962713	0.1665228977037287	0.2044338048420400	T	T	T
0.0000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.0000380050948792	0.2500760101897583	0.3854381412099173	T	T	T
0.1666666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.1659308222105480	0.3340691777894520	0.2935273412201198	T	T	T
0.083333332999970	0.4166666667000030	0.2047991552073682	T	T	T
0.2500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.4166666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.4181383556789200	0.3340691777894520	0.2935273412201198	T	T	T
0.3334771022962713	0.4169542046925514	0.2044338048420400	T	T	T
0.5000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.5000380050948792	0.2500760101897583	0.3854381412099173	T	T	T
0.6666666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.6659308222105480	0.3340691777894520	0.2935273412201198	T	T	T
0.583333332999970	0.4166666667000030	0.2047991552073682	T	T	T
0.7500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.9166666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.9181383556789200	0.3340691777894520	0.2935273412201198	T	T	T
0.8334771022962713	0.4169542046925514	0.2044338048420400	T	T	T
0.0000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.0000380050948792	0.4999619949051208	0.3854381412099173	T	T	T
0.1666666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.1659308222105480	0.5818616443210800	0.2935273412201198	T	T	T
0.0830457953074486	0.6665228977037287	0.2044338048420400	T	T	T
0.2500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.2499239898102417	0.4999619949051208	0.3854381412099173	T	T	T

	0.416666667000030	0.5833333332999970	0.0259047434999999	F	F	F
	0.416666667000030	0.5833333332999970	0.2942497797655079	T	T	T
	0.3334771022962713	0.6665228977037287	0.2044338048420400	T	T	T
	0.5000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.5000380050948792	0.4999619949051208	0.3854381412099173	T	T	T
	0.666666667000030	0.5833333332999970	0.0259047434999999	F	F	F
	0.6659308222105480	0.5818616443210800	0.2935273412201198	T	T	T
	0.5830457953074486	0.6665228977037287	0.2044338048420400	T	T	T
	0.7500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.7499239898102417	0.4999619949051208	0.3854381412099173	T	T	T
	0.916666667000030	0.5833333332999970	0.0259047434999999	F	F	F
	0.916666667000030	0.5833333332999970	0.2942497797655079	T	T	T
	0.8334771022962713	0.6665228977037287	0.2044338048420400	T	T	T
	0.0000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.0000380050948792	0.7500760101897583	0.3854381412099173	T	T	T
	0.166666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.1659308222105480	0.8340691777894520	0.2935273412201198	T	T	T
	0.0833333332999970	0.916666667000030	0.2047991552073682	T	T	T
	0.2500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.416666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.4181383556789200	0.8340691777894520	0.2935273412201198	T	T	T
	0.3334771022962713	0.9169542046925514	0.2044338048420400	T	T	T
	0.5000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.5000380050948792	0.7500760101897583	0.3854381412099173	T	T	T
	0.666666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.6659308222105480	0.8340691777894520	0.2935273412201198	T	T	T
	0.5833333332999970	0.916666667000030	0.2047991552073682	T	T	T
	0.7500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.916666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.9181383556789200	0.8340691777894520	0.2935273412201198	T	T	T
	0.8334771022962713	0.9169542046925514	0.2044338048420400	T	T	T
(10) 4X-PC						
4Cu/Ni(111)	1.0000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni	Cu				
	76	4				
	Selective dynamics					
	Direct					
	0.0000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.0017306852558434	0.0021052702482081	0.4008112824429304	T	T	T
	0.1666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.1669003503300956	0.0834114140107332	0.3140498335563038	T	T	T
	0.0832870811330011	0.1665283025836004	0.2266807875395074	T	T	T
	0.2500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.2495173531231529	0.9995331433159294	0.4009168128272833	T	T	T
	0.4166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.4160553476343551	0.0831816285186093	0.3141223721846274	T	T	T
	0.3332817399634536	0.1666604012196018	0.2266396517700997	T	T	T
	0.5000000000000000	0.0000000000000000	0.1392870000000030	F	F	F

0.5003840752138657	0.0023190348002160	0.4007934817552155	T	T	T
0.6666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
0.6666942912644700	0.0830669625721328	0.3142588077459223	T	T	T
0.5832078453672978	0.1666204790326944	0.2267462642386064	T	T	T
0.7500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
0.7526089366905211	0.0053877443355432	0.4008432583147368	T	T	T
0.9166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
0.9167114952572675	0.0832732230376081	0.3141834914547132	T	T	T
0.8333087855171399	0.1665974329693114	0.2267056193927104	T	T	T
0.0000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.9983008925797634	0.2487157562799283	0.4011072512920961	T	T	T
0.1666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.1673271960257807	0.3338192426403737	0.3147574411698741	T	T	T
0.0836644066463919	0.4166625483069097	0.2269741412650532	T	T	T
0.2500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.2481936736033248	0.2454572756587581	0.4009422741730120	T	T	T
0.4166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.4166446865807245	0.3337460757784925	0.3146656452572785	T	T	T
0.3332111866099723	0.4167192311265211	0.2270339324588591	T	T	T
0.5000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.5003575687550423	0.2478456985968407	0.4008757776558411	T	T	T
0.6666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.6662400759923841	0.3335105650925456	0.3141273328193463	T	T	T
0.5831012646389766	0.4167347478845755	0.2268568251298220	T	T	T
0.7500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.7500894549479185	0.2501156019230280	0.4011880323663490	T	T	T
0.9166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.9169006868705196	0.3332366859023068	0.3144252322228525	T	T	T
0.83330802455160438	0.4165640501272776	0.2267605053165838	T	T	T
0.0000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.9982784793229982	0.4996788987930643	0.4009662670567664	T	T	T
0.1666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.1674830073277960	0.5834382433744807	0.3146148121246739	T	T	T
0.0831465821132440	0.6666362190818944	0.2266471727863575	T	T	T
0.2500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.4166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.4170152472694539	0.5835282581389905	0.3153197673330439	T	T	T
0.3333394280515876	0.6666432901196799	0.2270310232568917	T	T	T
0.5000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.6666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.6665596816900958	0.5836515816868300	0.3150233126190400	T	T	T
0.5836510252935767	0.6671485584925989	0.2272572963509489	T	T	T
0.7500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.7523098650217719	0.4972414779799976	0.4007766574504856	T	T	T
0.9166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.9166433311238293	0.5838563784656756	0.3141784198248700	T	T	T
0.8333587942010894	0.6667591129886361	0.2268302743218413	T	T	T
0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.0015529888236685	0.7494586405252193	0.4008137942971715	T	T	T
0.1666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
0.1665701873597314	0.8332879872181351	0.3137419099998340	T	T	T

	0.0835891002822677	0.9167951769195142	0.2267019542282753	T	T	T
	0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.2477486871786283	0.7525235429874684	0.4006941629798462	T	T	T
	0.4166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.4168430917593966	0.8327453448055735	0.3145600944902256	T	T	T
	0.3331291729693433	0.9165654893815898	0.2266675271364704	T	T	T
	0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.6666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.6666247562259571	0.8332398258163067	0.3152067366561369	T	T	T
	0.5831974857477533	0.9163421488556907	0.2269241074350532	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.9166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.9158727362562473	0.8329079980168146	0.3146015043714385	T	T	T
	0.8332694615948668	0.9164467280023061	0.2269138768686858	T	T	T
	0.5000394400052173	0.7526072473479815	0.4057438729106266	T	T	T
	0.7521503854452050	0.7510851528322391	0.4059281191259672	T	T	T
	0.2480759493698272	0.4990363504658930	0.4058221964609317	T	T	T
	0.5001251236223183	0.4975013509137938	0.4057231166001714	T	T	T
4Ag/Ni(111)	1.0000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni	Ag				
	76	4				
	Selective dynamics					
	Direct					
	0.0000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.0075171386575548	0.0079880073303329	0.3988174234101933	T	T	T
	0.1666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.1675798463209404	0.0840039167218904	0.3122116619223263	T	T	T
	0.0837384685367866	0.1676738450104054	0.2263161356034260	T	T	T
	0.2500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.2496192370473551	0.9994759481144371	0.3989978741689910	T	T	T
	0.4166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.4155776033686038	0.0831785534718108	0.3121731084064763	T	T	T
	0.3337003122284727	0.1675260039200381	0.2261263289772728	T	T	T
	0.5000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.5006764639514216	0.0081775148944132	0.3990573519055047	T	T	T
	0.6666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.6665948033244007	0.0828914972560071	0.3133125632845335	T	T	T
	0.5834776313155245	0.1667012368877394	0.2260705736177968	T	T	T
	0.7500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.7559825456060878	0.0117183335726239	0.4000292673068415	T	T	T
	0.9166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.9165435109554707	0.0826359038558664	0.3127596263858692	T	T	T
	0.8332631916821427	0.1665930693746702	0.2261740673885271	T	T	T
	0.0000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.9924895441025328	0.2440091758187677	0.3996637526829190	T	T	T
	0.1666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.1679196676971770	0.3349081281840114	0.3156242449872906	T	T	T
	0.0841551627420216	0.4169797862012956	0.2270964936746154	T	T	T

0.2500000000000000	0.2500000000000000	0.1392870000000030	F F F
0.2457580164489244	0.2391076980746760	0.4002182035360207	T T T
0.4166669999999968	0.3333330000000032	0.0514190000000028	F F F
0.4176633520085176	0.3359687963150790	0.3153778385039629	T T T
0.3336339951128693	0.4177500919972417	0.2278013631093785	T T T
0.5000000000000000	0.2500000000000000	0.1392870000000030	F F F
0.5006794925803888	0.2422809051464085	0.3991563133210079	T T T
0.6666669999999968	0.3333330000000032	0.0514190000000028	F F F
0.6663786207662028	0.3334905975514388	0.3132127500491677	T T T
0.5831844467343785	0.4176753922062417	0.2271168087281552	T T T
0.7500000000000000	0.2500000000000000	0.1392870000000030	F F F
0.7498514822101541	0.2497668157945725	0.4007281658250932	T T T
0.9166669999999968	0.3333330000000032	0.0514190000000028	F F F
0.9166090226256500	0.3332174535789960	0.3135573926686916	T T T
0.8331472568296761	0.4166455063558701	0.2262240069551282	T T T
0.0000000000000000	0.5000000000000000	0.1392870000000030	F F F
0.9922560678488637	0.4983836044517318	0.3995427910011458	T T T
0.1666669999999968	0.5833330000000032	0.0514190000000028	F F F
0.1677883933482107	0.5828459138925552	0.3155405447896484	T T T
0.0834013051694598	0.6661639707905422	0.2263322171589834	T T T
0.2500000000000000	0.5000000000000000	0.1392870000000030	F F F
0.4166669999999968	0.5833330000000032	0.0514190000000028	F F F
0.4165645368205588	0.5837018953807842	0.3184048977480600	T T T
0.3336538897981072	0.6662601667241290	0.2279708435096595	T T T
0.5000000000000000	0.5000000000000000	0.1392870000000030	F F F
0.6666669999999968	0.5833330000000032	0.0514190000000028	F F F
0.6660406917623405	0.5842064810719307	0.3170601197155349	T T T
0.5826703508708491	0.6667328158195929	0.2285186321070540	T T T
0.7500000000000000	0.5000000000000000	0.1392870000000030	F F F
0.7556352991693842	0.4936905687643360	0.3999916792339633	T T T
0.9166669999999968	0.5833330000000032	0.0514190000000028	F F F
0.9160827103157771	0.5844082921102185	0.3127440257301970	T T T
0.8321909189375276	0.6667238649764258	0.2269501804497978	T T T
0.0000000000000000	0.7500000000000000	0.1392870000000030	F F F
0.0073970721782217	0.7491866576355264	0.3988725470511767	T T T
0.1666669999999968	0.8333330000000032	0.0514190000000028	F F F
0.1668353176567337	0.8333243391271878	0.3122528878111410	T T T
0.0825112838844646	0.9163387495263180	0.2263216612488179	T T T
0.2500000000000000	0.7500000000000000	0.1392870000000030	F F F
0.2454782002699716	0.7558060812871332	0.4001547187026731	T T T
0.4166669999999968	0.8333330000000032	0.0514190000000028	F F F
0.4174026180019865	0.8320311085147054	0.3153211171700079	T T T
0.3334729168368611	0.9160028177029034	0.2262326552179630	T T T
0.5000000000000000	0.7500000000000000	0.1392870000000030	F F F
0.6666669999999968	0.8333330000000032	0.0514190000000028	F F F
0.6660537227276251	0.8320362420954055	0.3172095614757637	T T T
0.5831086369152700	0.9154497942235977	0.2272271241115575	T T T
0.7500000000000000	0.7500000000000000	0.1392870000000030	F F F
0.9166669999999968	0.8333330000000032	0.0514190000000028	F F F
0.9143086754123075	0.8322340912071482	0.3151626166401797	T T T
0.8321063493705765	0.9156041942984814	0.2270807364703273	T T T

	0.5009624609189132	0.7631719753041111	0.4246479094871205	T	T	T
	0.7678685171887167	0.7587907239829121	0.4266118433152570	T	T	T
	0.2340190178928907	0.4918902017205085	0.4263259028999755	T	T	T
	0.5008719762037899	0.4876233189164481	0.4248144860214893	T	T	T
4Au/Ni(111)	1.000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni	Au				
	76	4				
	Selective dynamics					
	Direct					
	0.0000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.0085994558756539	0.0082659675736281	0.3997748787289837	T	T	T
	0.1666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.1678657142006585	0.0843184710058296	0.3128166509317083	T	T	T
	0.0833183069826617	0.1670009009044335	0.2264378686667783	T	T	T
	0.2500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.2504763873431841	0.0001932359628967	0.3991955925547188	T	T	T
	0.4166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.4162889790859481	0.0833990924533552	0.3126041773369721	T	T	T
	0.3334820759085275	0.1670440415732699	0.2262081729923651	T	T	T
	0.5000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.5005510436835081	0.0084776434929168	0.4001110683327269	T	T	T
	0.6666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.6668903711250422	0.0832001782311025	0.3136230398242645	T	T	T
	0.5835926805202263	0.1668293812639874	0.2262637349352090	T	T	T
	0.7500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.7552005690625592	0.0107880824462683	0.4013180508736269	T	T	T
	0.9166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.9165847594348264	0.0831553495339463	0.3133024003621401	T	T	T
	0.8332849187151865	0.1665832868555910	0.2262348796654834	T	T	T
	0.0000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.9913845745832575	0.2433648596507325	0.4005196908458188	T	T	T
	0.1666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.1667419059864841	0.3334009715332655	0.3151035186670725	T	T	T
	0.0839657985446749	0.4168279719499068	0.2270413344947073	T	T	T
	0.2500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.2459236856637546	0.2402211600955937	0.4015440260432896	T	T	T
	0.4166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.4171906015747453	0.3343701328918414	0.3150631363078062	T	T	T
	0.3331513711974097	0.4169069060480552	0.2276288394886237	T	T	T
	0.5000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.5004237367576181	0.2420589091970626	0.4001672852990126	T	T	T
	0.6666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.6666624450093863	0.3334553914494691	0.3135378165332696	T	T	T
	0.5831654986666663	0.4171341448622314	0.2271175482047454	T	T	T
	0.7500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.7493244120185381	0.2496833396499838	0.4006274006698547	T	T	T
	0.9166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.9161363139541052	0.3329520616468571	0.3136586901305023	T	T	T

	0.8332406343472343	0.4166704644838646	0.2263612670122370	T	T	T
	0.0000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.9911167654056285	0.4981141193473988	0.4004365922232651	T	T	T
	0.1666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.1666703835938677	0.5831316403536917	0.3149965954126301	T	T	T
	0.0833120076405720	0.6663508410152303	0.2264308553197978	T	T	T
	0.2500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.4166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.4165330423746454	0.5831790650803228	0.3169748238292129	T	T	T
	0.3334688766496257	0.6661849705173069	0.2277721805143145	T	T	T
	0.5000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.6666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.6662466071347666	0.5834084066507543	0.3160637260666945	T	T	T
	0.5827061650972993	0.6664440070058433	0.2281215320390118	T	T	T
	0.7500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.7548384083018291	0.4941634404231721	0.4014205034491738	T	T	T
	0.9166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.9161135745416331	0.5838647825724621	0.3132799565050348	T	T	T
	0.8325371233635792	0.6666634467555070	0.2269413205427426	T	T	T
	0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.0082338031011489	0.7501078148945979	0.3997659850669848	T	T	T
	0.1666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.1669296343235729	0.8332854511966019	0.3127689365952619	T	T	T
	0.0829384977586045	0.9164653761282082	0.2264230326114713	T	T	T
	0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.2457624142669772	0.7556788041348312	0.4013378121390971	T	T	T
	0.4166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.4170975534341395	0.8326472057135419	0.3150392594293407	T	T	T
	0.3335168585505386	0.9161562281220341	0.2263725292907779	T	T	T
	0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.6666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.6664137500211140	0.8330456318898669	0.3159524696421343	T	T	T
	0.5830725332600650	0.9156901169162239	0.2271352094058656	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.9166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.9158277462885991	0.8329742247868737	0.3146034282804919	T	T	T
	0.8323368464993095	0.9157402839925339	0.2270464402132575	T	T	T
	0.5006487610030135	0.7645624956264570	0.4229942798680142	T	T	T
	0.7680666628670991	0.7591073774342547	0.4212330534664446	T	T	T
	0.2331444553170314	0.4917152626286949	0.4209335758715582	T	T	T
	0.5006049235994396	0.4861416914207624	0.4233240016275204	T	T	T
4Ni/Cu(111)	1.0000000000000000					
	8.8905944857135406	-5.1329871195825199	-0.0000000000000010			
	0.0000000000000000	10.2659742391650006	0.0000000000000010			
	0.0000000000000000	0.0000000000000000	23.3821328661704015			
	Ni	Cu				
	4	76				
	Selective dynamics					
	Direct					
	0.2554760085567125	0.5027380042783633	0.3795913452782926	T	T	T
	0.5002006844501565	0.5048820624198100	0.3796221083510858	T	T	T

0.5002006844501565	0.7453186220303465	0.3796221083510858	T	T	T
0.7455471980296409	0.7477735990148204	0.3798039165446809	T	T	T
0.0000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.9975049554731967	0.9979020871516653	0.3839133856350898	T	T	T
0.1666666667000030	0.0833333332999970	0.0259047434999999	F	F	F
0.1665251965970498	0.0835605570289317	0.2953480953971166	T	T	T
0.0832230485940784	0.1665745986143889	0.2053714779317417	T	T	T
0.2500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.2498946354206169	0.9999473177103084	0.3839339218213809	T	T	T
0.4166666667000030	0.0833333332999970	0.0259047434999999	F	F	F
0.4167085371931734	0.0833542685465858	0.2952280837370509	T	T	T
0.3332771417252900	0.1665832941918737	0.2054167197233951	T	T	T
0.5000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.4998298648479604	0.9969394650687491	0.3836757847810190	T	T	T
0.6666666667000030	0.0833333332999970	0.0259047434999999	F	F	F
0.6666012163836683	0.0830879982042347	0.2948310091754891	T	T	T
0.5832504671432162	0.1666252336216090	0.2053917157976457	T	T	T
0.7500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.7475114158913598	0.9953662528537848	0.3836045620480064	T	T	T
0.9166666667000030	0.0833333332999970	0.0259047434999999	F	F	F
0.9164476638930878	0.0832847340781981	0.2950280332272470	T	T	T
0.8333043767590809	0.1666119556271823	0.2053698230384313	T	T	T
0.0000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.0028011043362000	0.2520409233337872	0.3834841390931771	T	T	T
0.1666666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.1670127948987385	0.3338273204048505	0.2943634074829120	T	T	T
0.0830658258437538	0.4165329129718813	0.2049428292374600	T	T	T
0.2500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.2523769158143949	0.2544324475994770	0.3838209288624768	T	T	T
0.4166666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.4169741180267792	0.3341871169185637	0.2944955251525627	T	T	T
0.3330593168448317	0.4162496422670685	0.2044256142285690	T	T	T
0.5000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.4998298648479604	0.2528903997792114	0.3836757847810190	T	T	T
0.6666666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.6666012163836683	0.3335132180794176	0.2948310091754891	T	T	T
0.5833282863195635	0.4164425576053006	0.2048892196099743	T	T	T
0.7500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.7500965742905024	0.2500482871452476	0.3832559790794932	T	T	T
0.9166666667000030	0.3333333332999970	0.0259047434999999	F	F	F
0.9168289439264257	0.3334144719132084	0.2947603735460049	T	T	T
0.8333043767590809	0.4166924212319074	0.2053698230384313	T	T	T
0.0000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.0028011043362000	0.5007601810024127	0.3834841390931771	T	T	T
0.1666666667000030	0.5833333332999970	0.0259047434999999	F	F	F
0.1670127948987385	0.5831854743938862	0.2943634074829120	T	T	T
0.0832230485940784	0.6666484500796983	0.2053714779317417	T	T	T
0.2500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.4166666667000030	0.5833333332999970	0.0259047434999999	F	F	F
0.4166933309487177	0.5833466654243509	0.2929753591354824	T	T	T
0.3330593168448317	0.6668096746777792	0.2044256142285690	T	T	T

	0.5000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.6666666667000030	0.5833333332999970	0.0259047434999999	F	F	F
	0.6663100595880920	0.5832318821629627	0.2937891654346316	T	T	T
	0.5834575083711968	0.6667287542355993	0.2040160347821072	T	T	T
	0.7500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.7475114158913598	0.5021451630375751	0.3836045620480064	T	T	T
	0.9166666667000030	0.5833333332999970	0.0259047434999999	F	F	F
	0.9164476638930878	0.5831629297148808	0.2950280332272470	T	T	T
	0.8335180421596888	0.6665588867777714	0.2049343128154746	T	T	T
	0.0000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.9975049554731967	0.7496028683215314	0.3839133856350898	T	T	T
	0.1666666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.1665251965970498	0.8329646394681092	0.2953480953971166	T	T	T
	0.0833313419865078	0.9166656710432619	0.2054554425093968	T	T	T
	0.2500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.2523769158143949	0.7479444682149179	0.3838209288624768	T	T	T
	0.4166666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.4169741180267792	0.8327870010082066	0.2944955251525627	T	T	T
	0.3332771417252900	0.9166938476334252	0.2054167197233951	T	T	T
	0.5000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.6666666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.6663100595880920	0.8330781773251132	0.2937891654346316	T	T	T
	0.5833282863195635	0.9168857288142647	0.2048892196099743	T	T	T
	0.7500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.9166666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.9157565126010212	0.8328782562505097	0.2947105293710521	T	T	T
	0.8335180421596888	0.9169591554819263	0.2049343128154746	T	T	T
4Pd/Cu(111)	1.0000000000000000					
	8.8905944857135406	-5.1329871195825199	-0.0000000000000010			
	0.0000000000000000	10.2659742391650006	0.0000000000000010			
	0.0000000000000000	0.0000000000000000	23.3821328661704015			
	Pd	Cu				
	4	76				
	Selective dynamics					
	Direct					
	0.2388553637119060	0.4944276818559530	0.3879366407066485	T	T	T
	0.5000470712628982	0.4918118226596278	0.3881235559680931	T	T	T
	0.5000470712628982	0.7582352486032704	0.3881235559680931	T	T	T
	0.7613193269109146	0.7556596634554609	0.3875025162242949	T	T	T
	0.0000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.0057965395263722	0.0045409569244796	0.3834416801086604	T	T	T
	0.1666666667000030	0.0833333332999970	0.0259047434999999	F	F	F
	0.1671073225515585	0.0835659773053692	0.2936932883504610	T	T	T
	0.0832034476735970	0.1670713167230957	0.2050477785413491	T	T	T
	0.2500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.2506137766917007	0.0003068883458468	0.3826749017222397	T	T	T
	0.4166666667000030	0.0833333332999970	0.0259047434999999	F	F	F
	0.4170664365887973	0.0835332182443977	0.2937212468456778	T	T	T
	0.3337700769524687	0.1673391702497540	0.2048077682044678	T	T	T
	0.5000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.4998558762495762	0.0047664505529497	0.3836106235752084	T	T	T

0.666666667000030	0.083333332999970	0.025904743499999	F F F
0.6666694026040290	0.0830653618316433	0.2943923091075007	T T T
0.5838092579297367	0.1669046290148728	0.2049461368145842	T T T
0.750000000000000	0.000000000000000	0.1155258754999977	F F F
0.7531465692559891	0.0060700317247111	0.3843406404205680	T T T
0.916666667000030	0.083333332999970	0.025904743499999	F F F
0.9162648936131319	0.0827121136992872	0.2943369759871572	T T T
0.8333450762639387	0.1667027833654160	0.2051349142467345	T T T
0.000000000000000	0.250000000000000	0.1155258754999977	F F F
0.9945016425538498	0.2453281392308924	0.3837050520245384	T T T
0.166666667000030	0.333333332999970	0.025904743499999	F F F
0.1660020479212179	0.3323994983771215	0.2944517632609021	T T T
0.0833263365813863	0.4166631683406976	0.2049885054294762	T T T
0.250000000000000	0.250000000000000	0.1155258754999977	F F F
0.2469778771754179	0.2437990299486543	0.3840261462715162	T T T
0.416666667000030	0.333333332999970	0.025904743499999	F F F
0.4163869637220543	0.3328676539125013	0.2942653427361464	T T T
0.3333775528172538	0.4171221993846572	0.2050724184773358	T T T
0.500000000000000	0.250000000000000	0.1155258754999977	F F F
0.4998558762495762	0.2450894256966265	0.3836106235752084	T T T
0.666666667000030	0.333333332999970	0.025904743499999	F F F
0.6666694026040290	0.3336040406723768	0.2943923091075007	T T T
0.5834964102118505	0.4170774419975274	0.2050827350003175	T T T
0.750000000000000	0.250000000000000	0.1155258754999977	F F F
0.7494001788426345	0.2497000894213173	0.3830010451051322	T T T
0.916666667000030	0.333333332999970	0.025904743499999	F F F
0.9166745983790605	0.3333372991395223	0.2944462243001524	T T T
0.8333450762639387	0.4166422929985316	0.2051349142467345	T T T
0.000000000000000	0.500000000000000	0.1155258754999977	F F F
0.9945016425538498	0.4991735033229645	0.3837050520245384	T T T
0.166666667000030	0.583333332999970	0.025904743499999	F F F
0.1660020479212179	0.5836025494440875	0.2944517632609021	T T T
0.0832034476735970	0.6661321310505031	0.2050477785413491	T T T
0.250000000000000	0.500000000000000	0.1155258754999977	F F F
0.416666667000030	0.583333332999970	0.025904743499999	F F F
0.4159739798098130	0.5829869898549020	0.2955747596635092	T T T
0.3333775528172538	0.6662553535326055	0.2050724184773358	T T T
0.500000000000000	0.500000000000000	0.1155258754999977	F F F
0.666666667000030	0.583333332999970	0.025904743499999	F F F
0.6667755533481454	0.5834481826132176	0.2947786710364113	T T T
0.5826916872199419	0.6663458436599754	0.2050713846517027	T T T
0.750000000000000	0.500000000000000	0.1155258754999977	F F F
0.7531465692559891	0.4970765375312780	0.3843406404205680	T T T
0.916666667000030	0.583333332999970	0.025904743499999	F F F
0.9162648936131319	0.5835527798138358	0.2943369759871572	T T T
0.8326608222332368	0.6662657544184896	0.2049361358464594	T T T
0.000000000000000	0.750000000000000	0.1155258754999977	F F F
0.0057965395263722	0.7512555826018925	0.3834416801086604	T T T
0.166666667000030	0.833333332999970	0.025904743499999	F F F
0.1671073225515585	0.8335413451461733	0.2936932883504610	T T T
0.0830782819831555	0.9165391410415822	0.2046192746670954	T T T

	0.2500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.2469778771754179	0.7531788472267635	0.3840261462715162	T	T	T
	0.4166666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.4163869637220543	0.8335193097095441	0.2942653427361464	T	T	T
	0.3337700769524687	0.9164309068027237	0.2048077682044678	T	T	T
	0.5000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.6666666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.6667755533481454	0.8333273706349189	0.2947786710364113	T	T	T
	0.5834964102118505	0.9164189683143249	0.2050827350003175	T	T	T
	0.7500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.9166666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.9180379395784826	0.8340189697392333	0.2937711580236169	T	T	T
	0.8326608222332368	0.9163950679147561	0.2049361358464594	T	T	T
4Pt/Cu(111)	1.0000000000000000					
	8.8905944857135406	-5.1329871195825199	-0.0000000000000010			
	0.0000000000000000	10.2659742391650006	0.0000000000000010			
	0.0000000000000000	0.0000000000000000	23.3821328661704015			
	Pt	Cu				
	4	76				
	Selective dynamics					
	Direct					
	0.2396110035812598	0.4948055017906299	0.3861162477251625	T	T	T
	0.5000598766450608	0.4930974882799006	0.3866946362013479	T	T	T
	0.5000598766450608	0.7569623883651602	0.3866946362013479	T	T	T
	0.7606230839406507	0.7553115419703218	0.3858607100432607	T	T	T
	0.0000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.0051034744095659	0.0037707963155853	0.3846704541625598	T	T	T
	0.1666666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.1669106461766106	0.0835348178631676	0.2944301520414854	T	T	T
	0.0831945393768976	0.1667609916342911	0.2050864571141631	T	T	T
	0.2500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.2506032542244938	0.0003016271122505	0.3833475430992195	T	T	T
	0.4166666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.4170245489028517	0.0835122744014214	0.2944644175472177	T	T	T
	0.3335663006820653	0.1669105511971338	0.2049952170832725	T	T	T
	0.5000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.4998080780987522	0.0038971302719446	0.3847446688755838	T	T	T
	0.6666666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.6670007412039496	0.0837297617370467	0.2947287364156708	T	T	T
	0.5835195038760475	0.1667597519880317	0.2052128037296796	T	T	T
	0.7500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.7528418896786064	0.0051992731730337	0.3854969681956533	T	T	T
	0.9166666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.9165535324328786	0.0834798067762677	0.2948175298703930	T	T	T
	0.8333481787654478	0.1667439061719733	0.2052787940289207	T	T	T
	0.0000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
	0.9952468041894207	0.2460158071427330	0.3846797418849377	T	T	T
	0.1666666667000030	0.333333332999970	0.0259047434999999	F	F	F
	0.1648915910559197	0.3309903063956767	0.2938831165859455	T	T	T
	0.0829188191219430	0.4164594096109724	0.2048474382333723	T	T	T
	0.2500000000000000	0.2500000000000000	0.1155258754999977	F	F	F

0.2472010505227686	0.2446812935824809	0.3853250635305656	T	T	T
0.4166666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.4162271251315062	0.3314707569951025	0.2939401812302762	T	T	T
0.3332332111765837	0.4166816100304089	0.2047103625090401	T	T	T
0.5000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.4998080780987522	0.2459109478268076	0.3847446688755838	T	T	T
0.6666666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.6670007412039496	0.3332709793668940	0.2947287364156708	T	T	T
0.5836120207270383	0.4166751979696173	0.2048951374702668	T	T	T
0.7500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.7494244039795745	0.2497122019897873	0.3832768661544605	T	T	T
0.9166666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.9162133219920605	0.3331066609460294	0.2947039883989362	T	T	T
0.8333481787654478	0.4166042726934833	0.2052787940289207	T	T	T
0.0000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.9952468041894207	0.4992309970466877	0.3846797418849377	T	T	T
0.1666666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.1648915910559197	0.5839012845602340	0.2938831165859455	T	T	T
0.0831945393768976	0.6664335478426082	0.2050864571141631	T	T	T
0.2500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.4166666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.4155354488610641	0.5827677243805311	0.2936787352803520	T	T	T
0.3332332111765837	0.6665516012461836	0.2047103625090401	T	T	T
0.5000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.6666666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.6674894124932891	0.5825112601082481	0.2936257392399924	T	T	T
0.5829786136981880	0.6664893068991020	0.2045423450928894	T	T	T
0.7500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.7528418896786064	0.4976426165055727	0.3854969681956533	T	T	T
0.9166666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.9165535324328786	0.5830737255566021	0.2948175298703930	T	T	T
0.8331440093192484	0.6662979316833102	0.2048105949838970	T	T	T
0.0000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
0.0051034744095659	0.7513326780939806	0.3846704541625598	T	T	T
0.1666666667000030	0.833333332999970	0.0259047434999999	F	F	F
0.1669106461766106	0.8333758282134340	0.2944301520414854	T	T	T
0.0833099802092008	0.9166549901546048	0.2048388789379061	T	T	T
0.2500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
0.2472010505227686	0.7525197569402877	0.3853250635305656	T	T	T
0.4166666667000030	0.833333332999970	0.0259047434999999	F	F	F
0.4162271251315062	0.8347563680363947	0.2939401812302762	T	T	T
0.3335663006820653	0.9166557495849332	0.2049952170832725	T	T	T
0.5000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
0.6666666667000030	0.833333332999970	0.0259047434999999	F	F	F
0.6674894124932891	0.8349781522850321	0.2936257392399924	T	T	T
0.5836120207270383	0.9169368228574299	0.2048951374702668	T	T	T
0.7500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
0.9166666667000030	0.833333332999970	0.0259047434999999	F	F	F
0.9190707952687234	0.8345353975843608	0.2935332643542807	T	T	T
0.8331440093192484	0.9168460777359471	0.2048105949838970	T	T	T
(11) 4X-PL					

4Cu/Ni(111)	1.00000000000000			
	8.6224000674449712	-4.9781450000000014	0.0000000000000000	
	0.0000000000000000	9.9562900000000010	0.0000000000000000	
	0.0000000000000000	0.0000000000000000	23.1292800000000014	
	Ni	Cu		
	76	4		
	Selective dynamics			
	Direct			
	0.0000000000000000	0.0000000000000000	0.1392870000000030	F F F
	0.1666669999999968	0.0833330000000032	0.0514190000000028	F F F
0.1668332361190465	0.0833125483210679	0.3149436966005155	T T T	
0.0833987759063533	0.1670039211050423	0.2271975292375217	T T T	
0.2500000000000000	0.0000000000000000	0.1392870000000030	F F F	
0.2524671079811611	0.9973334396251801	0.4006477025369790	T T T	
0.4166669999999968	0.0833330000000032	0.0514190000000028	F F F	
0.4163048536018081	0.0837148486150454	0.3141588761010610	T T T	
0.3332424971445889	0.1667533461759376	0.2267332346955442	T T T	
0.5000000000000000	0.0000000000000000	0.1392870000000030	F F F	
0.5001787556305146	0.9998184332921838	0.4012270438437753	T T T	
0.6666669999999968	0.0833330000000032	0.0514190000000028	F F F	
0.6669540633532804	0.0834433849693568	0.3141340914075386	T T T	
0.5832909274234623	0.1669056444344079	0.2268098814714392	T T T	
0.7500000000000000	0.0000000000000000	0.1392870000000030	F F F	
0.7479537728451220	0.0023321626317383	0.4009423178239260	T T T	
0.9166669999999968	0.0833330000000032	0.0514190000000028	F F F	
0.9170675485470667	0.0829324514529333	0.3149733703289002	T T T	
0.8333115942047655	0.1666884057952345	0.2266269547615138	T T T	
0.0000000000000000	0.2500000000000000	0.1392870000000030	F F F	
0.9976678373682617	0.2520462271548780	0.4009423178239260	T T T	
0.1666669999999968	0.3333330000000032	0.0514190000000028	F F F	
0.1670499538401700	0.3329709888761201	0.3149755407560590	T T T	
0.0832773991176978	0.4167015236299392	0.2266970821827599	T T T	
0.2500000000000000	0.2500000000000000	0.1392870000000030	F F F	
0.4166669999999968	0.3333330000000032	0.0514190000000028	F F F	
0.4166766399432902	0.3331436784034665	0.3149491583002373	T T T	
0.3329906025334068	0.4165969369575961	0.2271912686732378	T T T	
0.5000000000000000	0.2500000000000000	0.1392870000000030	F F F	
0.5026949285184159	0.2475710593805829	0.4006318451285011	T T T	
0.6666669999999968	0.3333330000000032	0.0514190000000028	F F F	
0.6663512459780989	0.3336487540219011	0.3139445281341935	T T T	
0.5830917398962612	0.4169082601037388	0.2267241163649771	T T T	
0.7500000000000000	0.2500000000000000	0.1392870000000030	F F F	
0.7500745400406927	0.2499254599593073	0.4011268631235438	T T T	
0.9166669999999968	0.3333330000000032	0.0514190000000028	F F F	
0.9165566150306432	0.3330459366467196	0.3141340914075386	T T T	
0.8330943555655921	0.4167090725765377	0.2268098814714392	T T T	
0.0000000000000000	0.5000000000000000	0.1392870000000030	F F F	
0.0001815667078162	0.4998212443694783	0.4012270438437753	T T T	
0.1666669999999968	0.5833330000000032	0.0514190000000028	F F F	
0.1669469095368896	0.5834365821689005	0.3141303657778067	T T T	
0.0832512943526353	0.6668719570112316	0.2268031882206998	T T T	

	0.2500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.2479697411381281	0.5023497397570580	0.4009335625449566	T	T	T
	0.4166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.4170852197163271	0.5829147802836729	0.3149340130451463	T	T	T
	0.3333251599991058	0.66667484000008942	0.2266070724587905	T	T	T
	0.5000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.6666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.6668563215965335	0.5833233600567098	0.3149491583002373	T	T	T
	0.5834030630424039	0.6670093974665932	0.2271912686732378	T	T	T
	0.7500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.7524289406194171	0.4973050714815841	0.4006318451285011	T	T	T
	0.9166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.9162851513849546	0.5836951463981919	0.3141588761010610	T	T	T
	0.8332456538240649	0.6667575028554111	0.2267332346955442	T	T	T
	0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.0026665603748199	0.7475328920188389	0.4006477025369790	T	T	T
	0.1666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.1663407874371217	0.8336592125628783	0.3139473954781380	T	T	T
	0.0830916474149319	0.9169083525850681	0.2267239694730137	T	T	T
	0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.2500747384822617	0.7499252615177383	0.4011150566374155	T	T	T
	0.4166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.4165634178310995	0.8330530904631104	0.3141303657778067	T	T	T
	0.3331280429887684	0.9167487056473647	0.2268031882206998	T	T	T
	0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.4976502602429420	0.7520302588618719	0.4009335625449566	T	T	T
	0.6666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.6670290111238799	0.8329500461598300	0.3149755407560590	T	T	T
	0.5832984763700608	0.9167226008823022	0.2266970821827599	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.9166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.9166874516789321	0.8331667638809535	0.3149436966005155	T	T	T
	0.8329960788949577	0.9166012240936467	0.2271975292375217	T	T	T
	0.2500555863526657	0.2499355458484303	0.4058362293801210	T	T	T
	0.7500644541515697	0.7499444136473343	0.4058362293801210	T	T	T
	0.0000940249985462	0.9999059750014538	0.4058556508240088	T	T	T
	0.5000697300020462	0.4999302699979538	0.4058477702576724	T	T	T
4Ag/Ni(111)	1.0000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni	Ag				
	76	4				
	Selective dynamics					
	Direct					
	0.0000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.1666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.1657254101754830	0.0809529198760757	0.3152600454954353	T	T	T
	0.0833639717310533	0.1666640769891288	0.2274980514610050	T	T	T
	0.2500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.2552620064426208	0.9913778507175763	0.4003911731608412	T	T	T

0.416666999999968	0.083333000000032	0.051419000000028	F	F	F
0.4164813685125281	0.0835378011087826	0.3136167208622922	T	T	T
0.3331211640129368	0.1668981655402035	0.2269765842163523	T	T	T
0.500000000000000	0.000000000000000	0.1392870000000030	F	F	F
0.5010816049841296	0.9989173241449834	0.4004323870380588	T	T	T
0.666666999999968	0.083333000000032	0.051419000000028	F	F	F
0.6676508852315379	0.0829570352200264	0.3133269014521360	T	T	T
0.5835267289436388	0.1665296989769800	0.2264166360450446	T	T	T
0.750000000000000	0.000000000000000	0.1392870000000030	F	F	F
0.7468729563804999	0.0062588175634559	0.4012695832247601	T	T	T
0.916666999999968	0.083333000000032	0.051419000000028	F	F	F
0.9185702221030638	0.0814297778969362	0.3165526214868919	T	T	T
0.8339119402335626	0.1660880597664374	0.2266540800310111	T	T	T
0.000000000000000	0.250000000000000	0.1392870000000030	F	F	F
0.9937411824365441	0.2531270436195001	0.4012695832247601	T	T	T
0.166666999999968	0.333333000000032	0.051419000000028	F	F	F
0.1669050763717124	0.3330681650813929	0.3148227526039875	T	T	T
0.0836554983214981	0.4163583481050779	0.2264004158505486	T	T	T
0.250000000000000	0.250000000000000	0.1392870000000030	F	F	F
0.416666999999968	0.333333000000032	0.051419000000028	F	F	F
0.4189781857328043	0.3342589350934020	0.3152710471668101	T	T	T
0.3333405778800085	0.4166346663265088	0.2275040475669101	T	T	T
0.500000000000000	0.250000000000000	0.1392870000000030	F	F	F
0.5086038491874589	0.2447106848552494	0.4003770014726626	T	T	T
0.666666999999968	0.333333000000032	0.051419000000028	F	F	F
0.6669126417988309	0.3330873582011691	0.3133768637039651	T	T	T
0.5832174869578921	0.4167825130421079	0.2267483762744149	T	T	T
0.750000000000000	0.250000000000000	0.1392870000000030	F	F	F
0.7511178251862418	0.2488821748137582	0.4005652671981466	T	T	T
0.916666999999968	0.333333000000032	0.051419000000028	F	F	F
0.9170429647799736	0.3323491147684621	0.3133269014521360	T	T	T
0.8334703010230200	0.4164732710563612	0.2264166360450446	T	T	T
0.000000000000000	0.500000000000000	0.1392870000000030	F	F	F
0.0010826758550166	0.4989183950158704	0.4004323870380588	T	T	T
0.166666999999968	0.583333000000032	0.051419000000028	F	F	F
0.1676205448439987	0.5829595000986245	0.3133420391651143	T	T	T
0.0835009591841640	0.6665277264760121	0.2264108766694619	T	T	T
0.250000000000000	0.500000000000000	0.1392870000000030	F	F	F
0.2468165073405899	0.5062319104882107	0.4012547332387726	T	T	T
0.416666999999968	0.583333000000032	0.051419000000028	F	F	F
0.4185702351504617	0.5814297648495383	0.3165737055792803	T	T	T
0.3339336451218031	0.6660663548781969	0.2266423972682929	T	T	T
0.500000000000000	0.500000000000000	0.1392870000000030	F	F	F
0.666666999999968	0.583333000000032	0.051419000000028	F	F	F
0.6657410649065980	0.5810218142671957	0.3152710471668101	T	T	T
0.5833653336734912	0.6666594221199915	0.2275040475669101	T	T	T
0.750000000000000	0.500000000000000	0.1392870000000030	F	F	F
0.7552893151447506	0.4913961508125411	0.4003770014726626	T	T	T
0.916666999999968	0.583333000000032	0.051419000000028	F	F	F
0.9164621988912174	0.5835186314874719	0.3136167208622922	T	T	T
0.8331008344597990	0.6668788359870632	0.2269765842163523	T	T	T

	0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.0086221492824237	0.7447379935573792	0.4003911731608412	T	T	T
	0.1666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.1668769377425008	0.8331230622574992	0.3133672987402605	T	T	T
	0.0832143648186161	0.9167856351813839	0.2267460055752792	T	T	T
	0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.2511334202162203	0.7488665797837797	0.4005562560541520	T	T	T
	0.4166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.4170404999013755	0.8323794551560013	0.3133420391651143	T	T	T
	0.3334722735239879	0.9164990408158360	0.2264108766694619	T	T	T
	0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.4937680895117893	0.7531834926594101	0.4012547332387726	T	T	T
	0.6666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.6669318349186071	0.8330949236282876	0.3148227526039875	T	T	T
	0.5836416518949221	0.9163445016785019	0.2264004158505486	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.9166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.9190470801239243	0.8342745898245170	0.3152600454954353	T	T	T
	0.8333359230108712	0.9166360282689467	0.2274980514610050	T	T	T
	0.2509326140890664	0.2489333726692564	0.4122911345382860	T	T	T
	0.7510666273307436	0.7490673859109336	0.4122911345382860	T	T	T
	0.0012489317598536	0.9987510682401464	0.4399325201293180	T	T	T
	0.5012360342615452	0.4987639657384548	0.4396953974474087	T	T	T
4Au/Ni(111)	1.0000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni Au					
	76 4					
	Selective dynamics					
	Direct					
	0.0000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.1666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.1669048632104406	0.0822433391808985	0.3150745505088963	T	T	T
	0.0835156183834798	0.1668342502255555	0.2273389169732027	T	T	T
	0.2500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.2570170447938764	0.9922077854666185	0.4016282669515263	T	T	T
	0.4166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.4167285889012504	0.0832706003141865	0.3137666708655260	T	T	T
	0.3332579588840048	0.1667561626221712	0.2269724845206511	T	T	T
	0.5000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.5011812674797014	0.9988032074656417	0.4004768240507133	T	T	T
	0.6666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.6672674925035835	0.0831644178096909	0.3135809788441293	T	T	T
	0.5833841593712208	0.1667508691452753	0.2265012609921513	T	T	T
	0.7500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.7453038375988683	0.0051205220306159	0.4018655060472796	T	T	T
	0.9166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.9170235538997318	0.0829764461002682	0.3150477801780198	T	T	T
	0.8335009346531876	0.1664990653468124	0.2264265666793790	T	T	T
	0.0000000000000000	0.2500000000000000	0.1392870000000030	F	F	F

0.9948794779693841	0.2546961624011317	0.4018655060472796	T	T	T
0.1666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.1666531940295712	0.3332997163982228	0.3146131871864668	T	T	T
0.0835135669537550	0.4165018525321855	0.2265093801078208	T	T	T
0.2500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.4166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.4177654556857391	0.3330912200704574	0.3150741242097652	T	T	T
0.3331825890596747	0.4164907659254382	0.2273348266002699	T	T	T
0.5000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.5078136159930438	0.2429901902208016	0.4016279289584972	T	T	T
0.6666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.6669441837360282	0.3330558162639718	0.3136450321804602	T	T	T
0.5832324994886093	0.4167675005113907	0.2269610595378921	T	T	T
0.7500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.7512913648764084	0.2487086351235916	0.4005524467696517	T	T	T
0.9166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.9168355821903091	0.3327325074964165	0.3135809788441293	T	T	T
0.8332491308547247	0.4166158406287792	0.2265012609921513	T	T	T
0.0000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.0011967925343583	0.4988187325202986	0.4004768240507133	T	T	T
0.1666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.1672741420044943	0.5831646652604618	0.3135923642777811	T	T	T
0.0833619012194262	0.6667473783060700	0.2265086803491130	T	T	T
0.2500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.2453472173373896	0.5051337393490343	0.4018659331492316	T	T	T
0.4166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.4170507258680729	0.5829492741319271	0.3150509123953000	T	T	T
0.3334810759071019	0.6665189240928981	0.2264569271644135	T	T	T
0.5000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.6666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.6669087799295426	0.5822345443142609	0.3150741242097652	T	T	T
0.5835092340745618	0.6668174109403253	0.2273348266002699	T	T	T
0.7500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.7570098097791984	0.4921863840069562	0.4016279289584972	T	T	T
0.9166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.9167293996858135	0.5832714110987496	0.3137666708655260	T	T	T
0.8332428373778313	0.6667420411159952	0.2269724845206511	T	T	T
0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.0077922145333886	0.7429829552061236	0.4016282669515263	T	T	T
0.1666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
0.1669501251266894	0.8330498748733106	0.3136376915038355	T	T	T
0.0832091450480448	0.9167908549519552	0.2269333078127502	T	T	T
0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.2512914366103374	0.7487085633896626	0.4005281639275182	T	T	T
0.4166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
0.4168353347395382	0.8327258579955057	0.3135923642777811	T	T	T
0.3332526216939300	0.9166380987805667	0.2265086803491130	T	T	T
0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.4948662606509657	0.7546527826626104	0.4018659331492316	T	T	T
0.6666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
0.6667002836017772	0.8333468059704288	0.3146131871864668	T	T	T

	0.5834981474678074	0.9164864330462450	0.2265093801078208	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.9166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.9177566608191015	0.8330951367895594	0.3150745505088963	T	T	T
	0.8331657497744445	0.9164843816165202	0.2273389169732027	T	T	T
	0.2511405465255336	0.2488597560481622	0.4162530704388914	T	T	T
	0.7511402439518378	0.7488594534744664	0.4162530704388914	T	T	T
	0.0011735553605021	0.9988264446394979	0.4211511591735402	T	T	T
	0.5011718573788713	0.4988281426211287	0.4211555323522447	T	T	T
4Ni/Cu(111)	1.0000000000000000					
	8.8905944857135406	-5.1329871195825199	-0.0000000000000010			
	0.0000000000000000	10.2659742391650006	0.0000000000000010			
	0.0000000000000000	0.0000000000000000	23.3821328661704015			
	Ni	Cu				
	4	76				
	Selective dynamics					
	Direct					
	0.0004645857279471	0.9995354142720529	0.3796462180270765	T	T	T
	0.2504645857279471	0.2495354142720529	0.3796462180270765	T	T	T
	0.5004645857279471	0.4995354142720529	0.3796462180270765	T	T	T
	0.7504645857279471	0.7495354142720529	0.3796462180270765	T	T	T
	0.0000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.1666666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.1663676545796733	0.0836323454203267	0.2939784658163305	T	T	T
	0.0831619554158465	0.1668380445841535	0.2044464745961321	T	T	T
	0.2500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.2480238361591276	0.0019761638408724	0.3834443634198337	T	T	T
	0.4166666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.4163940672573290	0.0836059327426710	0.2945965615355703	T	T	T
	0.3332665353743067	0.1667334646256933	0.2048154381846317	T	T	T
	0.5000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.5000357693976980	0.9999642306023020	0.3829812488833610	T	T	T
	0.6666666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.6668758405699009	0.0831241594300991	0.2945641909867760	T	T	T
	0.5832364154065388	0.1667635845934612	0.2051561558820012	T	T	T
	0.7500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.7523635550462018	0.9976364449537982	0.3831490130339859	T	T	T
	0.9166666667000030	0.083333332999970	0.0259047434999999	F	F	F
	0.9168786523772567	0.0831213476227433	0.2939514479829128	T	T	T
	0.8332996115289362	0.1667003884710638	0.2051082605118495	T	T	T
	0.0000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
	0.0023635550462018	0.2476364449537982	0.3831490130339859	T	T	T
	0.1666666667000030	0.333333332999970	0.0259047434999999	F	F	F
	0.1668786523772567	0.3331213476227433	0.2939514479829128	T	T	T
	0.0832996115289362	0.4167003884710638	0.2051082605118495	T	T	T
	0.2500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
	0.4166666667000030	0.333333332999970	0.0259047434999999	F	F	F
	0.4163676545796733	0.3336323454203267	0.2939784658163305	T	T	T
	0.3331619554158465	0.4168380445841535	0.2044464745961321	T	T	T
	0.5000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
	0.4980238361591276	0.2519761638408724	0.3834443634198337	T	T	T

	0.666666667000030	0.333333332999970	0.0259047434999999	F	F	F
	0.6663940672573290	0.3336059327426710	0.2945965615355703	T	T	T
	0.5832665353743067	0.4167334646256933	0.2048154381846317	T	T	T
	0.7500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
	0.7500357693976980	0.2499642306023020	0.3829812488833610	T	T	T
	0.916666667000030	0.333333332999970	0.0259047434999999	F	F	F
	0.9168758405699009	0.3331241594300991	0.2945641909867760	T	T	T
	0.8332364154065388	0.4167635845934612	0.2051561558820012	T	T	T
	0.0000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.0000357693976980	0.4999642306023020	0.3829812488833610	T	T	T
	0.166666667000030	0.583333332999970	0.0259047434999999	F	F	F
	0.1668758405699009	0.5831241594300991	0.2945641909867760	T	T	T
	0.0832364154065388	0.6667635845934612	0.2051561558820012	T	T	T
	0.2500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.2523635550462018	0.4976364449537982	0.3831490130339859	T	T	T
	0.416666667000030	0.583333332999970	0.0259047434999999	F	F	F
	0.4168786523772567	0.5831213476227433	0.2939514479829128	T	T	T
	0.3332996115289362	0.6667003884710638	0.2051082605118495	T	T	T
	0.5000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.666666667000030	0.583333332999970	0.0259047434999999	F	F	F
	0.6663676545796733	0.5836323454203267	0.2939784658163305	T	T	T
	0.5831619554158465	0.6668380445841535	0.2044464745961321	T	T	T
	0.7500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.7480238361591205	0.5019761638408724	0.3834443634198337	T	T	T
	0.916666667000030	0.583333332999970	0.0259047434999999	F	F	F
	0.9163940672573290	0.5836059327426710	0.2945965615355703	T	T	T
	0.8332665353743067	0.6667334646256933	0.2048154381846317	T	T	T
	0.0000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.9980238361591276	0.7519761638408724	0.3834443634198337	T	T	T
	0.166666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.1663940672573290	0.8336059327426710	0.2945965615355703	T	T	T
	0.0832665353743067	0.9167334646256933	0.2048154381846317	T	T	T
	0.2500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.2500357693976980	0.7499642306023020	0.3829812488833610	T	T	T
	0.416666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.4168758405699009	0.8331241594300991	0.2945641909867760	T	T	T
	0.3332364154065388	0.9167635845934612	0.2051561558820012	T	T	T
	0.5000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.5023635550462018	0.7476364449537982	0.3831490130339859	T	T	T
	0.666666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.6668786523772567	0.8331213476227433	0.2939514479829128	T	T	T
	0.5832996115289362	0.9167003884710638	0.2051082605118495	T	T	T
	0.7500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.916666667000030	0.833333332999970	0.0259047434999999	F	F	F
	0.9163676545796733	0.8336323454203267	0.2939784658163305	T	T	T
	0.8331619554158465	0.9168380445841535	0.2044464745961321	T	T	T
4Pd/Cu(111)	1.0000000000000000					
	8.8905944857135406	-5.1329871195825199	-0.0000000000000010			
	0.0000000000000000	10.2659742391650006	0.0000000000000010			
	0.0000000000000000	0.0000000000000000	23.3821328661704015			
	Pd	Cu				

Selective dynamics

Direct

0.0002070325746075	0.9997929674253925	0.3875316522478442	T	T	T
0.2502070325746075	0.2497929674253925	0.3875316522478442	T	T	T
0.5002070325746075	0.4997929674253925	0.3875316522478442	T	T	T
0.7502070325746075	0.7497929674253925	0.3875316522478442	T	T	T
0.0000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.1666666667000030	0.083333332999970	0.0259047434999999	F	F	F
0.1668678595280042	0.0831321404719958	0.2942521739017181	T	T	T
0.0831830103186704	0.1668169896813225	0.2048498335366773	T	T	T
0.2500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.2533100657368834	0.9966899342631166	0.3840136037513702	T	T	T
0.4166666667000030	0.083333332999970	0.0259047434999999	F	F	F
0.4165796440762080	0.0834203559237920	0.2940518386311552	T	T	T
0.3331476742860318	0.1668523257139682	0.2049408729932836	T	T	T
0.5000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.5000149864186696	0.9999850135813304	0.3827545867510906	T	T	T
0.6666666667000030	0.083333332999970	0.0259047434999999	F	F	F
0.6666236419075204	0.0833763580924796	0.2939705982810281	T	T	T
0.5832721424322571	0.1667278575677429	0.2048454248633291	T	T	T
0.7500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.7468573351808487	0.0031426648191513	0.3841283353929512	T	T	T
0.9166666667000030	0.083333332999970	0.0259047434999999	F	F	F
0.9164366206325028	0.0835633793674972	0.2945133705127816	T	T	T
0.8335574644153780	0.1664425355846220	0.2050725407500948	T	T	T
0.0000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.9968573351808487	0.2531426648191513	0.3841283353929512	T	T	T
0.1666666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.1664366206325028	0.3335633793674972	0.2945133705127816	T	T	T
0.0835574644153780	0.4164425355846220	0.2050725407500948	T	T	T
0.2500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.4166666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.4168678595280042	0.3331321404719958	0.2942521739017181	T	T	T
0.3331830103186704	0.4168169896813296	0.2048498335366773	T	T	T
0.5000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.5033100657368834	0.2466899342631166	0.3840136037513702	T	T	T
0.6666666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.6665796440762080	0.3334203559237920	0.2940518386311552	T	T	T
0.5831476742860318	0.4168523257139682	0.2049408729932836	T	T	T
0.7500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.7500149864186696	0.2499850135813304	0.3827545867510906	T	T	T
0.9166666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.9166236419075204	0.3333763580924796	0.2939705982810281	T	T	T
0.8332721424322571	0.4167278575677429	0.2048454248633291	T	T	T
0.0000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.0000149864186696	0.4999850135813304	0.3827545867510906	T	T	T
0.1666666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.1666236419075204	0.5833763580924796	0.2939705982810281	T	T	T
0.0832721424322571	0.6667278575677429	0.2048454248633291	T	T	T
0.2500000000000000	0.5000000000000000	0.1155258754999977	F	F	F

	0.2468573351808487	0.5031426648191513	0.3841283353929512	T	T	T
	0.4166666667000030	0.5833333332999970	0.0259047434999999	F	F	F
	0.4164366206325028	0.5835633793674972	0.2945133705127816	T	T	T
	0.3335574644153780	0.6664425355846220	0.2050725407500948	T	T	T
	0.5000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.6666666667000030	0.5833333332999970	0.0259047434999999	F	F	F
	0.6668678595280042	0.5831321404719958	0.2942521739017181	T	T	T
	0.5831830103186775	0.6668169896813225	0.2048498335366773	T	T	T
	0.7500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
	0.7533100657368834	0.4966899342631166	0.3840136037513702	T	T	T
	0.9166666667000030	0.5833333332999970	0.0259047434999999	F	F	F
	0.9165796440762080	0.5834203559237920	0.2940518386311552	T	T	T
	0.8331476742860318	0.6668523257139682	0.2049408729932836	T	T	T
	0.0000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.0033100657368834	0.7466899342631166	0.3840136037513702	T	T	T
	0.1666666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.1665796440762080	0.8334203559237920	0.2940518386311552	T	T	T
	0.0831476742860318	0.9168523257139682	0.2049408729932836	T	T	T
	0.2500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.2500149864186696	0.7499850135813304	0.3827545867510906	T	T	T
	0.4166666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.4166236419075204	0.8333763580924796	0.2939705982810281	T	T	T
	0.3332721424322571	0.9167278575677429	0.2048454248633291	T	T	T
	0.5000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.4968573351808487	0.7531426648191513	0.3841283353929512	T	T	T
	0.6666666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.6664366206325028	0.8335633793674972	0.2945133705127816	T	T	T
	0.5835574644153780	0.9164425355846220	0.2050725407500948	T	T	T
	0.7500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
	0.9166666667000030	0.8333333332999970	0.0259047434999999	F	F	F
	0.9168678595280042	0.8331321404719958	0.2942521739017181	T	T	T
	0.8331830103186775	0.9168169896813225	0.2048498335366773	T	T	T
4Pt/Cu(111)	1.0000000000000000					
	8.8905944857135406	-5.1329871195825199	-0.0000000000000010			
	0.0000000000000000	10.2659742391650006	0.0000000000000010			
	0.0000000000000000	0.0000000000000000	23.3821328661704015			
	Pt	Cu				
	4	76				
	Selective dynamics					
	Direct					
	0.0000225041513957	0.9999774958486043	0.3864342135986405	T	T	T
	0.2500225041513957	0.2499774958486043	0.3864342135986405	T	T	T
	0.5000225041513957	0.4999774958486043	0.3864342135986405	T	T	T
	0.7500225041513957	0.7499774958486043	0.3864342135986405	T	T	T
	0.0000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.1666666667000030	0.0833333332999970	0.0259047434999999	F	F	F
	0.1672008876086011	0.0827991123913989	0.2935327648435191	T	T	T
	0.0831882399830945	0.1668117600169055	0.2045786274443060	T	T	T
	0.2500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
	0.2525384034348193	0.9974615965651807	0.3852451994304644	T	T	T
	0.4166666667000030	0.0833333332999970	0.0259047434999999	F	F	F

0.4169399312630446	0.0830600687369554	0.2943595467013154	T	T	T
0.3333493063726749	0.1666506936273251	0.2048510746785084	T	T	T
0.5000000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.4999081136270718	0.0000918863729282	0.3829471490224208	T	T	T
0.6666666667000030	0.083333332999970	0.0259047434999999	F	F	F
0.6667445100230651	0.0832554899769278	0.2945084884830891	T	T	T
0.5834093468317363	0.1665906531682637	0.2050298626573337	T	T	T
0.7500000000000000	0.0000000000000000	0.1155258754999977	F	F	F
0.7473533643276582	0.0026466356723418	0.3852627328984681	T	T	T
0.9166666667000030	0.083333332999970	0.0259047434999999	F	F	F
0.9157354707709402	0.0842645292290598	0.2938471574666082	T	T	T
0.8334832746064080	0.1665167253935920	0.2051638597581444	T	T	T
0.0000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.9973533643276582	0.2526466356723418	0.3852627328984681	T	T	T
0.1666666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.1657354707709402	0.3342645292290598	0.2938471574666082	T	T	T
0.0834832746064080	0.4165167253935920	0.2051638597581444	T	T	T
0.2500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.4166666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.4172008876086011	0.3327991123913989	0.2935327648435191	T	T	T
0.3331882399830945	0.4168117600169055	0.2045786274443060	T	T	T
0.5000000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.5025384034348193	0.2474615965651807	0.3852451994304644	T	T	T
0.6666666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.6669399312630446	0.3330600687369554	0.2943595467013154	T	T	T
0.5833493063726749	0.4166506936273251	0.2048510746785084	T	T	T
0.7500000000000000	0.2500000000000000	0.1155258754999977	F	F	F
0.7499081136270718	0.2500918863729282	0.3829471490224208	T	T	T
0.9166666667000030	0.333333332999970	0.0259047434999999	F	F	F
0.9167445100230651	0.3332554899769278	0.2945084884830891	T	T	T
0.8334093468317363	0.4165906531682637	0.2050298626573337	T	T	T
0.0000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.9999081136270718	0.5000918863729282	0.3829471490224208	T	T	T
0.1666666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.1667445100230722	0.5832554899769349	0.2945084884830891	T	T	T
0.0834093468317363	0.6665906531682637	0.2050298626573337	T	T	T
0.2500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.2473533643276582	0.5026466356723418	0.3852627328984681	T	T	T
0.4166666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.4157354707709402	0.5842645292290598	0.2938471574666082	T	T	T
0.3334832746064080	0.6665167253935920	0.2051638597581444	T	T	T
0.5000000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.6666666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.6672008876086011	0.5827991123913989	0.2935327648435191	T	T	T
0.5831882399830945	0.6668117600169055	0.2045786274443060	T	T	T
0.7500000000000000	0.5000000000000000	0.1155258754999977	F	F	F
0.7525384034348193	0.4974615965651807	0.3852451994304644	T	T	T
0.9166666667000030	0.583333332999970	0.0259047434999999	F	F	F
0.9169399312630446	0.5830600687369554	0.2943595467013154	T	T	T
0.8333493063726749	0.6666506936273251	0.2048510746785084	T	T	T
0.0000000000000000	0.7500000000000000	0.1155258754999977	F	F	F

0.0025384034348193	0.7474615965651807	0.3852451994304644	T	T	T
0.1666666667000030	0.8333333332999970	0.0259047434999999	F	F	F
0.1669399312630446	0.8330600687369554	0.2943595467013154	T	T	T
0.0833493063726749	0.9166506936273251	0.2048510746785084	T	T	T
0.2500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
0.2499081136270718	0.7500918863729282	0.3829471490224208	T	T	T
0.4166666667000030	0.8333333332999970	0.0259047434999999	F	F	F
0.4167445100230722	0.8332554899769349	0.2945084884830891	T	T	T
0.3334093468317363	0.9165906531682637	0.2050298626573337	T	T	T
0.5000000000000000	0.7500000000000000	0.1155258754999977	F	F	F
0.4973533643276582	0.7526466356723418	0.3852627328984681	T	T	T
0.6666666667000030	0.8333333332999970	0.0259047434999999	F	F	F
0.6657354707709402	0.8342645292290598	0.2938471574666082	T	T	T
0.5834832746064080	0.9165167253935920	0.2051638597581444	T	T	T
0.7500000000000000	0.7500000000000000	0.1155258754999977	F	F	F
0.9166666667000030	0.8333333332999970	0.0259047434999999	F	F	F
0.9172008876086011	0.8327991123913989	0.2935327648435191	T	T	T
0.8331882399830945	0.9168117600169055	0.2045786274443060	T	T	T

(5) CO on Ni(111)

H site	1.0000000000000000				
	8.6223998537762103	-4.9781448766382903	0.0000000000000000		
	0.0000000000000000	9.9562897532765700	0.0000000000000000		
	0.0000000000000000	0.0000000000000000	23.1292765422759992		
Ni	C	O			
80	1	1			
Selective dynamics					
Direct					
0.0000000000000000	0.0000000000000000	0.1392871528000015	F	F	F
0.0003085258439878	0.0003040982147022	0.4011839662790347	T	T	T
0.1666666667000030	0.0833333332999970	0.0514193316000018	F	F	F
0.1674603584114005	0.0845898317215415	0.3148000695601521	T	T	T
0.0836658823950914	0.1667017002843181	0.2269004930242483	T	T	T
0.2500000000000000	0.0000000000000000	0.1392871528000015	F	F	F
0.2501047281781654	0.0001588527367800	0.4010587874785840	T	T	T
0.4166666667000030	0.0833333332999970	0.0514193316000018	F	F	F
0.4163498069604268	0.0836332980360884	0.3144068005415658	T	T	T
0.3332990342168900	0.1666375055099730	0.2268655379660180	T	T	T
0.5000000000000000	0.0000000000000000	0.1392871528000015	F	F	F
0.5000838928007141	0.0002496056046575	0.4011877634801267	T	T	T
0.6666666667000030	0.0833333332999970	0.0514193316000018	F	F	F
0.6671070023514216	0.0837039925029889	0.3144622347427874	T	T	T
0.5835160186959855	0.1669441994056080	0.2268486433173246	T	T	T
0.7500000000000000	0.0000000000000000	0.1392871528000015	F	F	F
0.7501782624379185	0.0000472374519430	0.4011030594439894	T	T	T
0.9166666667000030	0.0833333332999970	0.0514193316000018	F	F	F
0.9172256182297372	0.0836984878767860	0.3144586893879229	T	T	T
0.8334708326497329	0.1667638771358290	0.2268279360324035	T	T	T
0.0000000000000000	0.2500000000000000	0.1392871528000015	F	F	F
0.9969158567066817	0.2485886377841611	0.4008123296282297	T	T	T
0.1666666667000030	0.3333333332999970	0.0514193316000018	F	F	F
0.1670715828877576	0.3335472144046744	0.3144903906775910	T	T	T

0.0836560320118300	0.4169707119587311	0.2269069511343460	T	T	T
0.2500000000000000	0.2500000000000000	0.1392871528000015	F	F	F
0.2500891426733121	0.2502403640731389	0.4044009524881065	T	T	T
0.4166666667000030	0.3333333332999970	0.0514193316000018	F	F	F
0.4166031982747523	0.3334870136884074	0.3146025014355674	T	T	T
0.3334173298604406	0.4167248993743195	0.2270067468073984	T	T	T
0.5000000000000000	0.2500000000000000	0.1392871528000015	F	F	F
0.5018710703759232	0.2486990079390022	0.4007935767436281	T	T	T
0.6666666667000030	0.3333333332999970	0.0514193316000018	F	F	F
0.6667864241619932	0.3336952584265704	0.3142878068844195	T	T	T
0.5838253421920376	0.4170204755990252	0.2269445039066254	T	T	T
0.7500000000000000	0.2500000000000000	0.1392871528000015	F	F	F
0.7503582444787096	0.2504908299279875	0.4011243464029333	T	T	T
0.9166666667000030	0.3333333332999970	0.0514193316000018	F	F	F
0.9172553405964019	0.3336639234593171	0.3144502288700969	T	T	T
0.8334992902327516	0.4168530898691774	0.2268821689898793	T	T	T
0.0000000000000000	0.5000000000000000	0.1392871528000015	F	F	F
0.0003911832245259	0.5003086744685313	0.4011874604265657	T	T	T
0.1666666667000030	0.5833333332999970	0.0514193316000018	F	F	F
0.1674691741437096	0.5829417770512340	0.3148187458952791	T	T	T
0.0832743235427313	0.6670847063407759	0.2268094336357513	T	T	T
0.2500000000000000	0.5000000000000000	0.1392871528000015	F	F	F
0.2501633355287233	0.5001371832390251	0.4044266384478780	T	T	T
0.4166666667000030	0.5833333332999970	0.0514193316000018	F	F	F
0.4165913247070453	0.5831973399071910	0.3145845249715361	T	T	T
0.3332815522237855	0.6666631281226825	0.2268752063739642	T	T	T
0.5000000000000000	0.5000000000000000	0.1392871528000015	F	F	F
0.5000886978065828	0.5002926484867891	0.4044041825565597	T	T	T
0.6666666667000030	0.5833333332999970	0.0514193316000018	F	F	F
0.6660612953937016	0.5830895083641000	0.3149330665608447	T	T	T
0.5838306558886207	0.6668492010929430	0.2269510684985122	T	T	T
0.7500000000000000	0.5000000000000000	0.1392871528000015	F	F	F
0.7500606998480892	0.5001130474256892	0.4010922728997549	T	T	T
0.9166666667000030	0.5833333332999970	0.0514193316000018	F	F	F
0.9168662624202548	0.5836673852636093	0.3145999197949620	T	T	T
0.8338351572006849	0.6669437632047606	0.2268015960475475	T	T	T
0.0000000000000000	0.7500000000000000	0.1392871528000015	F	F	F
0.0001498022764466	0.7501595603116942	0.4011324045014079	T	T	T
0.1666666667000030	0.8333333332999970	0.0514193316000018	F	F	F
0.1667019791463426	0.8333644186525409	0.3144720298269676	T	T	T
0.0832610657389435	0.9161988466421127	0.2268056423237709	T	T	T
0.2500000000000000	0.7500000000000000	0.1392871528000015	F	F	F
0.2501277424068957	0.7501080400134467	0.4010749940447151	T	T	T
0.4166666667000030	0.8333333332999970	0.0514193316000018	F	F	F
0.4163257281287752	0.8328528331433516	0.3144054880915002	T	T	T
0.3332610492505905	0.9166608637845615	0.2268747910006475	T	T	T
0.5000000000000000	0.7500000000000000	0.1392871528000015	F	F	F
0.5018678300199161	0.7534611492127687	0.4007682631261614	T	T	T
0.6666666667000030	0.8333333332999970	0.0514193316000018	F	F	F
0.6667142452058075	0.8332644500590823	0.3142902681954497	T	T	T
0.5835232673823576	0.9167102497831505	0.2268453090877786	T	T	T

	0.7500000000000000	0.7500000000000000	0.1392871528000015	F	F	F
	0.7500973933493090	0.7501109474478381	0.4010724015497569	T	T	T
	0.9166666667000030	0.833333332999970	0.0514193316000018	F	F	F
	0.9167822923170652	0.8333852124735946	0.3145894883794225	T	T	T
	0.8334540553193198	0.9167163693301127	0.2268761463934017	T	T	T
	0.3336525155812761	0.4169127914702696	0.4612205599421416	T	T	T
	0.3338883481720632	0.4170057114465083	0.5129048405136966	T	T	T
B site	1.0000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni	C	O			
	80	1	1			
	Selective dynamics					
	Direct					
	0.0000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	-0.0001649196693644	0.0001621278942759	0.4012251582437920	T	T	T
	0.1666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.1673404484707858	0.0843874733646996	0.3149176357687001	T	T	T
	0.0838402547856818	0.1669521308723550	0.2270357677724400	T	T	T
	0.2500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.2490694491419920	-0.0016871301785902	0.4010816073588300	T	T	T
	0.4166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.4165699335920648	0.0838939028201064	0.3146838286113933	T	T	T
	0.3331918487815049	0.1664376421753893	0.2268347871366264	T	T	T
	0.5000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.4999680263615886	0.0000429938304666	0.4013497397633756	T	T	T
	0.6666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.6668612523206106	0.0836248403033710	0.3146272449857651	T	T	T
	0.5835113805990711	0.1670027848397977	0.2269767791128453	T	T	T
	0.7500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.7499739808133682	-0.0000549391416629	0.4011838918813284	T	T	T
	0.9166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.9171490864671120	0.0837653534575366	0.3145470313724874	T	T	T
	0.8334288465175131	0.1667300669947963	0.2268768878108280	T	T	T
	0.0000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	-0.0016621877883438	0.2492779900977925	0.4010915467116627	T	T	T
	0.1666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.1671939105972299	0.3333220415430207	0.3147205812349059	T	T	T
	0.0833531083916001	0.4169126958684942	0.2267927698556303	T	T	T
	0.2500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.2500715360973304	0.2500344181121359	0.4044605350512065	T	T	T
	0.4166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.4165827722852398	0.3330336707240129	0.3141438011486002	T	T	T
	0.3334020632042214	0.4168089472279294	0.2270047412928984	T	T	T
	0.5000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.5011936260121084	0.2487027162997131	0.4018864215455276	T	T	T
	0.6666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.6664746175768110	0.3334295476202354	0.3147770311234944	T	T	T
	0.5841572329046438	0.4171487995063166	0.2269889816250653	T	T	T
	0.7500000000000000	0.2500000000000000	0.1392870000000030	F	F	F

	0.7499907548738539	0.2499735606561722	0.4012701149126481	T	T	T
	0.9166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.9171204609798153	0.3334195691934350	0.3146107445919354	T	T	T
	0.8334618033265827	0.4167843631681281	0.2269857919675245	T	T	T
	0.0000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	-0.0000850965217380	0.5000523826187668	0.4014644374542776	T	T	T
	0.1666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.1674167901779143	0.5828546073106939	0.3147828150398440	T	T	T
	0.0838261635824130	0.6669910332269209	0.2271982846496779	T	T	T
	0.2500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.2485895222525563	0.5013091771851121	0.4019499798907525	T	T	T
	0.4166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.4168314422411798	0.5829166076577693	0.3147668072817855	T	T	T
	0.3333907175676010	0.6667894417382684	0.2267457019395617	T	T	T
	0.5000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.4994220580369594	0.4993767640990139	0.4047282132154806	T	T	T
	0.6666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.6656377148558889	0.5827179869684743	0.3150277332620540	T	T	T
	0.5837655229112975	0.6668641971805643	0.2270488978570055	T	T	T
	0.7500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.7515378210246895	0.5007345485160259	0.4011227386869406	T	T	T
	0.9166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.9163808835009611	0.5834382230264296	0.3146427998865845	T	T	T
	0.8341103272646558	0.6671044597078105	0.2267634233598131	T	T	T
	0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	-0.0003744693624817	0.7500717500440893	0.4013147445739175	T	T	T
	0.1666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.1666730085961786	0.8335488210655522	0.3146848688918903	T	T	T
	0.0831704242155864	0.9160687163450887	0.2267985619508648	T	T	T
	0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.2499505203274082	0.7500784750839198	0.4012603289783728	T	T	T
	0.4166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.4164475471139457	0.8329047990191540	0.3145132944934341	T	T	T
	0.3332795020607289	0.9166852510557164	0.2269715410581690	T	T	T
	0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.5004812772696663	0.7516501354495397	0.4010391331015508	T	T	T
	0.6666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.6666409454215991	0.8332276318127262	0.3144566461358603	T	T	T
	0.5834880647462386	0.9167492288837376	0.2269002448959374	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.7493512203180581	0.7498164621226586	0.4011636839015778	T	T	T
	0.9166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.9164403030181150	0.8331990590052626	0.3146212734102345	T	T	T
	0.8334518541970142	0.9167724050593037	0.2268942616346698	T	T	T
	0.3748783429171649	0.3737530988479459	0.4653944009764563	T	T	T
	0.3745618070756778	0.3731897984790886	0.5166970587119520	T	T	T
OT site	1.0000000000000000					
	8.6223998537762103	-4.9781448766382903	0.0000000000000000			
	0.0000000000000000	9.9562897532765700	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292765422759992			
	Ni	C	O			

80 1 1
Selective dynamics
Direct

0.0000000000000000	0.0000000000000000	0.1392871528000015	F F F
0.9976305941872888	0.9976664163418595	0.4009746324369091	T T T
0.1666666667000030	0.0833333329999970	0.0514193316000018	F F F
0.1674426406055249	0.0848112671617005	0.3150572415854060	T T T
0.0837490379975934	0.1670887795676547	0.2271380847187862	T T T
0.2500000000000000	0.0000000000000000	0.1392871528000015	F F F
0.2499594384290260	0.9974629384891166	0.4010730534150235	T T T
0.4166666667000030	0.0833333329999970	0.0514193316000018	F F F
0.4162530798723718	0.0834087992732327	0.3145229351091870	T T T
0.3333041755129623	0.1666721222879796	0.2271201719853001	T T T
0.5000000000000000	0.0000000000000000	0.1392871528000015	F F F
0.5001765893834922	0.9996483357010588	0.4012104215268267	T T T
0.6666666667000030	0.0833333329999970	0.0514193316000018	F F F
0.6668579190066547	0.0835129128701518	0.3144546462791960	T T T
0.5832191530524689	0.1666402172446379	0.2268712904358679	T T T
0.7500000000000000	0.0000000000000000	0.1392871528000015	F F F
0.7491947783423774	0.9994947855168674	0.4011376478356291	T T T
0.9166666667000030	0.0833333329999970	0.0514193316000018	F F F
0.9168304658154363	0.0836094131517904	0.3145311828818397	T T T
0.8333497481164447	0.1666398754027570	0.2268175299736766	T T T
0.0000000000000000	0.2500000000000000	0.1392871528000015	F F F
0.9974763580813455	0.2498772869793782	0.4011187146492142	T T T
0.1666666667000030	0.3333333329999970	0.0514193316000018	F F F
0.1672270987172396	0.3326795174916412	0.3152784111364555	T T T
0.0830724347505088	0.4168767334348277	0.2266632772228334	T T T
0.2500000000000000	0.2500000000000000	0.1392871528000015	F F F
0.2498113140270779	0.2497667278667259	0.4063519887086403	T T T
0.4166666667000030	0.3333333329999970	0.0514193316000018	F F F
0.4149776324068739	0.3324682730444028	0.3151477094911423	T T T
0.3329278508072919	0.4162429275569984	0.2271531682971589	T T T
0.5000000000000000	0.2500000000000000	0.1392871528000015	F F F
0.5023059590950495	0.2498154970144044	0.4010803783423401	T T T
0.6666666667000030	0.3333333329999970	0.0514193316000018	F F F
0.6659573704519699	0.3331831346250940	0.3144443491697216	T T T
0.5837449940305121	0.4168063150567156	0.2266877717422044	T T T
0.7500000000000000	0.2500000000000000	0.1392871528000015	F F F
0.7499092129319546	0.2498967875696181	0.4010938944279430	T T T
0.9166666667000030	0.3333333329999970	0.0514193316000018	F F F
0.9171877787057694	0.3330700080979138	0.3145446451335056	T T T
0.8329852603770534	0.4163675678711660	0.2271161346287869	T T T
0.0000000000000000	0.5000000000000000	0.1392871528000015	F F F
0.9997939778811857	0.5001335035812587	0.4012943182761723	T T T
0.1666666667000030	0.5833333329999970	0.0514193316000018	F F F
0.1668494579900586	0.5826786078721797	0.3145629114387481	T T T
0.0833902957181160	0.6667838267599606	0.2270974586688794	T T T
0.2500000000000000	0.5000000000000000	0.1392871528000015	F F F
0.2500873288289157	0.5023817195484200	0.4011289166362821	T T T
0.4166666667000030	0.5833333329999970	0.0514193316000018	F F F

	0.4163423449795710	0.5831020809762317	0.3145278125712837	T	T	T
	0.3333161305677985	0.6666218594481760	0.2268234321711273	T	T	T
	0.5000000000000000	0.5000000000000000	0.1392871528000015	F	F	F
	0.5021217951328188	0.5021555301761348	0.4009828066831594	T	T	T
	0.6666666667000030	0.5833333332999970	0.0514193316000018	F	F	F
	0.6661491505183424	0.5825971004541497	0.3145508429430318	T	T	T
	0.5832979566058217	0.6666201909384595	0.2268816181176103	T	T	T
	0.7500000000000000	0.5000000000000000	0.1392871528000015	F	F	F
	0.7503774509779011	0.5000418724205035	0.4011765233286474	T	T	T
	0.9166666667000030	0.5833333332999970	0.0514193316000018	F	F	F
	0.9165053803125839	0.5831622974705081	0.3146753494233001	T	T	T
	0.8333179577444638	0.6666719662887882	0.2271273349779054	T	T	T
	0.0000000000000000	0.7500000000000000	0.1392871528000015	F	F	F
	0.9996502130176506	0.7493100504647304	0.4011816439826785	T	T	T
	0.1666666667000030	0.8333333332999970	0.0514193316000018	F	F	F
	0.1665723650450330	0.8337185821163504	0.3144193236300128	T	T	T
	0.0831474319219672	0.9162454574677950	0.2266689972762592	T	T	T
	0.2500000000000000	0.7500000000000000	0.1392871528000015	F	F	F
	0.2499987608373894	0.7499966506744477	0.4010952520519264	T	T	T
	0.4166666667000030	0.8333333332999970	0.0514193316000018	F	F	F
	0.4163810723131949	0.8330062048673791	0.3144575549854667	T	T	T
	0.3331277623689012	0.9165630816047430	0.2268591947860880	T	T	T
	0.5000000000000000	0.7500000000000000	0.1392871528000015	F	F	F
	0.5003181173608533	0.7505564418872921	0.4011301315401662	T	T	T
	0.6666666667000030	0.8333333332999970	0.0514193316000018	F	F	F
	0.6666639392657930	0.8333181841381254	0.3143548123199044	T	T	T
	0.5833915064004522	0.9165567113394418	0.2268621928319390	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392871528000015	F	F	F
	0.7499093907359053	0.7499224138915760	0.4010754106964522	T	T	T
	0.9166666667000030	0.8333333332999970	0.0514193316000018	F	F	F
	0.9172720401899472	0.8337084277208465	0.3145244754362540	T	T	T
	0.8333620104501130	0.9167061310549077	0.2268819959962314	T	T	T
	0.2475057428593794	0.2465190208665286	0.4814495287960560	T	T	T
	0.2461507798526811	0.2446502816676871	0.5317334715172586	T	T	T
(6) CO on Cu(111)						
H site	1.0000000000000000					
	8.8905908144889398	-5.1329849999999997	0.0000000000000000			
	0.0000000000000000	10.2659699999999994	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.3821300000000001			
	C	Cu	O			
	1	80	1			
	Selective dynamics					
	Direct					
	0.5832955118651555	0.4169812614836236	0.4450020229025375	T	T	T
	0.0000000000000000	0.0000000000000000	0.1155260000000027	F	F	F
	0.9999317220351617	0.0002072545345966	0.3819490681939098	T	T	T
	0.1666669999999968	0.0833330000000032	0.0259050000000016	F	F	F
	0.1668573067811472	0.0832988444439329	0.2930624947515530	T	T	T
	0.0834186609041711	0.1667888942714026	0.2044723254176546	T	T	T
	0.2500000000000000	0.0000000000000000	0.1155260000000027	F	F	F
	0.2495658584091355	-0.0001641958485809	0.3821252972267242	T	T	T

0.416666999999968	0.083333000000032	0.025905000000016	F	F	F
0.4177301422224905	0.0856349513160878	0.2941465216376458	T	T	T
0.3331551349622195	0.1664638445204624	0.2043566127640461	T	T	T
0.5000000000000000	0.0000000000000000	0.1155260000000027	F	F	F
0.4999699899122078	-0.0001342783435895	0.3821379763797930	T	T	T
0.666666999999968	0.083333000000032	0.025905000000016	F	F	F
0.6662727888537971	0.0833168071135492	0.2930644675819989	T	T	T
0.5831927893090865	0.1664695393822767	0.2043493686490352	T	T	T
0.7500000000000000	0.0000000000000000	0.1155260000000027	F	F	F
0.7499953677875849	0.0002448128575794	0.3819388033107644	T	T	T
0.916666999999968	0.083333000000032	0.025905000000016	F	F	F
0.9166393374930595	0.0834440434434195	0.2934049624022028	T	T	T
0.8332597201072320	0.1667928223837111	0.2044814283916929	T	T	T
0.0000000000000000	0.2500000000000000	0.1155260000000027	F	F	F
-0.0001037136457084	0.2501381088242114	0.3819382988662284	T	T	T
0.166666999999968	0.333333000000032	0.025905000000016	F	F	F
0.1668403624003630	0.3338198300974876	0.2930521586559990	T	T	T
0.0833622652416577	0.4168636770290801	0.2043641193419086	T	T	T
0.2500000000000000	0.2500000000000000	0.1155260000000027	F	F	F
0.2473355136685324	0.2489034901127204	0.3814932519106503	T	T	T
0.416666999999968	0.333333000000032	0.025905000000016	F	F	F
0.4171797580294833	0.3337335696636844	0.2930775676453926	T	T	T
0.3331578545252762	0.4168650392306464	0.2043462234077106	T	T	T
0.5000000000000000	0.2500000000000000	0.1155260000000027	F	F	F
0.4993908453928866	0.2491603400241844	0.3851556663296735	T	T	T
0.666666999999968	0.333333000000032	0.025905000000016	F	F	F
0.6663499225731705	0.3337425103382884	0.2930755200493788	T	T	T
0.5833057979335845	0.4167448821844532	0.2042831410080359	T	T	T
0.7500000000000000	0.2500000000000000	0.1155260000000027	F	F	F
0.7512119405829181	0.2489306127636473	0.3815058066369257	T	T	T
0.916666999999968	0.333333000000032	0.025905000000016	F	F	F
0.9167700981878539	0.3338143127917624	0.2930631514014373	T	T	T
0.8335811520909050	0.4168587065172313	0.2043478247330338	T	T	T
0.0000000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.0002731757598016	0.5001626881536675	0.3821355392063515	T	T	T
0.166666999999968	0.583333000000032	0.025905000000016	F	F	F
0.1667660499328158	0.5837423834385380	0.2931685013116884	T	T	T
0.0827740627678801	0.6664751016447674	0.2047036897630317	T	T	T
0.2500000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.2495348613591326	0.5001725587055352	0.3821170460023179	T	T	T
0.416666999999968	0.583333000000032	0.025905000000016	F	F	F
0.4177062840011068	0.5823833773020846	0.2941350173835195	T	T	T
0.3335619383352303	0.6664893457531983	0.2047018199817023	T	T	T
0.5000000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.4993835521606914	0.5007733986602930	0.3851317030430482	T	T	T
0.666666999999968	0.583333000000032	0.025905000000016	F	F	F
0.6663585084161910	0.5829146866736737	0.2930739423809016	T	T	T
0.5831877512350858	0.6668970346461144	0.2043451412286064	T	T	T
0.7500000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.7510147818151144	0.5007827277255429	0.3851459969002898	T	T	T
0.916666999999968	0.583333000000032	0.025905000000016	F	F	F

	0.9144615770640645	0.5823649134610340	0.2941430983448117	T	T	T
	0.8335893595436364	0.6669000589112223	0.2043530930036282	T	T	T
	0.0000000000000000	0.7500000000000000	0.1155260000000027	F	F	F
	0.0003193795697458	0.7505855552726411	0.3821209682604897	T	T	T
	0.1666669999999968	0.8333330000000032	0.0259050000000016	F	F	F
	0.1667892365405755	0.8333106665684933	0.2931669158400935	T	T	T
	0.0833715290556116	0.9166806043274038	0.2043651108744315	T	T	T
	0.2500000000000000	0.7500000000000000	0.1155260000000027	F	F	F
	0.2499415788276573	0.7501974579307390	0.3821417450873755	T	T	T
	0.4166669999999968	0.8333330000000032	0.0259050000000016	F	F	F
	0.4163435639552154	0.8333244486556143	0.2931683100539997	T	T	T
	0.3335784223280970	0.9172803766969622	0.2047030755929793	T	T	T
	0.5000000000000000	0.7500000000000000	0.1155260000000027	F	F	F
	0.4999606297350946	0.7506038276392373	0.3821161084977815	T	T	T
	0.6666669999999968	0.8333330000000032	0.0259050000000016	F	F	F
	0.6662638662940760	0.8332485472884202	0.2930505787709185	T	T	T
	0.5831879056987026	0.9166903306614748	0.2043637915727251	T	T	T
	0.7500000000000000	0.7500000000000000	0.1155260000000027	F	F	F
	0.7512431040337076	0.7528211710905456	0.3814890795864271	T	T	T
	0.9166669999999968	0.8333330000000032	0.0259050000000016	F	F	F
	0.9167899418148705	0.8332313486120433	0.2930599123620830	T	T	T
	0.8332653372446314	0.9166383829737443	0.2044709733192838	T	T	T
	0.5831929178464907	0.4171304320854400	0.4956606335412757	T	T	T
B site	1.0000000000000000					
	8.8905908144889398	-5.1329849999999997	0.0000000000000000			
	0.0000000000000000	10.2659699999999994	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.3821300000000001			
	C	Cu	O			
	1	80	1			
	Selective dynamics					
	Direct					
	0.6294658675029290	0.5090596288703030	0.4490659627220569	T	T	T
	0.0000000000000000	0.0000000000000000	0.1155260000000027	F	F	F
	0.0005275350615778	0.0005869729133775	0.3821510271438652	T	T	T
	0.1666669999999968	0.8333330000000032	0.0259050000000016	F	F	F
	0.1665547724329059	0.0831083829106335	0.2930726172760093	T	T	T
	0.0834355699333384	0.1665961416047951	0.2044223834243772	T	T	T
	0.2500000000000000	0.0000000000000000	0.1155260000000027	F	F	F
	0.2494026617449038	0.9993953129530845	0.3820025958311157	T	T	T
	0.4166669999999968	0.8333330000000032	0.0259050000000016	F	F	F
	0.4167404026427769	0.0834783331950133	0.2932498611270756	T	T	T
	0.3333390010376733	0.1666712302175935	0.2045859595098481	T	T	T
	0.5000000000000000	0.0000000000000000	0.1155260000000027	F	F	F
	0.5000050145131886	0.9994277838626163	0.3820142408836341	T	T	T
	0.6666669999999968	0.8333330000000032	0.0259050000000016	F	F	F
	0.6665679117364761	0.0831080541950635	0.2930710746740481	T	T	T
	0.5833224749272844	0.1666618013962981	0.2045819507804674	T	T	T
	0.7500000000000000	0.0000000000000000	0.1155260000000027	F	F	F
	0.7500612570994473	0.0006055811976294	0.3821494902244375	T	T	T
	0.9166669999999968	0.8333330000000032	0.0259050000000016	F	F	F
	0.9167338398323526	0.0834631918619761	0.2934318416347656	T	T	T

0.8331536836422485	0.1665949451625227	0.2044265189501690	T	T	T
0.0000000000000000	0.2500000000000000	0.1155260000000027	F	F	F
0.0000397351864566	0.2500787699432870	0.3821040837940775	T	T	T
0.1666669999999968	0.3333330000000032	0.0259050000000016	F	F	F
0.1667584270258387	0.3334644648906767	0.2932361797660814	T	T	T
0.0832645924521117	0.4165334095577478	0.2044239052922413	T	T	T
0.2500000000000000	0.2500000000000000	0.1155260000000027	F	F	F
0.2489604865116098	0.2492972696924051	0.3819427962392640	T	T	T
0.4166669999999968	0.3333330000000032	0.0259050000000016	F	F	F
0.4178196123407927	0.3343627685294373	0.2937401884142513	T	T	T
0.3332280286939123	0.4165481672217757	0.2046208062832237	T	T	T
0.5000000000000000	0.2500000000000000	0.1155260000000027	F	F	F
0.4980697531476696	0.2461459589367277	0.3824048750668099	T	T	T
0.6666669999999968	0.3333330000000032	0.0259050000000016	F	F	F
0.6665543931124946	0.3343605642926591	0.2937432969644298	T	T	T
0.5831215912877206	0.4162523833731355	0.2041219298939352	T	T	T
0.7500000000000000	0.2500000000000000	0.1155260000000027	F	F	F
0.7503348483719466	0.2493113732856219	0.3819485295791810	T	T	T
0.9166669999999968	0.3333330000000032	0.0259050000000016	F	F	F
0.9167140851948504	0.3334569169043759	0.2932407616797588	T	T	T
0.8333175768369828	0.4165399978507556	0.2046211787255714	T	T	T
0.0000000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.0001821622245059	0.4998806672104766	0.3822953717133199	T	T	T
0.1666669999999968	0.5833330000000032	0.0259050000000016	F	F	F
0.1666094232548231	0.5831992718043522	0.2932281450047033	T	T	T
0.0826807726222522	0.6661376608505140	0.2047556834641581	T	T	T
0.2500000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.2496804099316552	0.4998769005904277	0.3822928818587302	T	T	T
0.4166669999999968	0.5833330000000032	0.0259050000000016	F	F	F
0.4180182871081906	0.5824746448997268	0.2941272381146466	T	T	T
0.3334567262221687	0.6661508122540923	0.2047537001675875	T	T	T
0.5000000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.4988981702024740	0.5001710419000247	0.3850586930263333	T	T	T
0.6666669999999968	0.5833330000000032	0.0259050000000016	F	F	F
0.6666697669789768	0.5833038727753121	0.2919438622677979	T	T	T
0.5830459148800892	0.6667981468474968	0.2040310429971600	T	T	T
0.7500000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.7512424978942902	0.5001788331352127	0.3850648334888766	T	T	T
0.9166669999999968	0.5833330000000032	0.0259050000000016	F	F	F
0.9144661666032102	0.5824706582470554	0.2941262105917877	T	T	T
0.8337547917694946	0.6668052226460423	0.2040220474594186	T	T	T
0.0000000000000000	0.7500000000000000	0.1155260000000027	F	F	F
0.0013107385057210	0.7508860894507950	0.3820297653578933	T	T	T
0.1666669999999968	0.8333330000000032	0.0259050000000016	F	F	F
0.1667348208496994	0.8330252204474710	0.2930247283578512	T	T	T
0.0829020807978681	0.9162234069401157	0.2044986976441657	T	T	T
0.2500000000000000	0.7500000000000000	0.1155260000000027	F	F	F
0.2499131796208039	0.7498244450079922	0.3820540168197498	T	T	T
0.4166669999999968	0.8333330000000032	0.0259050000000016	F	F	F
0.4163065116606621	0.8330259447418064	0.2930318243090722	T	T	T
0.3332920341302237	0.9165756062428893	0.2041895259030898	T	T	T

	0.5000000000000000 0.7500000000000000 0.1155260000000027 F F F
	0.4995743092533374 0.7508886532652430 0.3820371407081929 T T T
	0.6666669999999968 0.8333330000000032 0.0259050000000016 F F F
	0.6664435217633266 0.8324051845454439 0.2934378006911622 T T T
	0.5833115199511828 0.9162188312568766 0.2044992195488179 T T T
	0.7500000000000000 0.7500000000000000 0.1155260000000027 F F F
	0.7516070599494571 0.7532122039700874 0.3826040966503975 T T T
	0.9166669999999968 0.8333330000000032 0.0259050000000016 F F F
	0.9159753688030179 0.8324093523066746 0.2934462337547242 T T T
	0.8333020655881515 0.9166101482391281 0.2046754412205885 T T T
	0.6305332724341021 0.5111231591369602 0.4993922614864493 T T T
OT site	1.0000000000000000 8.8905908144889398 -5.1329849999999997 0.0000000000000000 0.0000000000000000 10.2659699999999994 0.0000000000000000 0.0000000000000000 0.0000000000000000 23.3821300000000001 C Cu O 1 80 1 Selective dynamics Direct 0.4992018534997938 0.4984570510709422 0.4660919846744054 T T T 0.0000000000000000 0.0000000000000000 0.1155260000000027 F F F 0.9999643683502265 -0.0000492256828297 0.3819900285438395 T T T 0.1666669999999968 0.0833330000000032 0.0259050000000016 F F F 0.1667228371091960 0.0832330036970940 0.2929456772681963 T T T 0.0835758432760530 0.1669345726912513 0.2044869113149860 T T T 0.2500000000000000 0.0000000000000000 0.1155260000000027 F F F 0.2497318506697336 0.9994740298398377 0.3818074262145784 T T T 0.4166669999999968 0.0833330000000032 0.0259050000000016 F F F 0.4164996443121675 0.0832338672291938 0.2929445889713928 T T T 0.3337482518596478 0.1675135166735753 0.2047267012828938 T T T 0.5000000000000000 0.0000000000000000 0.1155260000000027 F F F 0.4999732799402704 -0.0000481895417297 0.3819879739073242 T T T 0.6666669999999968 0.0833330000000032 0.0259050000000016 F F F 0.6666403517214277 0.0833028569832850 0.2931582547654385 T T T 0.5833403854834149 0.1669348589898652 0.2044862170011512 T T T 0.7500000000000000 0.0000000000000000 0.1155260000000027 F F F 0.7503311991768389 0.0006778497350464 0.3820681081953495 T T T 0.9166669999999968 0.0833330000000032 0.0259050000000016 F F F 0.9166525054724216 0.0833030403758578 0.2931588775956268 T T T 0.8333158785181256 0.1666509042329297 0.2043207626109815 T T T 0.0000000000000000 0.2500000000000000 0.1155260000000027 F F F 0.9992600641321518 0.2496116815892529 0.3820679831136499 T T T 0.1666669999999968 0.3333330000000032 0.0259050000000016 F F F 0.1671115183461719 0.3335395818348827 0.2932813953620876 T T T 0.0835768118024928 0.4166294484318678 0.2044851577321382 T T T 0.2500000000000000 0.2500000000000000 0.1155260000000027 F F F 0.2471343182019319 0.2473870980879123 0.3817181509080387 T T T 0.4166669999999968 0.3333330000000032 0.0259050000000016 F F F 0.4175778497547744 0.3351662849497204 0.2943507572507000 T T T 0.3335674362519597 0.4167819475252338 0.2044320637620967 T T T 0.5000000000000000 0.2500000000000000 0.1155260000000027 F F F

0.5002372123125185	0.2473964415377242	0.3817155129190438	T	T	T
0.6666669999999968	0.3333330000000032	0.0259050000000016	F	F	F
0.6664203362273126	0.3335406194500259	0.2932806452495351	T	T	T
0.5831962876864444	0.4167823761675885	0.2044321544252374	T	T	T
0.7500000000000000	0.2500000000000000	0.1155260000000027	F	F	F
0.7503360873424133	0.2496116395319180	0.3820673541801981	T	T	T
0.9166669999999968	0.3333330000000032	0.0259050000000016	F	F	F
0.9166528485688483	0.3333150863385422	0.2931553317752971	T	T	T
0.8330344933189606	0.4166300116558090	0.2044849518447122	T	T	T
0.0000000000000000	0.5000000000000000	0.1155260000000027	F	F	F
-0.0000226424288447	0.4999701597137435	0.3819881683732978	T	T	T
0.1666669999999968	0.5833330000000032	0.0259050000000016	F	F	F
0.1667234633490841	0.5834510078408501	0.2929465520625115	T	T	T
0.0832958450851871	0.6666086975642865	0.2041472247361275	T	T	T
0.2500000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.2471707601769901	0.4997072333287286	0.3817244040597899	T	T	T
0.4166669999999968	0.5833330000000032	0.0259050000000016	F	F	F
0.4175893017823911	0.5823563258204730	0.2943744125913052	T	T	T
0.3337527881686111	0.6662197749557217	0.2047365503396348	T	T	T
0.5000000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.4999642967875632	0.4999492995147166	0.3869469425744673	T	T	T
0.6666669999999968	0.5833330000000032	0.0259050000000016	F	F	F
0.6647517405765053	0.5823533098998938	0.2943758077198463	T	T	T
0.5831933985665031	0.6664045398629916	0.2044373232550389	T	T	T
0.7500000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.7525229583926434	0.4997144019250775	0.3817239960302892	T	T	T
0.9166669999999968	0.5833330000000032	0.0259050000000016	F	F	F
0.9167213162731596	0.5834545081460163	0.2929458689801947	T	T	T
0.8324475912223703	0.6662186217410481	0.2047375679915600	T	T	T
0.0000000000000000	0.7500000000000000	0.1155260000000027	F	F	F
0.0004566905933605	0.7502061071373106	0.3818082379768443	T	T	T
0.1666669999999968	0.8333330000000032	0.0259050000000016	F	F	F
0.1666478300953391	0.8333004057263029	0.2928352174355526	T	T	T
0.0832976784467449	0.9166751387377939	0.2041491349341931	T	T	T
0.2500000000000000	0.7500000000000000	0.1155260000000027	F	F	F
0.2497406425574502	0.7502051302300619	0.3818082568383281	T	T	T
0.4166669999999968	0.8333330000000032	0.0259050000000016	F	F	F
0.4165059755381499	0.8332316160371588	0.2929461534943237	T	T	T
0.3333604117119047	0.9166752587736228	0.2041489597485078	T	T	T
0.5000000000000000	0.7500000000000000	0.1155260000000027	F	F	F
0.5002501425212849	0.7527513868731751	0.3817240178282266	T	T	T
0.6666669999999968	0.8333330000000032	0.0259050000000016	F	F	F
0.6664238631238822	0.8328551162026737	0.2932795963519766	T	T	T
0.5833389989103193	0.9163917904982000	0.2044842763360958	T	T	T
0.7500000000000000	0.7500000000000000	0.1155260000000027	F	F	F
0.7524975917806451	0.7527553035855654	0.3817240107414863	T	T	T
0.9166669999999968	0.8333330000000032	0.0259050000000016	F	F	F
0.9167204423627044	0.8332329149617947	0.2929469352959077	T	T	T
0.8330346530503253	0.9163914821908289	0.2044847766587485	T	T	T
0.4988625467875422	0.4977544158334596	0.5155840014525463	T	T	T

(7) CO Pd(111)

H site	1.000000000000000			
	9.6381542603135379	-5.5645909566831619	-0.00000000000000020	
	0.00000000000000000	11.1291819133663008	0.00000000000000000	
	0.00000000000000000	0.00000000000000000	24.0869389807863001	
	C Pd O			
	1 80 1			
	Selective dynamics			
	Direct			
	0.5840407028956873	0.4163750895976616	0.4605139979532620	T T T
	0.1666666667000030	0.333333332999970	0.0263705027999990	F F F
	0.00000000000000000	0.00000000000000000	0.1206844688000004	F F F
	0.3336319049959187	0.1665387044013162	0.2149386594727397	T T T
	0.1669994664619582	0.3333571672438964	0.3086967595241993	T T T
	0.0005606357164149	-0.0002457533740299	0.4032126782153926	T T T
	0.1666666667000030	0.083333332999970	0.0263705027999990	F F F
	0.00000000000000000	0.25000000000000000	0.1206844688000004	F F F
	0.3337535445396056	0.4170464380935868	0.2149035431945675	T T T
	0.1670034911436331	0.0832476218948726	0.3086106202947576	T T T
	0.0005366382602563	0.2500451454643100	0.4033230882241571	T T T
	0.4166666667000030	0.083333332999970	0.0263705027999990	F F F
	0.25000000000000000	0.25000000000000000	0.1206844688000004	F F F
	0.0836025903250119	0.4168526709172563	0.2146635881565819	T T T
	0.4175999806472990	0.0845596872319170	0.3095190422073242	T T T
	0.2464390882999653	0.2477982379793616	0.4034831462725027	T T T
	0.4166666667000030	0.333333332999970	0.0263705027999990	F F F
	0.25000000000000000	0.00000000000000000	0.1206844688000004	F F F
	0.0835889381898291	0.1667771690862087	0.2146364114875670	T T T
	0.4171860911848373	0.3333826652184717	0.3098830173157863	T T T
	0.2504982938695641	-0.0001246280943821	0.4034456206438755	T T T
	0.6666666667000030	0.333333332999970	0.0263705027999990	F F F
	0.50000000000000000	0.00000000000000000	0.1206844688000004	F F F
	0.8333531490524561	0.1667012398317782	0.2147677848285582	T T T
	0.6667778600828503	0.3333387475902124	0.3097783055721033	T T T
	0.5004128290536860	-0.0002550504286775	0.4033921987169277	T T T
	0.6666666667000030	0.083333332999970	0.0263705027999990	F F F
	0.50000000000000000	0.25000000000000000	0.1206844688000004	F F F
	0.8336948530036893	0.4170597222697678	0.2148653344718304	T T T
	0.6668515019581092	0.0832203954744252	0.3086436539558303	T T T
	0.4997216567257083	0.2481030305771449	0.4076884329160385	T T T
	0.9166666667000030	0.083333332999970	0.0263705027999990	F F F
	0.75000000000000000	0.25000000000000000	0.1206844688000004	F F F
	0.5834932601762127	0.4166267644433655	0.2153047038074230	T T T
	0.9169235098947300	0.0832647226948035	0.3086762985148160	T T T
	0.7524335676903137	0.2478076103012644	0.4034335971220245	T T T
	0.9166666667000030	0.333333332999970	0.0263705027999990	F F F
	0.75000000000000000	0.00000000000000000	0.1206844688000004	F F F
	0.5830546417374530	0.1664320901501565	0.2148561545480289	T T T
	0.9169785795589375	0.3333670182755343	0.3086476947496663	T T T
	0.7502658035466521	-0.0002826114756370	0.4033202456333536	T T T
	0.1666666667000030	0.833333332999970	0.0263705027999990	F F F
	0.00000000000000000	0.50000000000000000	0.1206844688000004	F F F

	0.3332517844756150 0.6667879673946894 0.2147364039662499 T T T
	0.1668166640587556 0.8332732058735223 0.3088239491827812 T T T
	0.0005366192560807 0.4999044483702691 0.4034026202827029 T T T
	0.1666666667000030 0.5833333332999970 0.0263705027999990 F F F
	0.0000000000000000 0.7500000000000000 0.1206844688000004 F F F
	0.3331472922867003 0.9161122464824618 0.2145448149349369 T T T
	0.1669045952639960 0.5832049798564033 0.3088257595114843 T T T
	0.0004771472400370 0.7498427706480890 0.4034390271831912 T T T
	0.4166666667000030 0.5833333332999970 0.0263705027999990 F F F
	0.2500000000000000 0.7500000000000000 0.1206844688000004 F F F
	0.0835042746276182 0.9165301533168314 0.2146515252117512 T T T
	0.4176028166446101 0.5825602202349592 0.3096708453825980 T T T
	0.2504714220481851 0.7498580410434389 0.4034936903999738 T T T
	0.4166666667000030 0.8333333332999970 0.0263705027999990 F F F
	0.2500000000000000 0.5000000000000000 0.1206844688000004 F F F
	0.0839799312403942 0.6669427377859786 0.2145475952082778 T T T
	0.4169618582112439 0.8332856403263995 0.3088030243141980 T T T
	0.2505217547167885 0.4998465419907653 0.4035291537563555 T T T
	0.6666666667000030 0.8333333332999970 0.0263705027999990 F F F
	0.5000000000000000 0.5000000000000000 0.1206844688000004 F F F
	0.8335368836939476 0.6664309948584898 0.2149383137356439 T T T
	0.6667802115004865 0.8331625005335219 0.3086993899391032 T T T
	0.4997698320830287 0.5004189903564353 0.4077485963730184 T T T
	0.6666666667000030 0.5833333332999970 0.0263705027999990 F F F
	0.5000000000000000 0.7500000000000000 0.1206844688000004 F F F
	0.8332898770927365 0.9164847136712817 0.2146353117452145 T T T
	0.6668351851808940 0.5829980954355773 0.3098752765249654 T T T
	0.5004002397818411 0.7497257656384202 0.4035255814825658 T T T
	0.9166666667000030 0.5833333332999970 0.0263705027999990 F F F
	0.7500000000000000 0.7500000000000000 0.1206844688000004 F F F
	0.5832275928232870 0.9164927012035945 0.2146555262687293 T T T
	0.9156376886395833 0.5825835954536955 0.3095181336380993 T T T
	0.7524916803437928 0.7538320944808679 0.4034790545459201 T T T
	0.9166666667000030 0.8333333332999970 0.0263705027999990 F F F
	0.7500000000000000 0.5000000000000000 0.1206844688000004 F F F
	0.5830480833546671 0.6663536357453995 0.2149079908963154 T T T
	0.9169183571383985 0.8331819667935149 0.3086197639475451 T T T
	0.7521261302136584 0.5005776845500601 0.4076614920739882 T T T
	0.5841928988938316 0.4163137754931563 0.5100940488639714 T T T
OT site	1.0000000000000000 9.6381542603135379 -5.5645909566831619 -0.0000000000000020 0.0000000000000000 11.1291819133663008 0.0000000000000000 0.0000000000000000 0.0000000000000000 24.0869389807863001 C Pd O 1 80 1 Selective dynamics Direct 0.4997889760339228 0.4976391539079697 0.4855653161529060 T T T 0.1666666667000030 0.3333333332999970 0.0263705027999990 F F F 0.0000000000000000 0.0000000000000000 0.1206844688000004 F F F 0.3333265130638182 0.1666455617108639 0.2146944474896079 T T T

0.1666038672812816	0.3332943296357426	0.3089849220197655	T	T	T
-0.0000315360879688	0.0000499055180683	0.4032097168669262	T	T	T
0.1666666667000030	0.0833333332999970	0.0263705027999990	F	F	F
0.0000000000000000	0.2500000000000000	0.1206844688000004	F	F	F
0.3337891554445818	0.4168837997589802	0.2154227082643649	T	T	T
0.1670783448245160	0.0839420441501169	0.3087307399006289	T	T	T
-0.0004777203421632	0.2497530400061113	0.4035079595067769	T	T	T
0.4166666667000030	0.0833333332999970	0.0263705027999990	F	F	F
0.2500000000000000	0.2500000000000000	0.1206844688000004	F	F	F
0.0834498246866565	0.4166171348195547	0.2147102596123505	T	T	T
0.4168745749049106	0.0839448424998011	0.3087342387261305	T	T	T
0.2472081677810280	0.2470618573957681	0.4038057022058419	T	T	T
0.4166666667000030	0.3333333332999970	0.0263705027999990	F	F	F
0.2500000000000000	0.0000000000000000	0.1206844688000004	F	F	F
0.0834541366629262	0.1667940876607588	0.2147136541066024	T	T	T
0.4173626349611578	0.3347314121458155	0.3104693599576462	T	T	T
0.2496935043964242	-0.0006140345572870	0.4034371356379068	T	T	T
0.6666666667000030	0.3333333332999970	0.0263705027999990	F	F	F
0.5000000000000000	0.0000000000000000	0.1206844688000004	F	F	F
0.8333276241304733	0.1666711972430267	0.2147748967589508	T	T	T
0.6667009432671551	0.3333099250101569	0.3089860629183837	T	T	T
0.5000958239906980	0.0000651105112290	0.4032084022983684	T	T	T
0.6666666667000030	0.0833333332999970	0.0263705027999990	F	F	F
0.5000000000000000	0.2500000000000000	0.1206844688000004	F	F	F
0.8331777796547494	0.4166179357738251	0.2147107406458590	T	T	T
0.6666258244956277	0.0832988477474560	0.3087298055986004	T	T	T
0.4998318867192104	0.2470378237996860	0.4038092125677157	T	T	T
0.9166666667000030	0.0833333332999970	0.0263705027999990	F	F	F
0.7500000000000000	0.2500000000000000	0.1206844688000004	F	F	F
0.5831006197256569	0.4168873605088049	0.2154186278924754	T	T	T
0.9166846858734942	0.0832998521380566	0.3087313612612949	T	T	T
0.7502356817749084	0.2497498507281679	0.4035076863715891	T	T	T
0.9166666667000030	0.3333333332999970	0.0263705027999990	F	F	F
0.7500000000000000	0.0000000000000000	0.1206844688000004	F	F	F
0.5833574351691170	0.1667981663765456	0.2147132576625181	T	T	T
0.9166819997417979	0.3333510939491512	0.3087263810187226	T	T	T
0.7502176592256895	0.0004372061790285	0.4035005561107595	T	T	T
0.1666666667000030	0.8333333332999970	0.0263705027999990	F	F	F
0.0000000000000000	0.5000000000000000	0.1206844688000004	F	F	F
0.3333604506044400	0.6666357707851821	0.2147284560258248	T	T	T
0.1666658651416382	0.8332915892265661	0.3087930469359039	T	T	T
-0.0000632904614420	0.4998858409364659	0.4032063335032597	T	T	T
0.1666666667000030	0.5833333332999970	0.0263705027999990	F	F	F
0.0000000000000000	0.7500000000000000	0.1206844688000004	F	F	F
0.3333755810473492	0.9166560593988333	0.2147950325589086	T	T	T
0.1671125752217502	0.5830883365286975	0.3087361329736504	T	T	T
0.0005911470856479	0.7502898959114104	0.4034400582450746	T	T	T
0.4166666667000030	0.5833333332999970	0.0263705027999990	F	F	F
0.2500000000000000	0.7500000000000000	0.1206844688000004	F	F	F
0.0833125524404864	0.9166657499930251	0.2147973684531831	T	T	T
0.4174651191982057	0.5825353416569009	0.3105463716582116	T	T	T

	0.2497019337126371	0.7502882161546864	0.4034461422078602	T	T	T
	0.4166666667000030	0.8333333332999970	0.0263705027999990	F	F	F
	0.2500000000000000	0.5000000000000000	0.1206844688000004	F	F	F
	0.0833153009473592	0.6665936145969802	0.2147903186767314	T	T	T
	0.4168975188962947	0.8328835594575732	0.3087335616576564	T	T	T
	0.2472154980242333	0.5001632814063472	0.4038167042365586	T	T	T
	0.6666666667000030	0.8333333332999970	0.0263705027999990	F	F	F
	0.5000000000000000	0.5000000000000000	0.1206844688000004	F	F	F
	0.8333050177056242	0.6666421376259219	0.2147034224972998	T	T	T
	0.6666987021423170	0.8333715941902808	0.3089823404153001	T	T	T
	0.4999989864615945	0.4999392301931621	0.4086766244512867	T	T	T
	0.6666666667000030	0.5833333332999970	0.0263705027999990	F	F	F
	0.5000000000000000	0.7500000000000000	0.1206844688000004	F	F	F
	0.8331822328015956	0.9165271496831943	0.2147138382033642	T	T	T
	0.6651715412140773	0.5825738151882788	0.3105105105000748	T	T	T
	0.4998363940331527	0.7527594264700245	0.4038123210412618	T	T	T
	0.9166666667000030	0.5833333332999970	0.0263705027999990	F	F	F
	0.7500000000000000	0.7500000000000000	0.1206844688000004	F	F	F
	0.5833634698701690	0.9165306774643945	0.2147134094615953	T	T	T
	0.9160185191494326	0.5830955828362392	0.3087360510766162	T	T	T
	0.7529248096619605	0.7527678051239184	0.4038089806891553	T	T	T
	0.9166666667000030	0.8333333332999970	0.0263705027999990	F	F	F
	0.7500000000000000	0.5000000000000000	0.1206844688000004	F	F	F
	0.5831052241886926	0.6661908335943312	0.2154173853878939	T	T	T
	0.9160347785885649	0.8329041870108391	0.3087314009910831	T	T	T
	0.7529649786231937	0.5001649258599978	0.4038154106330321	T	T	T
	0.4996535534377358	0.4964293161862561	0.5336522649843588	T	T	T

(8) CO on Pt(111)

H site	1.0000000000000000					
	9.7149212688523594	-5.6089124097279299	0.0000000000000000			
	0.0000000000000000	11.2178248194559007	-0.0000000000000020			
	0.0000000000000000	0.0000000000000000	24.1593156105318982			
	C	Pt	O			
	1	80	1			
	Selective dynamics					
	Direct					
	0.5835731573031097	0.4161306510202992	0.4900286049669446	T	T	T
	0.1666666667000030	0.3333333332999970	0.0528360781000003	F	F	F
	0.0000000000000000	0.0000000000000000	0.1476164493000027	F	F	F
	0.3337600748893678	0.1666655156451672	0.2415270162902090	T	T	T
	0.1671545860519863	0.3335611222543053	0.3350658026098350	T	T	T
	0.0004732361303684	-0.0006375019264734	0.4310900783871529	T	T	T
	0.1666666667000030	0.0833333332999970	0.0528360781000003	F	F	F
	0.0000000000000000	0.2500000000000000	0.1476164493000027	F	F	F
	0.3337730095015804	0.4170520560296917	0.2415444586969708	T	T	T
	0.1671329111370092	0.0832338313080015	0.3350426084637385	T	T	T
	0.0003679964179608	0.2499081914616785	0.4310741092550978	T	T	T
	0.4166666667000030	0.0833333332999970	0.0528360781000003	F	F	F
	0.2500000000000000	0.2500000000000000	0.1476164493000027	F	F	F
	0.0834616273586755	0.4168463774295494	0.2414749611038239	T	T	T
	0.4179616451004543	0.0855999918851912	0.3361352878718453	T	T	T

0.2450503236254450	0.2469349596066322	0.4307189646314868	T	T	T
0.4166666667000030	0.3333333332999970	0.0528360781000003	F	F	F
0.2500000000000000	0.0000000000000000	0.1476164493000027	F	F	F
0.0835748278151082	0.1667818778531588	0.2413856849013344	T	T	T
0.4175359619151263	0.3335628944784676	0.3365349563146500	T	T	T
0.2503556847905317	-0.0005880907579142	0.4310069420142590	T	T	T
0.6666666667000030	0.3333333332999970	0.0528360781000003	F	F	F
0.5000000000000000	0.0000000000000000	0.1476164493000027	F	F	F
0.8332352320406994	0.1667600436504947	0.2413745780155756	T	T	T
0.6664035550811287	0.3335650203510239	0.3364849140614994	T	T	T
0.5001496567173287	-0.0004911069112289	0.4309871132173703	T	T	T
0.6666666667000030	0.0833333332999970	0.0528360781000003	F	F	F
0.5000000000000000	0.2500000000000000	0.1476164493000027	F	F	F
0.8333364365512541	0.4170775575964855	0.2415383047934453	T	T	T
0.6664123107346294	0.0831933000155799	0.3350307329760328	T	T	T
0.4986231996176370	0.2465732116751531	0.4356805348549943	T	T	T
0.9166666667000030	0.0833333332999970	0.0528360781000003	F	F	F
0.7500000000000000	0.2500000000000000	0.1476164493000027	F	F	F
0.5833492665014165	0.4166595925851708	0.2421860722438527	T	T	T
0.9167695567499939	0.0832083642715346	0.3352578859651801	T	T	T
0.7527354013741493	0.2470799238083229	0.4306582925656870	T	T	T
0.9166666667000030	0.3333333332999970	0.0528360781000003	F	F	F
0.7500000000000000	0.0000000000000000	0.1476164493000027	F	F	F
0.5829321104856113	0.1666650617903276	0.2415378335343613	T	T	T
0.9167496826539261	0.3335295166949087	0.3350275219296120	T	T	T
0.7499109254882400	-0.0005583521205504	0.4310843799377108	T	T	T
0.1666666667000030	0.8333333332999970	0.0528360781000003	F	F	F
0.0000000000000000	0.5000000000000000	0.1476164493000027	F	F	F
0.3332399762723807	0.6667683719145381	0.2413382909621572	T	T	T
0.1668572566107250	0.8330599744700723	0.3351658336973610	T	T	T
0.0002467099886485	0.4997019566341152	0.4309880043288516	T	T	T
0.1666666667000030	0.5833333332999970	0.0528360781000003	F	F	F
0.0000000000000000	0.7500000000000000	0.1476164493000027	F	F	F
0.3331947853155197	0.9162991971544383	0.2412947311672860	T	T	T
0.1669670780020731	0.5833505939802620	0.3351886903404696	T	T	T
0.0002801855575103	0.7493699487373829	0.4310251792051223	T	T	T
0.4166666667000030	0.5833333332999970	0.0528360781000003	F	F	F
0.2500000000000000	0.7500000000000000	0.1476164493000027	F	F	F
0.0834636090583243	0.9165403621781985	0.2414786336445905	T	T	T
0.4181088355760819	0.5818497663349688	0.3362221799720452	T	T	T
0.2503078068941582	0.7494986690433172	0.4311430908151174	T	T	T
0.4166666667000030	0.8333333332999970	0.0528360781000003	F	F	F
0.2500000000000000	0.5000000000000000	0.1476164493000027	F	F	F
0.0837091156046727	0.6668049156977147	0.2412989643431958	T	T	T
0.4165750223350880	0.8329803884122037	0.3351907196005109	T	T	T
0.2503399701437594	0.4996422816756859	0.4310886219507631	T	T	T
0.6666666667000030	0.8333333332999970	0.0528360781000003	F	F	F
0.5000000000000000	0.5000000000000000	0.1476164493000027	F	F	F
0.8333420989767957	0.6662544747743558	0.2415277744974482	T	T	T
0.6663929929668055	0.8327905759415470	0.3350712565655102	T	T	T
0.4986584472391897	0.5010652643886975	0.4358992189758655	T	T	T

	0.666666667000030 0.583333332999970 0.0528360781000003 F F F
	0.500000000000000 0.750000000000000 0.1476164493000027 F F F
	0.8332289819512084 0.9164307108941518 0.2413933696346369 T T T
	0.6664315488723987 0.5824669374406383 0.3365457638662285 T T T
	0.5001254067876042 0.7493667113781431 0.4310754110624935 T T T
	0.916666667000030 0.583333332999970 0.0528360781000003 F F F
	0.750000000000000 0.750000000000000 0.1476164493000027 F F F
	0.5831675576226526 0.9165350851540617 0.2414779967304858 T T T
	0.9143564826002252 0.5819954273420161 0.3361293569181432 T T T
	0.7528970232428470 0.7548264531450931 0.4307311581006333 T T T
	0.916666667000030 0.833333332999970 0.0528360781000003 F F F
	0.750000000000000 0.500000000000000 0.1476164493000027 F F F
	0.5829658680601082 0.6662300135415224 0.2415478361405134 T T T
	0.9167510812055750 0.8328340117539628 0.3350520627165106 T T T
	0.7531581619474778 0.5011468907071315 0.4356707446626842 T T T
	0.5837867464876054 0.4158583671017952 0.5395899145860444 T T T
OT site	1.000000000000000
	9.7149212688523594 -5.6089124097279299 0.000000000000000
	0.000000000000000 11.2178248194559007 -0.000000000000020
	0.000000000000000 0.000000000000000 24.1593156105318982
	C Pt O
	1 80 1
	Selective dynamics
	Direct
	0.5014296588607464 0.4985209341593655 0.5149256343444657 T T T
	0.166666667000030 0.333333332999970 0.0528360781000003 F F F
	0.000000000000000 0.000000000000000 0.1476164493000027 F F F
	0.3341904651329254 0.1684017185042602 0.2410756413978779 T T T
	0.1661279867990694 0.3330592625130167 0.3354946693627265 T T T
	0.0002360066124940 -0.0002459872663328 0.4307433500071445 T T T
	0.166666667000030 0.083333332999970 0.0528360781000003 F F F
	0.000000000000000 0.250000000000000 0.1476164493000027 F F F
	0.3344006306064702 0.4172403712213101 0.2427309609094120 T T T
	0.1677266391952936 0.0840674462592456 0.3346610657667329 T T T
	-0.0011381603281529 0.2493634615669560 0.4313025497342643 T T T
	0.416666667000030 0.083333332999970 0.0528360781000003 F F F
	0.250000000000000 0.250000000000000 0.1476164493000027 F F F
	0.0836943621144117 0.4166710031850627 0.2413013599159541 T T T
	0.4163971299668829 0.0840998607171984 0.3346383516965509 T T T
	0.2450460459742331 0.2451354377959856 0.4310206309992692 T T T
	0.416666667000030 0.333333332999970 0.0528360781000003 F F F
	0.250000000000000 0.000000000000000 0.1476164493000027 F F F
	0.0836966404825829 0.1670198352699860 0.2413005656849403 T T T
	0.4178178998702120 0.3356087168328883 0.3383319652361033 T T T
	0.2496185477579427 -0.0009060477520553 0.4309766259781860 T T T
	0.666666667000030 0.333333332999970 0.0528360781000003 F F F
	0.500000000000000 0.000000000000000 0.1476164493000027 F F F
	0.8333420759898185 0.1666609489189961 0.2414947639985307 T T T
	0.6669226329871568 0.3330724974662477 0.3354775079995372 T T T
	0.4996358139991236 -0.0002774685128336 0.4307483258087615 T T T
	0.666666667000030 0.083333332999970 0.0528360781000003 F F F

0.5000000000000000	0.2500000000000000	0.1476164493000027	F F F
0.8329804066697455	0.4166595141468060	0.2412913389036288	T T T
0.6662987021954671	0.0831448754343653	0.3351251418751001	T T T
0.5001602327102616	0.2450301363568592	0.4309904821742280	T T T
0.9166666667000030	0.0833333329999970	0.0528360781000003	F F F
0.7500000000000000	0.2500000000000000	0.1476164493000027	F F F
0.5827909116894079	0.4172094160477051	0.2427006040866245	T T T
0.9168870333494378	0.0831131284645448	0.3351231802378504	T T T
0.7506655092793576	0.2493274477494007	0.4313018054821600	T T T
0.9166666667000030	0.3333333329999970	0.0528360781000003	F F F
0.7500000000000000	0.0000000000000000	0.1476164493000027	F F F
0.5833356578121012	0.1670180187246108	0.2412914810112433	T T T
0.9168514548892038	0.3336986365469574	0.3351244532291273	T T T
0.7506253096334735	0.0011239846673414	0.4313031609574797	T T T
0.1666666667000030	0.8333333329999970	0.0528360781000003	F F F
0.0000000000000000	0.5000000000000000	0.1476164493000027	F F F
0.3342313477153657	0.6657709123145832	0.2411400815452835	T T T
0.1667094161293815	0.8332833075843463	0.3352124637416776	T T T
0.0002733460350837	0.5003578234791742	0.4307455017889766	T T T
0.1666666667000030	0.5833333329999970	0.0528360781000003	F F F
0.0000000000000000	0.7500000000000000	0.1476164493000027	F F F
0.3333113087071050	0.9166452677064394	0.2414277044716572	T T T
0.1677671538571543	0.5835634525021741	0.3346851551125725	T T T
0.0009030778461859	0.7503754358290734	0.4309811534256734	T T T
0.4166666667000030	0.5833333329999970	0.0528360781000003	F F F
0.2500000000000000	0.7500000000000000	0.1476164493000027	F F F
0.0833575562804076	0.9166693873693063	0.2414287733625649	T T T
0.4179605602547665	0.5820364288237233	0.3384733544051020	T T T
0.2496385222510677	0.7503531184145910	0.4310120345213186	T T T
0.4166666667000030	0.8333333329999970	0.0528360781000003	F F F
0.2500000000000000	0.5000000000000000	0.1476164493000027	F F F
0.0833588038533299	0.6666886782118577	0.2414275298893650	T T T
0.4164358130741131	0.8322301158411781	0.3346860947970656	T T T
0.2451202635350258	0.4997994821554791	0.4310633121358622	T T T
0.6666666667000030	0.8333333329999970	0.0528360781000003	F F F
0.5000000000000000	0.5000000000000000	0.1476164493000027	F F F
0.8316103646691748	0.6658084054857920	0.2410780611985198	T T T
0.6669409594968636	0.8338689659048950	0.3354956998555360	T T T
0.5000796780472850	0.4999047948414388	0.4387382103552376	T T T
0.6666666667000030	0.5833333329999970	0.0528360781000003	F F F
0.5000000000000000	0.7500000000000000	0.1476164493000027	F F F
0.8329837049538008	0.9163008129293989	0.2413007070464530	T T T
0.6643858056146364	0.5821767977923269	0.3383291030072096	T T T
0.5001967111561610	0.7548787095059174	0.4310661625423344	T T T
0.9166666667000030	0.5833333329999970	0.0528360781000003	F F F
0.7500000000000000	0.7500000000000000	0.1476164493000027	F F F
0.5833271203760123	0.9163044325749033	0.2413023820207311	T T T
0.9158960499658253	0.5835971287637385	0.3346413240262719	T T T
0.7548502979254342	0.7549369807987594	0.4310216728475711	T T T
0.9166666667000030	0.8333333329999970	0.0528360781000003	F F F
0.7500000000000000	0.5000000000000000	0.1476164493000027	F F F

	0.5827677929961929	0.6656025205132338	0.2427307025794282	T	T	T
	0.9159292644091644	0.8322691045352452	0.3346621337180758	T	T	T
	0.7549565212140444	0.4998305950595230	0.4309920377168659	T	T	T
	0.5024491566769353	0.4974637325559024	0.5628530622054494	T	T	T
(9) CO on nX/M(111)						
2Cu/Ni(111) ^{PC}	1.000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni	C	Cu	O		
	78	1	2	1		
	Selective dynamics					
	Direct					
	0.0000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.0002198745097119	0.9999609818084402	0.4012163595785791	T	T	T
	0.1666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.1673012787329708	0.0834659464892771	0.3141993936131457	T	T	T
	0.0836591455608749	0.1670470001775787	0.2270305860504970	T	T	T
	0.2500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.2486740129885585	0.0015774504543078	0.4006607900739575	T	T	T
	0.4166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.4166776601028080	0.0829976352693331	0.3145143067974516	T	T	T
	0.3333646483217609	0.1669680502907746	0.2266139301014776	T	T	T
	0.5000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.5006081470065661	0.0012674345558067	0.4041624233174947	T	T	T
	0.6666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.6662138709199049	0.0828250402715338	0.3147633149578338	T	T	T
	0.5835912746910228	0.1668635796993748	0.2269369230453297	T	T	T
	0.7500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.7538299966305343	0.0025630086580643	0.4010301685360669	T	T	T
	0.9166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.9167171200031947	0.0834582878598517	0.3144017778874025	T	T	T
	0.8338398635655053	0.1669588696716723	0.2267289016711946	T	T	T
	0.0000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.9981492448510617	0.2489339184426432	0.4011121694220808	T	T	T
	0.1666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.1675034400613670	0.3343612142662524	0.3150032649007438	T	T	T
	0.0836773572772435	0.4166245389929845	0.2269573048717592	T	T	T
	0.2500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.2481537280350194	0.2459695589757916	0.4010164050022245	T	T	T
	0.4166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.4168566054748099	0.3338737433603379	0.3149051039393123	T	T	T
	0.3332258981169458	0.4166728159600511	0.2271822579814007	T	T	T
	0.5000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.5008810420624170	0.2487529855366802	0.4009544449734861	T	T	T
	0.6666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.6666869262600891	0.3333960501874173	0.3143550281109451	T	T	T
	0.5833564745799825	0.4168385680521912	0.2270079721225861	T	T	T
	0.7500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.7502023953533346	0.2507429915726041	0.4011772476999268	T	T	T
	0.9166669999999968	0.3333330000000032	0.0514190000000028	F	F	F

	0.9171535864801487	0.3334656124964521	0.3144834317507041	T	T	T
	0.8334825050108876	0.4167614692121480	0.2268044718495124	T	T	T
	0.0000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.9976447592030330	0.5000079468026022	0.4007294157187016	T	T	T
	0.1666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.1678113008552651	0.5841510824581284	0.3147639562700957	T	T	T
	0.0835784960450418	0.6671519631909307	0.2267517575049569	T	T	T
	0.2500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.4166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.4170274167536163	0.5844522208328444	0.3153449278478187	T	T	T
	0.3333289673443737	0.6666631561683101	0.2269267792377540	T	T	T
	0.5000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.6666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.6663560303145484	0.5838094470252544	0.3147221754657921	T	T	T
	0.5835646388326923	0.6671312013466796	0.2270551870630548	T	T	T
	0.7500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.7522850435517783	0.5002026233882128	0.4009198992926808	T	T	T
	0.9166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.9171094204533301	0.5839791877729649	0.3140253028691745	T	T	T
	0.8334007831097489	0.6667442862202461	0.2266553876962862	T	T	T
	0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.0000955318777367	0.7498214219823979	0.4007105727587976	T	T	T
	0.1666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.1672744294052735	0.8331400611529292	0.3141908886337416	T	T	T
	0.0832886401555257	0.9171093696544672	0.2266539970534978	T	T	T
	0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.2499918198112581	0.7522029301354013	0.4037318653367213	T	T	T
	0.4166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.4166708330883782	0.8330721574045705	0.3140747065077979	T	T	T
	0.3333371203458598	0.9170620017515098	0.2268496214016004	T	T	T
	0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.5033107980070546	0.7549533232200618	0.4038445413029959	T	T	T
	0.6666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.6664690313806001	0.8332821395541896	0.3146136723457472	T	T	T
	0.5840211494650579	0.9169734812669844	0.2269754546851728	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.7525449219795874	0.7524295336088929	0.4008961356881579	T	T	T
	0.9166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.9167173923816389	0.8330949093612049	0.3142324608815111	T	T	T
	0.8338318389097265	0.9169597985748692	0.2267123535853499	T	T	T
	0.4154759043346890	0.8335903492933482	0.4607045537746863	T	T	T
	0.2485194237646984	0.4986179689004954	0.4057513685570824	T	T	T
	0.5015276867089197	0.5005195840857813	0.4058296836583096	T	T	T
	0.4140312448562484	0.8332712822150371	0.5123942017513662	T	T	T
3Cu/Ni(111) ^{PC}	1.0000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni C Cu O					
	77 1 3 1					
	Selective dynamics					

Direct			
0.0000000000000000	0.0000000000000000	0.1392870000000030	F F F
0.0016136366108401	0.0018419165279904	0.4007415147814012	T T T
0.1666669999999968	0.0833330000000032	0.0514190000000028	F F F
0.1671066372338271	0.0831822936770477	0.3140364829932297	T T T
0.0832597083230183	0.1667218846624179	0.2267833765224198	T T T
0.2500000000000000	0.0000000000000000	0.1392870000000030	F F F
0.2493688069992477	0.9999216241832053	0.4005470475152436	T T T
0.4166669999999968	0.0833330000000032	0.0514190000000028	F F F
0.4168857987327468	0.0841004308928409	0.3143005803384497	T T T
0.3333854980042719	0.1666232604024526	0.2267227995300777	T T T
0.5000000000000000	0.0000000000000000	0.1392870000000030	F F F
0.4984057878624212	0.9987680260994625	0.4004772252465882	T T T
0.6666669999999968	0.0833330000000032	0.0514190000000028	F F F
0.6664342870364545	0.0836576580896514	0.3144059130823422	T T T
0.5830507503305221	0.1662677753227141	0.2267346301682985	T T T
0.7500000000000000	0.0000000000000000	0.1392870000000030	F F F
0.7523581406006570	0.0046873962873317	0.4006808891895930	T T T
0.9166669999999968	0.0833330000000032	0.0514190000000028	F F F
0.9160177324358173	0.0829725642300947	0.3142688600121120	T T T
0.8332004947084419	0.1665829722537054	0.2267882124976954	T T T
0.0000000000000000	0.2500000000000000	0.1392870000000030	F F F
-0.0006017839058249	0.2493919808495224	0.4012499393603836	T T T
0.1666669999999968	0.3333330000000032	0.0514190000000028	F F F
0.1669085584124897	0.3332549623156855	0.3142844198815160	T T T
0.0839070409633283	0.4167524982108034	0.2267376111972439	T T T
0.2500000000000000	0.2500000000000000	0.1392870000000030	F F F
0.2469793645851531	0.2472677052289396	0.4008651559546804	T T T
0.4166669999999968	0.3333330000000032	0.0514190000000028	F F F
0.4171629537802035	0.3331532609513854	0.3148130096479350	T T T
0.3333080085819035	0.4168020791439648	0.2268850180403084	T T T
0.5000000000000000	0.2500000000000000	0.1392870000000030	F F F
0.4997598960621268	0.2480973379360983	0.4039906143222044	T T T
0.6666669999999968	0.3333330000000032	0.0514190000000028	F F F
0.6661050653180910	0.3331464434718902	0.3137056329519270	T T T
0.5829938420389998	0.4166698588388653	0.2268435836710758	T T T
0.7500000000000000	0.2500000000000000	0.1392870000000030	F F F
0.7500076841570785	0.2493107830424450	0.4039369440105470	T T T
0.9166669999999968	0.3333330000000032	0.0514190000000028	F F F
0.9156309716718228	0.3329294281595571	0.3146269768304388	T T T
0.8335439440238488	0.4167661440771954	0.2268328234657236	T T T
0.0000000000000000	0.5000000000000000	0.1392870000000030	F F F
0.0026581606631350	0.5013328879361598	0.4007482023435978	T T T
0.1666669999999968	0.5833330000000032	0.0514190000000028	F F F
0.1668614958861717	0.5835452621275975	0.3143403984919753	T T T
0.0836854783926991	0.6668177780447334	0.2265921066677408	T T T
0.2500000000000000	0.5000000000000000	0.1392870000000030	F F F
0.4166669999999968	0.5833330000000032	0.0514190000000028	F F F
0.4170704165514387	0.5831892053387994	0.3151013331157884	T T T
0.3333722185857504	0.6667441976176416	0.2272279280843648	T T T
0.5000000000000000	0.5000000000000000	0.1392870000000030	F F F

	0.666666999999968	0.583333000000032	0.051419000000028	F	F	F
	0.6664016820829671	0.5828261838586783	0.3152696007727945	T	T	T
	0.5832902077560197	0.6671199419943236	0.2272127357950570	T	T	T
	0.7500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.7514992265706729	0.4973893679725470	0.4036410525998167	T	T	T
	0.916666999999968	0.583333000000032	0.051419000000028	F	F	F
	0.9155214585748092	0.5831125869968078	0.3143819133155044	T	T	T
	0.8331980290412087	0.6666079873939573	0.2269308987600917	T	T	T
	0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.0019615540756649	0.7500001006858078	0.4006040164532195	T	T	T
	0.166666999999968	0.833333000000032	0.051419000000028	F	F	F
	0.1666840278653510	0.8334274621951162	0.3138271177617809	T	T	T
	0.0832928427770896	0.9165977753925520	0.2266588531229698	T	T	T
	0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.2476166139826009	0.7499073599062007	0.4008845788935896	T	T	T
	0.416666999999968	0.833333000000032	0.051419000000028	F	F	F
	0.4171123089078050	0.8333123380146742	0.3147203742399873	T	T	T
	0.3329844685719938	0.9162968393240474	0.2265748375368804	T	T	T
	0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.666666999999968	0.833333000000032	0.051419000000028	F	F	F
	0.6663903740229143	0.8331642616988878	0.3151421197739617	T	T	T
	0.5829148265337941	0.9159723099263236	0.2267777461110376	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.916666999999968	0.833333000000032	0.051419000000028	F	F	F
	0.9157477609247079	0.8324363324912397	0.3144575113406264	T	T	T
	0.8330503965165900	0.9163159976078752	0.2269072553091309	T	T	T
	0.2449245625560613	0.4969426305448437	0.4007790865767764	T	T	T
	0.6661791147681951	0.3319452721720029	0.4608423020067738	T	T	T
	0.4987598566525851	0.7505022703438327	0.4060544963086176	T	T	T
	0.7521757325379564	0.7509345777470073	0.4055825216774780	T	T	T
	0.4974485462267944	0.4983577716780734	0.4057275648633605	T	T	T
	0.6669256563784243	0.3313801403976782	0.5125084883303238	T	T	T
4Cu/Ni(111) ^{PC}	1.0000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni	C	Cu	O		
	76	1	4	1		
	Selective dynamics					
	Direct					
	0.0000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.0018441892787786	0.0022927205684771	0.4008085799488251	T	T	T
	0.166666999999968	0.083333000000032	0.051419000000028	F	F	F
	0.1672580567135758	0.0836748165077584	0.3140282782988363	T	T	T
	0.0834125649723829	0.1665895668142234	0.2267695905699340	T	T	T
	0.2500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.2497928632451292	0.0005277789909704	0.4008245791216293	T	T	T
	0.416666999999968	0.083333000000032	0.051419000000028	F	F	F
	0.4170569616242260	0.0843906223171719	0.3144909751338622	T	T	T
	0.3334064766169519	0.1666964093366167	0.2268268533880588	T	T	T
	0.5000000000000000	0.0000000000000000	0.1392870000000030	F	F	F

0.4987949334954771	0.9995397544631124	0.4006715484375303	T	T	T
0.6666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
0.6667470647246679	0.0841050250890468	0.3145792984249915	T	T	T
0.5832414026420217	0.1665432909376225	0.2268814402850856	T	T	T
0.7500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
0.7528819033920359	0.0054799913119540	0.4008000200346111	T	T	T
0.9166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
0.9166074195688462	0.0835075572187962	0.3141979758182336	T	T	T
0.8333343159079746	0.1667214202081604	0.2268809984958197	T	T	T
0.0000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.9984286821723268	0.2487840679312407	0.4010793885673651	T	T	T
0.1666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.1674109134710326	0.3339573392568487	0.3148347225699978	T	T	T
0.0841186891143516	0.4168590864566806	0.2269655440138571	T	T	T
0.2500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.2477722339235798	0.2453792589689963	0.4008247294725472	T	T	T
0.4166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.4175454541587797	0.3336635026493376	0.3149351690570079	T	T	T
0.3331613039015271	0.4167697600368148	0.2271009441449608	T	T	T
0.5000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.5008511753334316	0.2489850039640907	0.4043456073549436	T	T	T
0.6666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.6665477363497330	0.3337485852700273	0.3139455992376985	T	T	T
0.5832126420200352	0.4168300068710892	0.2269670958110013	T	T	T
0.7500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
0.7504832288898077	0.2501961356678936	0.4042951173253326	T	T	T
0.9166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
0.9161873593162607	0.3335589994008267	0.3147482653097161	T	T	T
0.8336219269617847	0.4168717567801492	0.2268752039489126	T	T	T
0.0000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.0016541630310290	0.5019031904041563	0.4006403914503867	T	T	T
0.1666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.1671678164862253	0.5833218480793592	0.3147075526348808	T	T	T
0.0838228852257142	0.6670445711319380	0.2265647217997049	T	T	T
0.2500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.4166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.4172856595621092	0.5835083620173995	0.3152931802723521	T	T	T
0.3333739892391123	0.6666836679478538	0.2273954417117265	T	T	T
0.5000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.6666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.6669130147567851	0.5833304709409418	0.3152176984079769	T	T	T
0.5834946906965772	0.6671685504753938	0.2272257366924913	T	T	T
0.7500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
0.7522619376109047	0.4984037862294007	0.4036876690902649	T	T	T
0.9166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
0.9161732172685821	0.5835653656083165	0.3143473246211680	T	T	T
0.8334298211944503	0.6667498581759034	0.2269821884743483	T	T	T
0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
0.0022424749405223	0.7506718860517754	0.4006905379030130	T	T	T
0.1666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
0.1667599177461636	0.8334379986680116	0.3137726934971080	T	T	T

	0.0838059676932910	0.9168175319063092	0.2267277984661924	T	T	T
	0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.2480091340043792	0.7530788479916600	0.4007172743237236	T	T	T
	0.4166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.4172718586226679	0.8335460578665177	0.3146928540926788	T	T	T
	0.3331902359723934	0.9163906536842058	0.2266396080937230	T	T	T
	0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.6666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.6666139508380795	0.8333348127873945	0.3150967514378498	T	T	T
	0.5831485996212332	0.9160720178815329	0.2268639546037786	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.9166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.9159340099437161	0.8327309781383790	0.3145204887305936	T	T	T
	0.8333683952912484	0.9164913394372347	0.2269178099077236	T	T	T
	0.6679139303487747	0.3346592635787021	0.4611490434060674	T	T	T
	0.5002850960098502	0.7524877087362298	0.4057762379185531	T	T	T
	0.7525937577508154	0.7517321808296401	0.4056634988817861	T	T	T
	0.2484146403447386	0.4992110090007513	0.4058543710415389	T	T	T
	0.4991854507844017	0.4987390781697633	0.4054155935988684	T	T	T
	0.6694582784639940	0.3361631859102474	0.5128342634882552	T	T	T
2Ag/Ni(111) ^{S1}	1.0000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni	C	Ag	O		
	78	1	2	1		
	Selective dynamics					
	Direct					
	0.7516479112000027	0.9975668909000035	0.1392870000000030	F	F	F
	0.7535523515779755	0.0027586152338484	0.4003710961493672	T	T	T
	0.9183149111999995	0.0808998908999996	0.0514190000000028	F	F	F
	0.9187392529996389	0.0808661729377830	0.3138190372572361	T	T	T
	0.8351055988992362	0.1643344124862840	0.2267469022925230	T	T	T
	0.0016479112000027	0.9975668909000035	0.1392870000000030	F	F	F
	0.0079504581719208	0.0041650389787814	0.4000385924975519	T	T	T
	0.1683149111999995	0.0808998908999996	0.0514190000000028	F	F	F
	0.1689986221559734	0.0807980735508798	0.3129429569020012	T	T	T
	0.0850422443292177	0.1646366716334582	0.2267001681093896	T	T	T
	0.2516479112000027	0.9975668909000035	0.1392870000000030	F	F	F
	0.2485058866243463	0.9956924909617872	0.4001195123769133	T	T	T
	0.4183149111999995	0.0808998908999996	0.0514190000000028	F	F	F
	0.4189038467334993	0.0808426415441138	0.3143239817278847	T	T	T
	0.3353619482875038	0.1644745812504086	0.2266301949094810	T	T	T
	0.5016479112000027	0.9975668909000035	0.1392870000000030	F	F	F
	0.5020753497102707	0.9996702395969834	0.4045407101506645	T	T	T
	0.6683149111999995	0.0808998908999996	0.0514190000000028	F	F	F
	0.6680734063771793	0.0807157378495695	0.3139189030856985	T	T	T
	0.5849799948064434	0.1642369432817118	0.2268002350649041	T	T	T
	0.7516479112000027	0.2475668909000035	0.1392870000000030	F	F	F
	0.7507030462707007	0.2471889482188517	0.4044368546377302	T	T	T
	0.9183149111999995	0.3308998908999996	0.0514190000000028	F	F	F

0.9172429809990104	0.3302159099841134	0.3146147980457181	T	T	T
0.8349795148131719	0.4138410811784869	0.2267164469593484	T	T	T
0.0016479112000027	0.2475668909000035	0.1392870000000030	F	F	F
0.9956298270926627	0.2430319500560804	0.4006123905997723	T	T	T
0.1683149111999995	0.3308998908999996	0.0514190000000028	F	F	F
0.1692911384911205	0.3319930669387008	0.3158349089294633	T	T	T
0.0855038854233255	0.4144569810455904	0.2272544327519731	T	T	T
0.2516479112000027	0.2475668909000035	0.1392870000000030	F	F	F
0.2537071661525699	0.2417230723557320	0.4003919433884771	T	T	T
0.4183149111999995	0.3308998908999996	0.0514190000000028	F	F	F
0.4192224028241726	0.3301724060462348	0.3141668769978446	T	T	T
0.3344296379994769	0.4144652303674676	0.2271731905631658	T	T	T
0.5016479112000027	0.2475668909000035	0.1392870000000030	F	F	F
0.5022680374119692	0.2459382611434696	0.4046642762969258	T	T	T
0.6683149111999995	0.3308998908999996	0.0514190000000028	F	F	F
0.6678226438197425	0.3302733159464729	0.3139417207530412	T	T	T
0.5848021238083404	0.4143399780014325	0.2268561421646053	T	T	T
0.7516479112000027	0.4975668909000035	0.1392870000000030	F	F	F
0.7533087601613647	0.4939239681453579	0.4003946110011304	T	T	T
0.9183149111999995	0.5808998908999996	0.0514190000000028	F	F	F
0.9184358618949857	0.5807235575955929	0.3138257730370563	T	T	T
0.8346856264213282	0.6640567020452006	0.2271445832652619	T	T	T
0.0016479112000027	0.4975668909000035	0.1392870000000030	F	F	F
0.9957526505323473	0.4962693771580796	0.4006792343117107	T	T	T
0.1683149111999995	0.5808998908999996	0.0514190000000028	F	F	F
0.1690700238902134	0.5803633375662528	0.3157220248113665	T	T	T
0.0849453975748738	0.6637338709496499	0.2266394496293183	T	T	T
0.2516479112000027	0.4975668909000035	0.1392870000000030	F	F	F
0.4183149111999995	0.5808998908999996	0.0514190000000028	F	F	F
0.4177838981536605	0.5803068877175354	0.3161619466062889	T	T	T
0.3345195274954482	0.6631822127310270	0.2270838841563059	T	T	T
0.5016479112000027	0.4975668909000035	0.1392870000000030	F	F	F
0.5023241337120268	0.4897881590290088	0.4004735608656035	T	T	T
0.6683149111999995	0.5808998908999996	0.0514190000000028	F	F	F
0.6690923793612026	0.5819453586030264	0.3151596905613734	T	T	T
0.5847171399025205	0.6640926003177541	0.2272050205556730	T	T	T
0.7516479112000027	0.7475668909000035	0.1392870000000030	F	F	F
0.9183149111999995	0.8308998908999996	0.0514190000000028	F	F	F
0.9173622720411226	0.8303250904479871	0.3153457240746419	T	T	T
0.8345842955767165	0.9136451715416964	0.2270495055634597	T	T	T
0.0016479112000027	0.7475668909000035	0.1392870000000030	F	F	F
0.0076669595027886	0.7468100022784525	0.4001021485796728	T	T	T
0.1683149111999995	0.8308998908999996	0.0514190000000028	F	F	F
0.1684747863766632	0.8310392281335158	0.3129886084532669	T	T	T
0.0845152787377625	0.9138188904213016	0.2265058258431944	T	T	T
0.2516479112000027	0.7475668909000035	0.1392870000000030	F	F	F
0.2536068091128698	0.7551416617817952	0.4002777534398846	T	T	T
0.4183149111999995	0.8308998908999996	0.0514190000000028	F	F	F
0.4190860860809338	0.8318122547624427	0.3141027452133643	T	T	T
0.3350225451598687	0.9139442410159114	0.2265957805432781	T	T	T
0.5016479112000027	0.7475668909000035	0.1392870000000030	F	F	F

	0.5022353531974436	0.7555257456380676	0.4003218899540459	T	T	T
	0.6683149111999995	0.8308998908999996	0.0514190000000028	F	F	F
	0.6690744627809251	0.8301394689920423	0.3151644919678485	T	T	T
	0.5846556408737404	0.9136285901439946	0.2267749474964071	T	T	T
	0.5845484218464211	0.1634499716068122	0.4619467717585731	T	T	T
	0.7530908318894738	0.7481175631529939	0.4231337796695667	T	T	T
	0.2518345236419189	0.4974474620221416	0.4236308761218103	T	T	T
	0.5862427118598329	0.1638444859110051	0.5135896808991056	T	T	T
3Ag/Ni(111) ^{PC}	1.00000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni	C	Ag	O		
	77	1	3	1		
	Selective dynamics					
	Direct					
	0.0000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.0005443577159103	0.9993720278169876	0.3992930399001389	T	T	T
	0.1666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.1684953203621818	0.0836073429688374	0.3130787878284609	T	T	T
	0.0839087898306347	0.1676293690921123	0.2263582221286665	T	T	T
	0.2500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.2497018254701086	0.9999325708587148	0.4035289837398748	T	T	T
	0.4166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.4161730142928456	0.0835248515135611	0.3127703770378338	T	T	T
	0.3338015484136659	0.1675539255039585	0.2263780357025267	T	T	T
	0.5000000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.5017023598503750	0.0084271455045115	0.4027103399292241	T	T	T
	0.6666669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.6663020489232218	0.0831614581536549	0.3139791769792018	T	T	T
	0.5840790108848929	0.1669398094902427	0.2264746730033996	T	T	T
	0.7500000000000000	0.0000000000000000	0.1392870000000030	F	F	F
	0.7572645158755545	0.0075987520415373	0.3995870945406091	T	T	T
	0.9166669999999968	0.0833330000000032	0.0514190000000028	F	F	F
	0.9172080128682331	0.0829347167182954	0.3125058773462006	T	T	T
	0.8335856230793264	0.1667714279185770	0.2261577477587127	T	T	T
	0.0000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.9924731766738372	0.2425144990248994	0.3995317060707670	T	T	T
	0.1666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.1681684003647219	0.3345087074126274	0.3155827329384048	T	T	T
	0.0842947305555918	0.4169172847953465	0.2273622036068080	T	T	T
	0.2500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.2420334622701220	0.2393262262392185	0.4003504386343372	T	T	T
	0.4166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.4172382313854832	0.3345059350817053	0.3158546128184085	T	T	T
	0.3337469476252774	0.4176930144869535	0.2277604750127591	T	T	T
	0.5000000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.5014744286724503	0.2446155622481630	0.4023319008971118	T	T	T
	0.6666669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.6660917857336467	0.3332268682110264	0.3137053382079051	T	T	T
	0.5833514409721162	0.4168803689561794	0.2271778077602866	T	T	T

	0.7500000000000000	0.2500000000000000	0.1392870000000030	F	F	F
	0.7532281395562654	0.2519082490892853	0.4002085267928576	T	T	T
	0.9166669999999968	0.3333330000000032	0.0514190000000028	F	F	F
	0.9166697919971409	0.3332031533683166	0.3136827085200959	T	T	T
	0.8339826404872147	0.4169173059551947	0.2261457704296317	T	T	T
	0.0000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.9925331773484448	0.5004262335479491	0.3994497542294287	T	T	T
	0.1666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.1682513089914510	0.5837587170503653	0.3155157580042269	T	T	T
	0.0837768361029931	0.6662133829991020	0.2263784683144225	T	T	T
	0.2500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.4166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.4162905626018258	0.5836504285969233	0.3180217051827076	T	T	T
	0.3337818257465810	0.6663758651447068	0.2279599656925511	T	T	T
	0.5000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.6666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.6647962382835532	0.5828066699003873	0.3154390319566251	T	T	T
	0.5827020121696362	0.6665576147796346	0.2277864623218793	T	T	T
	0.7500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.7575726487426828	0.5002691771140337	0.3995194571709562	T	T	T
	0.9166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.9168393854736219	0.5847361169873658	0.3124926843580481	T	T	T
	0.8327274963100036	0.6664468534248208	0.2262261565386254	T	T	T
	0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.0005834793515205	0.7516298986299794	0.3994760214837187	T	T	T
	0.1666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.1677200216150461	0.8344996920323824	0.3130512392548181	T	T	T
	0.0836203059487610	0.9166867637738733	0.2262611415073207	T	T	T
	0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.2420410934803784	0.7530875138026722	0.4003880034657420	T	T	T
	0.4166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.4172317062067571	0.8335155116874273	0.3160327425534566	T	T	T
	0.3336884326760254	0.9160915373808385	0.2265472993157587	T	T	T
	0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.6666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.6651440524464974	0.8324426243721987	0.3154988740601385	T	T	T
	0.5831798879667270	0.9159584796773500	0.2272923445475430	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.7625704294976362	0.7565629827567473	0.4005657987582006	T	T	T
	0.9166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.9164138616463752	0.8330304560257072	0.3126644043564731	T	T	T
	0.8323962473978063	0.9160879053663107	0.2263528397357198	T	T	T
	0.4155757477776162	0.0840816373912737	0.4610142936488769	T	T	T
	0.5066033838302775	0.7630308282753504	0.4228732322869970	T	T	T
	0.2356850062790278	0.4931160789609709	0.4241509826743594	T	T	T
	0.5068088698393206	0.4946752403903245	0.4228109941985568	T	T	T
	0.4149158225340323	0.0844370687268022	0.5126695235364753	T	T	T
4Ag/Ni(111) ^{PC}	1.0000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			

Ni C Ag O
76 1 4 1

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.1392870000000030	F F F
0.0072636778015718	0.0086180408570391	0.3982258516619234	T T T
0.1666669999999968	0.0833330000000032	0.0514190000000028	F F F
0.1680518690748827	0.0844265925436210	0.3118384003114181	T T T
0.0837015970804282	0.1676560794316160	0.2261919733285848	T T T
0.2500000000000000	0.0000000000000000	0.1392870000000030	F F F
0.2466986658433618	0.9982128803510475	0.3983856341790364	T T T
0.4166669999999968	0.0833330000000032	0.0514190000000028	F F F
0.4162559709985598	0.0836289393858761	0.3121646012624820	T T T
0.3338215865886198	0.1678705952996388	0.2260492595104797	T T T
0.5000000000000000	0.0000000000000000	0.1392870000000030	F F F
0.4999543989890938	0.0079767485548489	0.4019746927700650	T T T
0.6666669999999968	0.0833330000000032	0.0514190000000028	F F F
0.6662945906795815	0.0831694431688162	0.3130831892709948	T T T
0.5833195566379640	0.1666140234504289	0.2260141548207397	T T T
0.7500000000000000	0.0000000000000000	0.1392870000000030	F F F
0.7576865801855782	0.0110656120754457	0.3993024495898599	T T T
0.9166669999999968	0.0833330000000032	0.0514190000000028	F F F
0.9163401281420617	0.0830237734884734	0.3122877312644894	T T T
0.8333728170898038	0.1666762224081207	0.2260257714494924	T T T
0.0000000000000000	0.2500000000000000	0.1392870000000030	F F F
0.9923836954530406	0.2445910073663254	0.3992531850308687	T T T
0.1666669999999968	0.3333330000000032	0.0514190000000028	F F F
0.1679084084534252	0.3349513285728061	0.3155274383156564	T T T
0.0847053795111634	0.4172959615949617	0.2269821869121772	T T T
0.2500000000000000	0.2500000000000000	0.1392870000000030	F F F
0.2454336871886274	0.2391019787801107	0.4000750650576906	T T T
0.4166669999999968	0.3333330000000032	0.0514190000000028	F F F
0.4178740480153350	0.3350880433855229	0.3154702915590427	T T T
0.3333695843479510	0.4178731153010017	0.2276565341753358	T T T
0.5000000000000000	0.2500000000000000	0.1392870000000030	F F F
0.5000506898117454	0.2425937909937182	0.4017477193521202	T T T
0.6666669999999968	0.3333330000000032	0.0514190000000028	F F F
0.6662821808004877	0.3332926065298246	0.3128861813317441	T T T
0.5829103565428079	0.4177568815995041	0.2270240367477852	T T T
0.7500000000000000	0.2500000000000000	0.1392870000000030	F F F
0.7499471129138461	0.2503240854209414	0.4036914526308108	T T T
0.9166669999999968	0.3333330000000032	0.0514190000000028	F F F
0.9153761631410430	0.3326813389378045	0.3134942799193740	T T T
0.8333656280681633	0.4166062982321688	0.2260146986849987	T T T
0.0000000000000000	0.5000000000000000	0.1392870000000030	F F F
0.9922573821066878	0.4982934845511791	0.3991351198058948	T T T
0.1666669999999968	0.5833330000000032	0.0514190000000028	F F F
0.1679261577010220	0.5829241977802072	0.3154310702800313	T T T
0.0834193110469529	0.6660828945846841	0.2262306540948176	T T T
0.2500000000000000	0.5000000000000000	0.1392870000000030	F F F
0.4166669999999968	0.5833330000000032	0.0514190000000028	F F F

	0.4166742208745681	0.5835879323339684	0.3178893506722273	T	T	T
	0.3334642219701927	0.6659855907348853	0.2278598450118747	T	T	T
	0.5000000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.6666669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.6659340282726411	0.5839416117542217	0.3166173992934838	T	T	T
	0.5826738553513697	0.6666492164990850	0.2282976470059247	T	T	T
	0.7500000000000000	0.5000000000000000	0.1392870000000030	F	F	F
	0.7576453080047586	0.4970541780153062	0.3993069231054833	T	T	T
	0.9166669999999968	0.5833330000000032	0.0514190000000028	F	F	F
	0.9158954694592736	0.5839185783240217	0.3123437072531007	T	T	T
	0.8322651001539025	0.6667143736826266	0.2267292902722815	T	T	T
	0.0000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.0072062764223033	0.7489465585478242	0.3984269271059281	T	T	T
	0.1666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.1671445158169522	0.8334054600438989	0.3120204919365256	T	T	T
	0.0828264517090637	0.9164568441183246	0.2260879765784489	T	T	T
	0.2500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.2451489984596546	0.7557072799274616	0.4000383990683463	T	T	T
	0.4166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.4176301326672232	0.8331427165147944	0.3155886511734203	T	T	T
	0.3336180585047449	0.9158906815107176	0.2261741953277976	T	T	T
	0.5000000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.6666669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.6659074521276847	0.8322122608885276	0.3167277424722293	T	T	T
	0.5828874551627702	0.9151469580426214	0.2271617955505109	T	T	T
	0.7500000000000000	0.7500000000000000	0.1392870000000030	F	F	F
	0.9166669999999968	0.8333330000000032	0.0514190000000028	F	F	F
	0.9144465092016304	0.8322472676934637	0.3146484240483400	T	T	T
	0.8321192895007796	0.9154426118873900	0.2268282338051058	T	T	T
	0.5844584161229767	0.1674832980023733	0.4610985878710105	T	T	T
	0.5008464660904411	0.7622901271830799	0.4227675922387683	T	T	T
	0.7681809167092807	0.7592762120569594	0.4262151248992160	T	T	T
	0.2335414359857646	0.4917972688647914	0.4259305674502311	T	T	T
	0.5009208076653195	0.4890018519463530	0.4225962395628018	T	T	T
	0.5849604120644085	0.1678799456320050	0.5127078013914022	T	T	T
2Au/Ni(111) ^{SI}	1.0000000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni C Au O					
	78 1 2 1					
	Selective dynamics					
	Direct					
	0.7516479112000027	0.9975668909000035	0.1392870000000030	F	F	F
	0.7535344730255613	0.0026534520677505	0.4010501753817407	T	T	T
	0.9183149111999995	0.0808998908999996	0.0514190000000028	F	F	F
	0.9187271872799047	0.0812127369377080	0.3141630952006086	T	T	T
	0.8352064077722308	0.1643419810989314	0.2267993460719064	T	T	T
	0.0016479112000027	0.9975668909000035	0.1392870000000030	F	F	F
	0.0078192046442398	0.0036475615028023	0.4009941588631807	T	T	T
	0.1683149111999995	0.0808998908999996	0.0514190000000028	F	F	F

0.1691179165440451	0.0811324749812891	0.3136361305942275	T	T	T
0.0850175659707974	0.1644623387772245	0.2267433354102713	T	T	T
0.2516479112000027	0.9975668909000035	0.1392870000000030	F	F	F
0.2492401124097264	0.9960022767963154	0.4002684301031444	T	T	T
0.4183149111999995	0.0808998908999996	0.0514190000000028	F	F	F
0.4188363778645667	0.0807527495956345	0.3142393166854095	T	T	T
0.3350977562350059	0.1644064519905413	0.2267362120103206	T	T	T
0.5016479112000027	0.9975668909000035	0.1392870000000030	F	F	F
0.5015991719914165	0.9994173428116359	0.4043676030884069	T	T	T
0.6683149111999995	0.0808998908999996	0.0514190000000028	F	F	F
0.6683044586416815	0.0806571796499882	0.3140795516454334	T	T	T
0.5850100756479838	0.1642042510223984	0.2268261750574946	T	T	T
0.7516479112000027	0.2475668909000035	0.1392870000000030	F	F	F
0.7505675708472770	0.2470454022825488	0.4042257742366857	T	T	T
0.9183149111999995	0.3308998908999996	0.0514190000000028	F	F	F
0.9171854202026691	0.3300990818014148	0.3146841710165481	T	T	T
0.8351238820731539	0.4139759611332642	0.2267658453153826	T	T	T
0.0016479112000027	0.2475668909000035	0.1392870000000030	F	F	F
0.9957463534777398	0.2432322743030624	0.4013604108901227	T	T	T
0.1683149111999995	0.3308998908999996	0.0514190000000028	F	F	F
0.1687621884680905	0.3306491917989340	0.3150840387284797	T	T	T
0.0855360276511551	0.4145109682730084	0.2271403502754247	T	T	T
0.2516479112000027	0.2475668909000035	0.1392870000000030	F	F	F
0.2531824782071310	0.2418140420817299	0.4013207628867486	T	T	T
0.4183149111999995	0.3308998908999996	0.0514190000000028	F	F	F
0.4193154353334934	0.3300619707281329	0.3145251952431778	T	T	T
0.3346081956249798	0.4144509040388824	0.2270538236459778	T	T	T
0.5016479112000027	0.2475668909000035	0.1392870000000030	F	F	F
0.5018785778176384	0.2454827927226215	0.4044725978464544	T	T	T
0.6683149111999995	0.3308998908999996	0.0514190000000028	F	F	F
0.6680370093374224	0.3303526508232303	0.3140822107806364	T	T	T
0.5846063588143842	0.4140959632531626	0.2268351311017742	T	T	T
0.7516479112000027	0.4975668909000035	0.1392870000000030	F	F	F
0.7531658016945287	0.4938483217619836	0.4011586819531907	T	T	T
0.9183149111999995	0.5808998908999996	0.0514190000000028	F	F	F
0.9185461517915130	0.5803388304183682	0.3142808266932368	T	T	T
0.8347241791457513	0.6639624326949376	0.2270948200602849	T	T	T
0.0016479112000027	0.4975668909000035	0.1392870000000030	F	F	F
0.9960802671465497	0.4962051298258038	0.4014529190291589	T	T	T
0.1683149111999995	0.5808998908999996	0.0514190000000028	F	F	F
0.1685912719943866	0.5809346844059139	0.3150798611473979	T	T	T
0.0848404680374998	0.6639392297890117	0.2267193710677258	T	T	T
0.2516479112000027	0.4975668909000035	0.1392870000000030	F	F	F
0.4183149111999995	0.5808998908999996	0.0514190000000028	F	F	F
0.4185495779145169	0.5805053587009226	0.3153686638172350	T	T	T
0.3345579951704864	0.6632852542675368	0.2270670886493938	T	T	T
0.5016479112000027	0.4975668909000035	0.1392870000000030	F	F	F
0.5020346615976818	0.4893743588776114	0.4018635812634160	T	T	T
0.6683149111999995	0.5808998908999996	0.0514190000000028	F	F	F
0.6684083441304105	0.5804987671599265	0.3147341053037834	T	T	T
0.5848790631169688	0.6641178138161117	0.2271261961631597	T	T	T

	0.7516479112000027	0.7475668909000035	0.1392870000000030	F	F	F
	0.9183149111999995	0.8308998908999996	0.0514190000000028	F	F	F
	0.9187269021068987	0.8309218309058973	0.3146380467057184	T	T	T
	0.8346388221744803	0.9137729411446975	0.2270035829701427	T	T	T
	0.0016479112000027	0.7475668909000035	0.1392870000000030	F	F	F
	0.0075704254824964	0.7474053807807904	0.4010379377362219	T	T	T
	0.1683149111999995	0.8308998908999996	0.0514190000000028	F	F	F
	0.1686297071951543	0.8308553475067683	0.3135289958575806	T	T	T
	0.0847932937447224	0.9140007349270785	0.2265525403447403	T	T	T
	0.2516479112000027	0.7475668909000035	0.1392870000000030	F	F	F
	0.2527593433838148	0.7540954326176966	0.4012801083830068	T	T	T
	0.4183149111999995	0.8308998908999996	0.0514190000000028	F	F	F
	0.4190056097659566	0.8318307690641513	0.3144857962688236	T	T	T
	0.3350274699811784	0.9137731903298241	0.2266592052438771	T	T	T
	0.5016479112000027	0.7475668909000035	0.1392870000000030	F	F	F
	0.5020083713111513	0.7555336004085662	0.4017268992826972	T	T	T
	0.6683149111999995	0.8308998908999996	0.0514190000000028	F	F	F
	0.6682411591127291	0.8307029642909917	0.3146968547861324	T	T	T
	0.5845182775431377	0.9136431102771702	0.2268235933200010	T	T	T
	0.5847411336623749	0.1636324066727710	0.4617554461502418	T	T	T
	0.7530503862621319	0.7481395331704879	0.4171892376151213	T	T	T
	0.2511192396164995	0.4970229275829896	0.4177106852392274	T	T	T
	0.5865383410060325	0.1640917565939649	0.5134031558694498	T	T	T
3Au/Ni(111) ^{SI}	1.00000000000000					
	8.6224000674449712	-4.9781450000000014	0.0000000000000000			
	0.0000000000000000	9.9562900000000010	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.1292800000000014			
	Ni	C	Au	O		
	77	1	3	1		
	Selective dynamics					
	Direct					
	0.7444199999999981	0.9828789999999969	0.1392870000000030	F	F	F
	0.7463185242091646	0.9893200260551126	0.4009961675150329	T	T	T
	0.9110870000000020	0.0662120000000002	0.0514190000000028	F	F	F
	0.9124041959107529	0.0664615076525496	0.3135557129236989	T	T	T
	0.8283378972099693	0.1496995767904449	0.2266959628549196	T	T	T
	0.9944199999999981	0.9828789999999969	0.1392870000000030	F	F	F
	0.9980814996236000	0.9902041665607704	0.4003624898080205	T	T	T
	0.1610870000000020	0.0662120000000002	0.0514190000000028	F	F	F
	0.1615728956381874	0.0658786513707161	0.3136481696285381	T	T	T
	0.0782520237037840	0.1500386462637222	0.2263875907191162	T	T	T
	0.2444199999999981	0.9828789999999969	0.1392870000000030	F	F	F
	0.2388361072477803	0.9791244085595283	0.4035745633967209	T	T	T
	0.4110870000000020	0.0662120000000002	0.0514190000000028	F	F	F
	0.4107267417399322	0.0660250718214340	0.3144910458956872	T	T	T
	0.3283888953517652	0.1496879046215444	0.2268908738583763	T	T	T
	0.4944199999999981	0.9828789999999969	0.1392870000000030	F	F	F
	0.4993248987952535	0.9806626726087264	0.4001912587010270	T	T	T
	0.6610870000000020	0.0662120000000002	0.0514190000000028	F	F	F
	0.6613552351657793	0.0662420565601335	0.3136554864390537	T	T	T
	0.5785271709243768	0.1500477769036905	0.2267111909653260	T	T	T

0.7444199999999981	0.2328789999999969	0.1392870000000030	F	F	F
0.7500602687297573	0.2327941640257307	0.4010114412534652	T	T	T
0.9110870000000020	0.3162120000000002	0.0514190000000028	F	F	F
0.9114070970000832	0.3168187961656507	0.3136147889390277	T	T	T
0.8281899147719467	0.3993811778044865	0.2263439284075421	T	T	T
0.9944199999999981	0.2328789999999969	0.1392870000000030	F	F	F
0.9896943697074146	0.2287845734104479	0.4010038443828710	T	T	T
0.1610870000000020	0.3162120000000002	0.0514190000000028	F	F	F
0.1618280772133449	0.3164847652867178	0.3145015204221807	T	T	T
0.0787366866799022	0.3996235984445364	0.2267087653067751	T	T	T
0.2444199999999981	0.2328789999999969	0.1392870000000030	F	F	F
0.2392573079429976	0.2276217356406437	0.4014322019307858	T	T	T
0.4110870000000020	0.3162120000000002	0.0514190000000028	F	F	F
0.4116382226555202	0.3160965906805901	0.3145124135364110	T	T	T
0.3284578388576980	0.3998329723037790	0.2269948134710879	T	T	T
0.4944199999999981	0.2328789999999969	0.1392870000000030	F	F	F
0.6610870000000020	0.3162120000000002	0.0514190000000028	F	F	F
0.6615511299264647	0.3167853573030097	0.3144330482187817	T	T	T
0.5783499341980245	0.3995255374007906	0.2267986144065657	T	T	T
0.7444199999999981	0.4828789999999969	0.1392870000000030	F	F	F
0.7513240638042590	0.4835751905903335	0.4013098959204275	T	T	T
0.9110870000000020	0.5662120000000002	0.0514190000000028	F	F	F
0.9125265348522202	0.5669770726154878	0.3136487897742747	T	T	T
0.8283431341925649	0.6498059659644515	0.2269475054594035	T	T	T
0.9944199999999981	0.4828789999999969	0.1392870000000030	F	F	F
0.9886765948151367	0.4797456862160964	0.4002598230608798	T	T	T
0.1610870000000020	0.5662120000000002	0.0514190000000028	F	F	F
0.1622569664929603	0.5676922390950562	0.3147813051463249	T	T	T
0.0783617891843231	0.6494017847021862	0.2265969657600891	T	T	T
0.2444199999999981	0.4828789999999969	0.1392870000000030	F	F	F
0.4110870000000020	0.5662120000000002	0.0514190000000028	F	F	F
0.4109055637427565	0.5665319652185589	0.3145339190228220	T	T	T
0.3285419484443646	0.6497390474050295	0.2269115374117860	T	T	T
0.4944199999999981	0.4828789999999969	0.1392870000000030	F	F	F
0.4952355273490107	0.4835619245598786	0.4013789658656322	T	T	T
0.6610870000000020	0.5662120000000002	0.0514190000000028	F	F	F
0.6623461158492534	0.5673608288448876	0.3146245438848936	T	T	T
0.5785953832185106	0.6498255396572103	0.2270131343330021	T	T	T
0.7444199999999981	0.7328789999999969	0.1392870000000030	F	F	F
0.9110870000000020	0.8162120000000002	0.0514190000000028	F	F	F
0.9121294989316583	0.8158710490842950	0.3148011126412164	T	T	T
0.8281439928010312	0.8995233866568411	0.2268040702851092	T	T	T
0.9944199999999981	0.7328789999999969	0.1392870000000030	F	F	F
0.0002144681883059	0.7312661929686936	0.4040581652702453	T	T	T
0.1610870000000020	0.8162120000000002	0.0514190000000028	F	F	F
0.1615235624729408	0.8161507800355667	0.3135323504926510	T	T	T
0.0781483236161546	0.8997076352133342	0.2265673937844546	T	T	T
0.2444199999999981	0.7328789999999969	0.1392870000000030	F	F	F
0.2480530640583518	0.7402669542074219	0.4041113868488479	T	T	T
0.4110870000000020	0.8162120000000002	0.0514190000000028	F	F	F
0.4109895095355509	0.8166857363069351	0.3137428843726006	T	T	T

	0.3286307976265493 0.8998934155592675 0.2265743913430036 T T T
	0.4944199999999981 0.7328789999999969 0.1392870000000030 F F F
	0.4954608290711532 0.7393729807721100 0.4014154777537375 T T T
	0.6610870000000020 0.8162120000000002 0.0514190000000028 F F F
	0.6614547342348491 0.8161618510248787 0.3145131968560206 T T T
	0.5787592872132458 0.8998755673564871 0.2263904706972161 T T T
	0.1629338162395329 0.8185178430337617 0.4620067194720375 T T T
	0.4953763682504062 0.2313839726214835 0.4170939601196201 T T T
	0.7476765843096813 0.7357347318704373 0.4172552248712147 T T T
	0.2431268879131687 0.4835443300397885 0.4173785754418072 T T T
	0.1637069673859577 0.8203253910115255 0.5135789478969460 T T T
4Au/Ni(111) ^{S1}	1.0000000000000000
	8.6224000674449712 -4.9781450000000014 0.0000000000000000
	0.0000000000000000 9.9562900000000010 0.0000000000000000
	0.0000000000000000 0.0000000000000000 23.1292800000000014
	Ni C Au O
	76 1 4 1
	Selective dynamics
	Direct
	0.0034156355999997 0.2472240844000027 0.1392870000000030 F F F
	0.1700826355999965 0.3305570843999988 0.0514190000000028 F F F
	0.1707383515652600 0.3310961626369431 0.3144030099498499 T T T
	0.0868700854239144 0.4142276356226858 0.2267186650975352 T T T
	0.2534156355999997 0.2472240844000027 0.1392870000000030 F F F
	0.2568542248471577 0.2506354356717776 0.4045120660093142 T T T
	0.4200826355999965 0.3305570843999988 0.0514190000000028 F F F
	0.4195920449905520 0.3306980150996386 0.3136638775295869 T T T
	0.3368473513684703 0.4141820892842646 0.2267583724672554 T T T
	0.5034156355999997 0.2472240844000027 0.1392870000000030 F F F
	0.5041609994524857 0.2462860869998458 0.4006310148987902 T T T
	0.6700826355999965 0.3305570843999988 0.0514190000000028 F F F
	0.6698633212032626 0.3309824573962729 0.3137159637431141 T T T
	0.5870657711410425 0.4143245923387974 0.2266782664747511 T T T
	0.7534156355999997 0.2472240844000027 0.1392870000000030 F F F
	0.7477514893962141 0.2427961305890030 0.4005167549996190 T T T
	0.9200826355999965 0.3305570843999988 0.0514190000000028 F F F
	0.9209059083209544 0.3309510355758953 0.3142617995845921 T T T
	0.8368399680664226 0.4140263208036833 0.2267001231006999 T T T
	0.0034156355999997 0.4972240844000027 0.1392870000000030 F F F
	0.0089379496309776 0.5028355468726701 0.4010326494493867 T T T
	0.1700826355999965 0.5805570843999988 0.0514190000000028 F F F
	0.1707354039302058 0.5801264308864318 0.3139021404949463 T T T
	0.0867896588330623 0.6642127246877281 0.2264936426357659 T T T
	0.2534156355999997 0.4972240844000027 0.1392870000000030 F F F
	0.2528153707841747 0.4970102138621905 0.4054733592170728 T T T
	0.4200826355999965 0.5805570843999988 0.0514190000000028 F F F
	0.4197935112814647 0.5800439773131393 0.3148357676176316 T T T
	0.3368380391898860 0.6642114036896913 0.2268528568239994 T T T
	0.5034156355999997 0.4972240844000027 0.1392870000000030 F F F
	0.4984511613837695 0.4920285053715581 0.4047606755763334 T T T
	0.6700826355999965 0.5805570843999988 0.0514190000000028 F F F

0.6693186981077448	0.5797223081152297	0.3148818252154211	T	T	T
0.5870915932514655	0.6639690531418926	0.2269940991528544	T	T	T
0.7534156355999997	0.4972240844000027	0.1392870000000030	F	F	F
0.9200826355999965	0.5805570843999988	0.0514190000000028	F	F	F
0.9201392774658381	0.5804519908620434	0.3142725499688627	T	T	T
0.8370751210295211	0.6640367091680810	0.2266962039942939	T	T	T
0.0034156355999997	0.7472240844000027	0.1392870000000030	F	F	F
0.0028581628043070	0.7478327162374010	0.4012187341718467	T	T	T
0.1700826355999965	0.8305570843999988	0.0514190000000028	F	F	F
0.1701463059471174	0.8303874095772478	0.3140737581438972	T	T	T
0.0866546336277850	0.9134355149315824	0.2265317072694986	T	T	T
0.2534156355999997	0.7472240844000027	0.1392870000000030	F	F	F
0.2482372883274638	0.7417834551479036	0.4008879665497589	T	T	T
0.4200826355999965	0.8305570843999988	0.0514190000000028	F	F	F
0.4203204721507105	0.8302452498434516	0.3142282764784419	T	T	T
0.3367275607703719	0.9139610444619696	0.2267119122633690	T	T	T
0.5034156355999997	0.7472240844000027	0.1392870000000030	F	F	F
0.6700826355999965	0.8305570843999988	0.0514190000000028	F	F	F
0.6700828675725768	0.8301418729015434	0.3138174142030905	T	T	T
0.5867125364293124	0.9136805002660945	0.2264642666977940	T	T	T
0.7534156355999997	0.7472240844000027	0.1392870000000030	F	F	F
0.7581597492590681	0.7519478815075124	0.4008009855770520	T	T	T
0.9200826355999965	0.8305570843999988	0.0514190000000028	F	F	F
0.9198910955534251	0.8305910821059937	0.3133720254087402	T	T	T
0.8370058981356877	0.9140754912913944	0.2264118537986686	T	T	T
0.0034156355999997	0.9972240844000027	0.1392870000000030	F	F	F
0.9982218605019846	0.9919548095588787	0.4009142501624171	T	T	T
0.1700826355999965	0.0805570843999988	0.0514190000000028	F	F	F
0.1705172451776241	0.0809412325462603	0.3147539750943368	T	T	T
0.0873194812879501	0.1642724898237302	0.2269731552197976	T	T	T
0.2534156355999997	0.9972240844000027	0.1392870000000030	F	F	F
0.4200826355999965	0.0805570843999988	0.0514190000000028	F	F	F
0.4196425623103545	0.0807083839841487	0.3140138678517542	T	T	T
0.3363124601887393	0.1636492317100068	0.2267986281969724	T	T	T
0.5034156355999997	0.9972240844000027	0.1392870000000030	F	F	F
0.5085349001657554	0.0032156352411081	0.4006645135907829	T	T	T
0.6700826355999965	0.0805570843999988	0.0514190000000028	F	F	F
0.6702595944625022	0.0809963385402305	0.3130050106658929	T	T	T
0.5867442185382343	0.1641077858565959	0.2263547711958247	T	T	T
0.7534156355999997	0.9972240844000027	0.1392870000000030	F	F	F
0.7528100843280682	0.9975085806717228	0.4005791450076725	T	T	T
0.9200826355999965	0.0805570843999988	0.0514190000000028	F	F	F
0.9208317853746192	0.0808553623008576	0.3140880981515062	T	T	T
0.8372788331034513	0.1644199821791693	0.2266629671828833	T	T	T
0.3377762202174136	0.4112544615306324	0.4628646778099570	T	T	T
0.9993297779963336	0.2456603812288362	0.4170605329389278	T	T	T
0.7538415611353527	0.4973896884901245	0.4176217063362148	T	T	T
0.2532382635821824	0.9963560513608656	0.4175917061880071	T	T	T
0.5048361322904120	0.7508051088370189	0.4169694355448929	T	T	T
0.3370657905313718	0.4120656830512655	0.5144561099215895	T	T	T
2Ni/Cu(111) ^{S1}	1.00000000000000				

8.8905908144889398 -5.1329849999999997 0.0000000000000000
0.0000000000000000 10.2659699999999994 0.0000000000000000
0.0000000000000000 0.0000000000000000 23.3821300000000001

Ni C Cu O
2 1 78 1

Selective dynamics

Direct

0.2508138199286947	0.5008475097829859	0.3861264633166712	T	T	T
0.7511973924742819	0.7507216788480449	0.3793913987915687	T	T	T
0.2524419789338879	0.5034480547095654	0.4608335849257088	T	T	T
0.0000000000000000	0.0000000000000000	0.1155260000000027	F	F	F
0.9983702783180419	0.9980916458111722	0.3832629434865282	T	T	T
0.1666669999999968	0.0833330000000032	0.0259050000000016	F	F	F
0.1666579478460974	0.0840193724168543	0.2946294163127519	T	T	T
0.0835778960916400	0.1671885511225497	0.2052415717263187	T	T	T
0.2500000000000000	0.0000000000000000	0.1155260000000027	F	F	F
0.2498953271391073	0.0000825357590202	0.3831739236115013	T	T	T
0.4166669999999968	0.0833330000000032	0.0259050000000016	F	F	F
0.4167239649983756	0.0834071735528354	0.2944075211067982	T	T	T
0.3333482873283842	0.1670069167575718	0.2051835368047037	T	T	T
0.5000000000000000	0.0000000000000000	0.1155260000000027	F	F	F
0.5005061389920940	0.0003003709058973	0.3831657492646627	T	T	T
0.6666669999999968	0.0833330000000032	0.0259050000000016	F	F	F
0.6669141566690513	0.0832147061223694	0.2943790700438100	T	T	T
0.5833636390976977	0.1666935660102027	0.2050168099963017	T	T	T
0.7500000000000000	0.0000000000000000	0.1155260000000027	F	F	F
0.7501141835280336	0.9981803606840032	0.3831644227680826	T	T	T
0.9166669999999968	0.0833330000000032	0.0259050000000016	F	F	F
0.9172097427625161	0.0838410601716149	0.2944774089610149	T	T	T
0.8337125664288934	0.1669839647802505	0.2051447118605836	T	T	T
0.0000000000000000	0.2500000000000000	0.1155260000000027	F	F	F
0.9997858936339128	0.2496706474791353	0.3831341564705326	T	T	T
0.1666669999999968	0.3333330000000032	0.0259050000000016	F	F	F
0.1679532554574550	0.3357242970498575	0.2949578428928135	T	T	T
0.0833500507326406	0.4167025642292685	0.2047211099533044	T	T	T
0.2500000000000000	0.2500000000000000	0.1155260000000027	F	F	F
0.2503577400730137	0.2503440466689852	0.3832078374213808	T	T	T
0.4166669999999968	0.3333330000000032	0.0259050000000016	F	F	F
0.4165706605535533	0.3341413068943027	0.2946411152655415	T	T	T
0.3333493510739700	0.4167361137444843	0.2047454953467849	T	T	T
0.5000000000000000	0.2500000000000000	0.1155260000000027	F	F	F
0.5004504077379224	0.2503777002664407	0.3831849619056413	T	T	T
0.6666669999999968	0.3333330000000032	0.0259050000000016	F	F	F
0.6669040093869256	0.3337754025091328	0.2943891340725386	T	T	T
0.5831069800352893	0.4167923827441484	0.2051420324771200	T	T	T
0.7500000000000000	0.2500000000000000	0.1155260000000027	F	F	F
0.7498592850304249	0.2500000228681998	0.3830187688561750	T	T	T
0.9166669999999968	0.3333330000000032	0.0259050000000016	F	F	F
0.9175096760496260	0.3338044611669417	0.2945443948927249	T	T	T
0.8337068631927309	0.4167792210420487	0.2051441074958120	T	T	T
0.0000000000000000	0.5000000000000000	0.1155260000000027	F	F	F

	0.9996858859783870	0.5003076302322427	0.3830998491127318	T	T	T
	0.1666669999999968	0.5833330000000032	0.0259050000000016	F	F	F
	0.1678774347579477	0.5824464211745024	0.2948778851391722	T	T	T
	0.0835398071363613	0.6664647882715613	0.2052131425600336	T	T	T
	0.2500000000000000	0.5000000000000000	0.1155260000000027	F	F	F
	0.4166669999999968	0.5833330000000032	0.0259050000000016	F	F	F
	0.4148341448588155	0.5824886826927340	0.2948980634098461	T	T	T
	0.3333453786568796	0.6666564617644966	0.2047302247753322	T	T	T
	0.5000000000000000	0.5000000000000000	0.1155260000000027	F	F	F
	0.5024241970591348	0.5021085344093237	0.3832924860037537	T	T	T
	0.6666669999999968	0.5833330000000032	0.0259050000000016	F	F	F
	0.6664271468338967	0.5838075521306081	0.2941302831011754	T	T	T
	0.5827006685967717	0.6663669330537161	0.2048776039936584	T	T	T
	0.7500000000000000	0.5000000000000000	0.1155260000000027	F	F	F
	0.7500277545848917	0.5020642785724618	0.3831646167739251	T	T	T
	0.9166669999999968	0.5833330000000032	0.0259050000000016	F	F	F
	0.9171624867947088	0.5834714143977280	0.2944723654390700	T	T	T
	0.8333878514972355	0.6664581452961755	0.2047977518364092	T	T	T
	0.0000000000000000	0.7500000000000000	0.1155260000000027	F	F	F
	0.9983185184113168	0.7504743941489522	0.3832601253069541	T	T	T
	0.1666669999999968	0.8333330000000032	0.0259050000000016	F	F	F
	0.1666360672456193	0.8327890277650241	0.2946231948448457	T	T	T
	0.0835768951695286	0.9168323459242700	0.2051559474768254	T	T	T
	0.2500000000000000	0.7500000000000000	0.1155260000000027	F	F	F
	0.2503454661961868	0.7504032557025369	0.3831750675493879	T	T	T
	0.4166669999999968	0.8333330000000032	0.0259050000000016	F	F	F
	0.4165736740563872	0.8325262570489116	0.2946270462551581	T	T	T
	0.3333452992340540	0.9163955398235899	0.2051802333300685	T	T	T
	0.5000000000000000	0.7500000000000000	0.1155260000000027	F	F	F
	0.5025477127487079	0.7506137701188962	0.3832920282347558	T	T	T
	0.6666669999999968	0.8333330000000032	0.0259050000000016	F	F	F
	0.6664522292730766	0.8327280875345409	0.2941196113134339	T	T	T
	0.5831116507170933	0.9163612787523689	0.2051356825024655	T	T	T
	0.7500000000000000	0.7500000000000000	0.1155260000000027	F	F	F
	0.9166669999999968	0.8333330000000032	0.0259050000000016	F	F	F
	0.9166545475364387	0.8333931277152899	0.2938700127726079	T	T	T
	0.8334099860719348	0.9170164704443380	0.2047947901669076	T	T	T
	0.2536738942300616	0.5052176477067576	0.5106403660460472	T	T	T
3Ni/Cu(111) ^{SI}	1.0000000000000000					
	8.8905908144889398	-5.1329849999999997	0.0000000000000000			
	0.0000000000000000	10.2659699999999994	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.3821300000000001			
	Ni	C	Cu	O		
	3	1	77	1		
	Selective dynamics					
	Direct					
	0.2501994792971365	0.2502687602055756	0.3864063407588248	T	T	T
	0.7504315169006288	0.5009680220877604	0.3795242485204296	T	T	T
	0.5007084776611667	0.7511309953698651	0.3794494403133997	T	T	T
	0.2496918361531995	0.2507038790395605	0.4611322791610858	T	T	T
	0.0000000000000000	0.0000000000000000	0.1155260000000027	F	F	F

-0.0008149568780899	-0.0007047888598864	0.3832005748281520	T	T	T
0.1666669999999968	0.0833330000000032	0.0259050000000016	F	F	F
0.1678168700465630	0.0855861725494618	0.2950912346252376	T	T	T
0.0833730288152890	0.1667141918287835	0.2048519318156109	T	T	T
0.2500000000000000	0.0000000000000000	0.1155260000000027	F	F	F
0.2504581749741018	-0.0000376331618427	0.3833150564840150	T	T	T
0.4166669999999968	0.0833330000000032	0.0259050000000016	F	F	F
0.4166560857276777	0.0840715919492045	0.2947917842013258	T	T	T
0.3333278950263539	0.1667505562411292	0.2048746735118235	T	T	T
0.5000000000000000	0.0000000000000000	0.1155260000000027	F	F	F
0.5003814620326258	0.9985036953827234	0.3832283029471377	T	T	T
0.6666669999999968	0.0833330000000032	0.0259050000000016	F	F	F
0.6667919963857180	0.0835697630406962	0.2943619821401556	T	T	T
0.5831142042516886	0.1667595294865883	0.2052000833158677	T	T	T
0.7500000000000000	0.0000000000000000	0.1155260000000027	F	F	F
0.7479512014862597	0.9981166537161092	0.3830677306343636	T	T	T
0.9166669999999968	0.0833330000000032	0.0259050000000016	F	F	F
0.9172470727564083	0.0836899546714231	0.2946543627136161	T	T	T
0.8336415952243000	0.1667359530864604	0.2051825747088871	T	T	T
0.0000000000000000	0.2500000000000000	0.1155260000000027	F	F	F
-0.0004057062750035	0.2503143735506984	0.3830904672678928	T	T	T
0.1666669999999968	0.3333330000000032	0.0259050000000016	F	F	F
0.1680509088308318	0.3326930972302064	0.2951008960253552	T	T	T
0.0835193579975009	0.4164694607168486	0.2052883409295580	T	T	T
0.2500000000000000	0.2500000000000000	0.1155260000000027	F	F	F
0.4166669999999968	0.3333330000000032	0.0259050000000016	F	F	F
0.4146915083327085	0.3326577121384398	0.2951549177737526	T	T	T
0.3333714216541440	0.4166775627705270	0.2048552428082198	T	T	T
0.5000000000000000	0.2500000000000000	0.1155260000000027	F	F	F
0.5021434273630173	0.2521666611035980	0.3833415887721139	T	T	T
0.6666669999999968	0.3333330000000032	0.0259050000000016	F	F	F
0.6662795692423635	0.3337767256310906	0.2942304856333556	T	T	T
0.5827044474268855	0.4163532499923852	0.2049658570413080	T	T	T
0.7500000000000000	0.2500000000000000	0.1155260000000027	F	F	F
0.7497264893129262	0.2517369171043021	0.3830765542984436	T	T	T
0.9166669999999968	0.3333330000000032	0.0259050000000016	F	F	F
0.9171339728398721	0.3333906842290171	0.2945193399138766	T	T	T
0.8333626579641895	0.4164482259880286	0.2048586470908503	T	T	T
0.0000000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.9986266241167258	0.5007066363333823	0.3831571917782697	T	T	T
0.1666669999999968	0.5833330000000032	0.0259050000000016	F	F	F
0.1668116431669646	0.5828500346806642	0.2946014337154156	T	T	T
0.0834794433058327	0.6667363814738664	0.2052395046413907	T	T	T
0.2500000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.2525013423289483	0.5023876097254254	0.3832459638503477	T	T	T
0.4166669999999968	0.5833330000000032	0.0259050000000016	F	F	F
0.4167972878713321	0.5830533004540170	0.2942601511084039	T	T	T
0.3331425366291315	0.6663238084216971	0.2048381059553923	T	T	T
0.5000000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.5020399729190269	0.5024469805680342	0.3833599086059212	T	T	T
0.6666669999999968	0.5833330000000032	0.0259050000000016	F	F	F

	0.6662045734017631	0.5828391257613227	0.2940933603386058	T	T	T
	0.5831909352094619	0.6662778342841700	0.2047919032591651	T	T	T
	0.7500000000000000	0.5000000000000000	0.1155260000000027	F	F	F
	0.9166669999999968	0.5833330000000032	0.0259050000000016	F	F	F
	0.9164597572775138	0.5832720439308146	0.2940059574780517	T	T	T
	0.8333756355278840	0.6668978726523225	0.2048634675383412	T	T	T
	0.0000000000000000	0.7500000000000000	0.1155260000000027	F	F	F
	0.9980902104114625	0.7480011463254914	0.3832285880349115	T	T	T
	0.1666669999999968	0.8333330000000032	0.0259050000000016	F	F	F
	0.1666862134359593	0.8337976241531573	0.2947902255761268	T	T	T
	0.0835214576602036	0.9170861909859439	0.2053141017882069	T	T	T
	0.2500000000000000	0.7500000000000000	0.1155260000000027	F	F	F
	0.2519419535244845	0.7501792795676742	0.3832272614608599	T	T	T
	0.4166669999999968	0.8333330000000032	0.0259050000000016	F	F	F
	0.4167847849857433	0.8333156605599624	0.2940242260835641	T	T	T
	0.3333124615613856	0.9169788095228399	0.2052267452956246	T	T	T
	0.5000000000000000	0.7500000000000000	0.1155260000000027	F	F	F
	0.6666669999999968	0.8333330000000032	0.0259050000000016	F	F	F
	0.6665778424523802	0.8330637388611376	0.2939929418329614	T	T	T
	0.5834342962758019	0.9168803760458099	0.2047144595739946	T	T	T
	0.7500000000000000	0.7500000000000000	0.1155260000000027	F	F	F
	0.7481129011980754	0.7484406814656396	0.3831958629699698	T	T	T
	0.9166669999999968	0.8333330000000032	0.0259050000000016	F	F	F
	0.9168893170348286	0.8336877035107078	0.2945721535490203	T	T	T
	0.8336671234546316	0.9169259256202323	0.2051727892761757	T	T	T
	0.2496948487956715	0.2512289816536036	0.5109425123961404	T	T	T
4Ni/Cu(111) ^{PC}	1.0000000000000000					
	8.8905908144889398	-5.1329849999999997	0.0000000000000000			
	0.0000000000000000	10.2659699999999994	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.3821300000000001			
	Ni	C	Cu	O		
	4	1	76	1		
	Selective dynamics					
	Direct					
	0.2535080523539001	0.2540076744524531	0.3822661433499226	T	T	T
	0.4989872384241210	0.2521940920475040	0.3824307733487788	T	T	T
	0.2511689024293861	0.5001843385469931	0.3794823187976107	T	T	T
	0.4970649210248836	0.4973254921310180	0.3822702773542936	T	T	T
	0.4164316971530276	0.3340507121018939	0.4369182160820224	T	T	T
	0.0000000000000000	0.0000000000000000	0.1155260000000027	F	F	F
	0.0030861524161146	0.0027459556131514	0.3829543675368158	T	T	T
	0.1666669999999968	0.0833330000000032	0.0259050000000016	F	F	F
	0.1682110734612620	0.0846828167501248	0.2944556626178895	T	T	T
	0.0837849069767738	0.1667329012043758	0.2048293587784339	T	T	T
	0.2500000000000000	0.0000000000000000	0.1155260000000027	F	F	F
	0.2513988229859014	0.0015959324338689	0.3830867910747979	T	T	T
	0.4166669999999968	0.0833330000000032	0.0259050000000016	F	F	F
	0.4176115557245277	0.0845040401776584	0.2945152222179397	T	T	T
	0.3337953677923277	0.1665276161970715	0.2047060553535038	T	T	T
	0.5000000000000000	0.0000000000000000	0.1155260000000027	F	F	F
	0.5004874559384500	0.0018717856195954	0.3829506777228709	T	T	T

0.6666669999999968	0.0833330000000032	0.0259050000000016	F	F	F
0.6672509257323213	0.0837691974622781	0.2945719577206129	T	T	T
0.5839237291274746	0.1667491627568979	0.2048952892257387	T	T	T
0.7500000000000000	0.0000000000000000	0.1155260000000027	F	F	F
0.7507635012070143	0.0002931752980953	0.3830964327069610	T	T	T
0.9166669999999968	0.0833330000000032	0.0259050000000016	F	F	F
0.9178049174143506	0.0839934026290923	0.2945717320783791	T	T	T
0.8339614451716904	0.1669831187366352	0.2052292377726300	T	T	T
0.0000000000000000	0.2500000000000000	0.1155260000000027	F	F	F
0.0049078435360575	0.2523100340022340	0.3829514738280587	T	T	T
0.1666669999999968	0.3333330000000032	0.0259050000000016	F	F	F
0.1681878664022875	0.3336422446311955	0.2939398805521077	T	T	T
0.0837929054943699	0.4167680340982851	0.2047816368009776	T	T	T
0.2500000000000000	0.2500000000000000	0.1155260000000027	F	F	F
0.4166669999999968	0.3333330000000032	0.0259050000000016	F	F	F
0.4173951204769091	0.3334657983020384	0.2932691798857265	T	T	T
0.3338375316268157	0.4168234297933524	0.2043271775658424	T	T	T
0.5000000000000000	0.2500000000000000	0.1155260000000027	F	F	F
0.6666669999999968	0.3333330000000032	0.0259050000000016	F	F	F
0.6665033188184376	0.3334558588497848	0.2945302433961693	T	T	T
0.5840546974187478	0.4168110841146508	0.2046824697989954	T	T	T
0.7500000000000000	0.2500000000000000	0.1155260000000027	F	F	F
0.7493775491776176	0.2507198951501080	0.3829354659865035	T	T	T
0.9166669999999968	0.3333330000000032	0.0259050000000016	F	F	F
0.9175806330059221	0.3336507680106010	0.2944684726329400	T	T	T
0.8336520308281401	0.4167278284164324	0.2051705566250674	T	T	T
0.0000000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.0028307708723730	0.5000810260803362	0.3833262680535957	T	T	T
0.1666669999999968	0.5833330000000032	0.0259050000000016	F	F	F
0.1679097684991921	0.5831602494466493	0.2943047701780777	T	T	T
0.0838466491680663	0.6667735040944781	0.2052578136941667	T	T	T
0.2500000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.4166669999999968	0.5833330000000032	0.0259050000000016	F	F	F
0.4173526832435662	0.5827348456573813	0.2939773255157349	T	T	T
0.3339821692609506	0.6669124131712155	0.2047965205002739	T	T	T
0.5000000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.6666669999999968	0.5833330000000032	0.0259050000000016	F	F	F
0.6661972944300746	0.5827027118908603	0.2944748792628188	T	T	T
0.5838903999219117	0.6668888768764679	0.2048277086586304	T	T	T
0.7500000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.7496785175709069	0.4998017481983318	0.3831084419400963	T	T	T
0.9166669999999968	0.5833330000000032	0.0259050000000016	F	F	F
0.9172680048758749	0.5833272656540540	0.2947242893035688	T	T	T
0.8336890760681154	0.6666382757800775	0.2051732327362911	T	T	T
0.0000000000000000	0.7500000000000000	0.1155260000000027	F	F	F
0.0009168368784967	0.7504099421772228	0.3833368073271601	T	T	T
0.1666669999999968	0.8333330000000032	0.0259050000000016	F	F	F
0.1677006577155802	0.8336786128101168	0.2947280551502332	T	T	T
0.0839652717410700	0.9168415706787791	0.2051748869090519	T	T	T
0.2500000000000000	0.7500000000000000	0.1155260000000027	F	F	F
0.2510584451039515	0.7484520351064786	0.3833577552166147	T	T	T

	0.416666999999968 0.8333330000000032 0.0259050000000016 F F F
	0.4174085826748065 0.8334134390637232 0.2945053866394844 T T T
	0.3339535236662524 0.9169537077278855 0.2051903393702654 T T T
	0.5000000000000000 0.7500000000000000 0.1155260000000027 F F F
	0.4988486255028184 0.7462041241398093 0.3830001513551097 T T T
	0.666666999999968 0.8333330000000032 0.0259050000000016 F F F
	0.6668878783288926 0.8330237640508980 0.2945863048645385 T T T
	0.5837915004301680 0.9167775051616376 0.2052521720935874 T T T
	0.7500000000000000 0.7500000000000000 0.1155260000000027 F F F
	0.7484221028308204 0.7480277103512002 0.3829965471279013 T T T
	0.916666999999968 0.8333330000000032 0.0259050000000016 F F F
	0.9173508456452255 0.8334834581279232 0.2946159341921837 T T T
	0.8339322892998853 0.9167772411042538 0.2052517305928542 T T T
	0.4166327898820530 0.3338319120675253 0.4881740956339279 T T T
2Pd/Cu(111) ^{s1}	1.0000000000000000
	8.8905908144889398 -5.1329849999999997 0.0000000000000000
	0.0000000000000000 10.2659699999999994 0.0000000000000000
	0.0000000000000000 0.0000000000000000 23.3821300000000001
	C Pd Cu O
	1 2 78 1
	Selective dynamics
	Direct
	0.7510796294802117 0.7514342419261274 0.4768804152844329 T T T
	0.2488740397923401 0.4994484860269107 0.3869531730165413 T T T
	0.7506218322527042 0.7503552012931342 0.3955202653965459 T T T
	0.0000000000000000 0.0000000000000000 0.1155260000000027 F F F
	0.0045503781856492 0.0044250780714837 0.3832452324798561 T T T
	0.166666999999968 0.0833330000000032 0.0259050000000016 F F F
	0.1663325384175703 0.0829114588819230 0.2940169175631727 T T T
	0.0831387647206780 0.1666962072893106 0.2051397289943289 T T T
	0.2500000000000000 0.0000000000000000 0.1155260000000027 F F F
	0.2509886800740955 0.0005045833528783 0.3827876177882474 T T T
	0.416666999999968 0.0833330000000032 0.0259050000000016 F F F
	0.4166676887121952 0.0833542560552683 0.2937445528860173 T T T
	0.3333121539998525 0.1669411739838901 0.2048948423563457 T T T
	0.5000000000000000 0.0000000000000000 0.1155260000000027 F F F
	0.4997166763922626 0.0014625023664975 0.3829355083893323 T T T
	0.666666999999968 0.0833330000000032 0.0259050000000016 F F F
	0.6665836630795328 0.0829152128676908 0.2940680835487068 T T T
	0.5835561895132801 0.1667842832513933 0.2047807818901334 T T T
	0.7500000000000000 0.0000000000000000 0.1155260000000027 F F F
	0.7499210206293671 0.0048730869535350 0.3832704896605077 T T T
	0.916666999999968 0.0833330000000032 0.0259050000000016 F F F
	0.9161624961155305 0.0824835727514675 0.2944413795578602 T T T
	0.8334438353059868 0.1665081570222966 0.2050675948250591 T T T
	0.0000000000000000 0.2500000000000000 0.1155260000000027 F F F
	0.9968815132989172 0.2476056251124364 0.3835319766092254 T T T
	0.166666999999968 0.3333330000000032 0.0259050000000016 F F F
	0.1664424258099354 0.3328023000217899 0.2941960277341080 T T T
	0.0833448184286484 0.4166827736833666 0.2048214921715863 T T T
	0.2500000000000000 0.2500000000000000 0.1155260000000027 F F F

0.2502798057400341	0.2466390987258079	0.3833715661415674	T	T	T
0.4166669999999968	0.3333330000000032	0.0259050000000016	F	F	F
0.4170157053102310	0.3338308049828936	0.2942941463974265	T	T	T
0.3336851960377315	0.4170676003373854	0.2049961878052272	T	T	T
0.5000000000000000	0.2500000000000000	0.1155260000000027	F	F	F
0.4997285318140122	0.2482842275129252	0.3829502278484175	T	T	T
0.6666669999999968	0.3333330000000032	0.0259050000000016	F	F	F
0.6665854716674909	0.3337013779476755	0.2940716972131768	T	T	T
0.5836414756867248	0.4174595883720625	0.2052805403907102	T	T	T
0.7500000000000000	0.2500000000000000	0.1155260000000027	F	F	F
0.7493106481703150	0.2496715315681041	0.3828280822975949	T	T	T
0.9166669999999968	0.3333330000000032	0.0259050000000016	F	F	F
0.9168621241019782	0.3334416139887491	0.2942644105322285	T	T	T
0.8334489670917468	0.4169611368001887	0.2050695123101963	T	T	T
0.0000000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.9968787669580057	0.4993023937409187	0.3835336330974771	T	T	T
0.1666669999999968	0.5833330000000032	0.0259050000000016	F	F	F
0.1664394669753634	0.5836425851934827	0.2942002190362786	T	T	T
0.0831354990336480	0.6664507596213103	0.2051435084040472	T	T	T
0.2500000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.4166669999999968	0.5833330000000032	0.0259050000000016	F	F	F
0.4180722375802406	0.5840413547190211	0.2946876661277589	T	T	T
0.3336745806968618	0.6666297305894676	0.2049965991350195	T	T	T
0.5000000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.4986825521145953	0.4942864765754546	0.3838954569444702	T	T	T
0.6666669999999968	0.5833330000000032	0.0259050000000016	F	F	F
0.6678063178808819	0.5854585802330092	0.2955087816710196	T	T	T
0.5832467735618969	0.6666239985701599	0.2051064785711144	T	T	T
0.7500000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.7499125638939727	0.4950834362282975	0.3832910970386194	T	T	T
0.9166669999999968	0.5833330000000032	0.0259050000000016	F	F	F
0.9161555000965197	0.5836909856164467	0.2944515733774989	T	T	T
0.8332154905528967	0.6667361795828899	0.2048691777984587	T	T	T
0.0000000000000000	0.7500000000000000	0.1155260000000027	F	F	F
0.0045238636327796	0.7501500585548305	0.3832526520947009	T	T	T
0.1666669999999968	0.8333330000000032	0.0259050000000016	F	F	F
0.1663201543008636	0.8334312180686094	0.2940193918264720	T	T	T
0.0824975924039474	0.9162545435804185	0.2051247390527302	T	T	T
0.2500000000000000	0.7500000000000000	0.1155260000000027	F	F	F
0.2502593426324006	0.7536588846567952	0.3833685674914500	T	T	T
0.4166669999999968	0.8333330000000032	0.0259050000000016	F	F	F
0.4170021685025903	0.8332046785717839	0.2942906859592139	T	T	T
0.3333131642244525	0.9163874780716610	0.2048973915559399	T	T	T
0.5000000000000000	0.7500000000000000	0.1155260000000027	F	F	F
0.4986889364615516	0.7544236366338621	0.3838777905929029	T	T	T
0.6666669999999968	0.8333330000000032	0.0259050000000016	F	F	F
0.6677886931231999	0.8323884275362489	0.2954807014920349	T	T	T
0.5836340816535373	0.9162004538016375	0.2052732148091435	T	T	T
0.7500000000000000	0.7500000000000000	0.1155260000000027	F	F	F
0.9166669999999968	0.8333330000000032	0.0259050000000016	F	F	F
0.9146115619973779	0.8323174383882596	0.2953873238029754	T	T	T

	0.8332214542630363	0.9164912160855063	0.2048659267777560	T	T	T
	0.7515411994616943	0.7523746726084798	0.5263970366307343	T	T	T
3Pd/Cu(111) ^{S1}	1.000000000000000					
	8.8905908144889398	-5.1329849999999997	0.0000000000000000			
	0.0000000000000000	10.2659699999999994	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.3821300000000001			
	C	Pd	Cu	O		
	1	3	77	1		
	Selective dynamics					
	Direct					
	0.7515346262747195	0.5044810137481434	0.4773887358747249	T	T	T
	0.2480531995153146	0.2485349711325794	0.3868252739875564	T	T	T
	0.7512048436754496	0.5005711566252015	0.3960033986280816	T	T	T
	0.4995850066725295	0.7513932099670414	0.3867595308180180	T	T	T
	0.0000000000000000	0.0000000000000000	0.1155260000000027	F	F	F
	0.9976043759537845	0.9981639212474983	0.3832885313168330	T	T	T
	0.1666669999999968	0.0833330000000032	0.0259050000000016	F	F	F
	0.1663495823808418	0.0827698919422280	0.2938465551649709	T	T	T
	0.0833113800545963	0.1667856263268097	0.2046596895982729	T	T	T
	0.2500000000000000	0.0000000000000000	0.1155260000000027	F	F	F
	0.2498233602419309	0.9970774924311385	0.3831254332293071	T	T	T
	0.4166669999999968	0.0833330000000032	0.0259050000000016	F	F	F
	0.4170444983513221	0.0841865251141880	0.2941225159823653	T	T	T
	0.3337344738549978	0.1671749584431045	0.2048132040978801	T	T	T
	0.5000000000000000	0.0000000000000000	0.1155260000000027	F	F	F
	0.4995631119664199	0.0022639481562276	0.3833135382041057	T	T	T
	0.6666669999999968	0.0833330000000032	0.0259050000000016	F	F	F
	0.6664734488217348	0.0835676256932476	0.2942453543919920	T	T	T
	0.5837737098456047	0.1675261545507458	0.2053390151810522	T	T	T
	0.7500000000000000	0.0000000000000000	0.1155260000000027	F	F	F
	0.7528720148389524	0.0031957609817419	0.3832514517047058	T	T	T
	0.9166669999999968	0.0833330000000032	0.0259050000000016	F	F	F
	0.9168947577922197	0.0836512739486187	0.2940702659642040	T	T	T
	0.8332363809827458	0.1669732688032992	0.2050983363677472	T	T	T
	0.0000000000000000	0.2500000000000000	0.1155260000000027	F	F	F
	0.9968462040925787	0.2495949576025167	0.3832987502521942	T	T	T
	0.1666669999999968	0.3333330000000032	0.0259050000000016	F	F	F
	0.1663555528062582	0.3337117372540432	0.2940203355820230	T	T	T
	0.0831419183172380	0.4166804936704214	0.2051577390891946	T	T	T
	0.2500000000000000	0.2500000000000000	0.1155260000000027	F	F	F
	0.4166669999999968	0.3333330000000032	0.0259050000000016	F	F	F
	0.4178305210770215	0.3339817814122304	0.2944161800491444	T	T	T
	0.3338023095566990	0.4170426194987118	0.2050433558691542	T	T	T
	0.5000000000000000	0.2500000000000000	0.1155260000000027	F	F	F
	0.4986709807261357	0.2452173456734657	0.3837241590873041	T	T	T
	0.6666669999999968	0.3333330000000032	0.0259050000000016	F	F	F
	0.6678744880707579	0.3357552496878468	0.2955013293528893	T	T	T
	0.5833954646402146	0.4168866184999842	0.2051682463520497	T	T	T
	0.7500000000000000	0.2500000000000000	0.1155260000000027	F	F	F
	0.7501251091312998	0.2460591824312202	0.3831972804636224	T	T	T
	0.9166669999999968	0.3333330000000032	0.0259050000000016	F	F	F

	0.9160528491237789	0.3337951681650603	0.2943168993781972	T	T	T
	0.8331513272876084	0.4168025111745629	0.2048060707466961	T	T	T
	0.0000000000000000	0.5000000000000000	0.1155260000000027	F	F	F
	0.0035006574032579	0.4999235782064229	0.3831294183866119	T	T	T
	0.1666669999999968	0.5833330000000032	0.0259050000000016	F	F	F
	0.1664814764441919	0.5835828454939942	0.2941531562785946	T	T	T
	0.0825218677537007	0.6661828174270290	0.2051376484219035	T	T	T
	0.2500000000000000	0.5000000000000000	0.1155260000000027	F	F	F
	0.2461479767525984	0.5000004499561697	0.3838483953666856	T	T	T
	0.4166669999999968	0.5833330000000032	0.0259050000000016	F	F	F
	0.4166705992728857	0.5827192001706428	0.2943315279330738	T	T	T
	0.3333168906170438	0.6665046609134279	0.2048813812579776	T	T	T
	0.5000000000000000	0.5000000000000000	0.1155260000000027	F	F	F
	0.4983864483932693	0.4998432784900052	0.3841468486783884	T	T	T
	0.6666669999999968	0.5833330000000032	0.0259050000000016	F	F	F
	0.6677701920984080	0.5825981943501805	0.2956962728827946	T	T	T
	0.5836029723664655	0.6662702145731298	0.2052480284080007	T	T	T
	0.7500000000000000	0.5000000000000000	0.1155260000000027	F	F	F
	0.9166669999999968	0.5833330000000032	0.0259050000000016	F	F	F
	0.9145177320483467	0.5823590713418344	0.2952840151986186	T	T	T
	0.8329838986790312	0.6663616840183543	0.2048981761053813	T	T	T
	0.0000000000000000	0.7500000000000000	0.1155260000000027	F	F	F
	0.0042713715431530	0.7547242722280983	0.3829878200009829	T	T	T
	0.1666669999999968	0.8333330000000032	0.0259050000000016	F	F	F
	0.1661948925192807	0.8329343846570302	0.2938201026564566	T	T	T
	0.0830785756206869	0.9166514724829840	0.2049425973905238	T	T	T
	0.2500000000000000	0.7500000000000000	0.1155260000000027	F	F	F
	0.2472118248726116	0.7505442786230923	0.3831713650801500	T	T	T
	0.4166669999999968	0.8333330000000032	0.0259050000000016	F	F	F
	0.4163800786134005	0.8338074539763841	0.2938333275289835	T	T	T
	0.3335124430593349	0.9168545887374180	0.2049996337758153	T	T	T
	0.5000000000000000	0.7500000000000000	0.1155260000000027	F	F	F
	0.6666669999999968	0.8333330000000032	0.0259050000000016	F	F	F
	0.6671169516390661	0.8333006118731555	0.2941045734969085	T	T	T
	0.5834995797130496	0.9168470758989971	0.2047648121063315	T	T	T
	0.7500000000000000	0.7500000000000000	0.1155260000000027	F	F	F
	0.7540701230660102	0.7555708571307281	0.3836795523869114	T	T	T
	0.9166669999999968	0.8333330000000032	0.0259050000000016	F	F	F
	0.9161709546527721	0.8325942877792778	0.2941620168511247	T	T	T
	0.8330607972485531	0.9164221185655992	0.2051266050002470	T	T	T
	0.7514920980334349	0.5080862827296094	0.5268710145048476	T	T	T
4Pd/Cu(111) ^{S1}	1.0000000000000000					
	8.8905908144889398	-5.1329849999999997	0.0000000000000000			
	0.0000000000000000	10.2659699999999994	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.3821300000000001			
	C Pd Cu O					
	1 4 76 1					
	Selective dynamics					
	Direct					
	0.7504305946840859	0.4979094911886283	0.4777062467910088	T	T	T
	0.0002459671478988	0.2480510038668128	0.3866727396310351	T	T	T

0.7500406649444229	0.4984265081759575	0.3962678469241873	T	T	T
0.4998103270271710	0.7484529242714166	0.3866037115123278	T	T	T
0.2499606182049249	0.9984544860892086	0.3864296047468170	T	T	T
0.0000000000000000	0.2484235322000004	0.1155260000000027	F	F	F
0.1666669999999968	0.3317565322000036	0.0259050000000016	F	F	F
0.1671236230132817	0.3322012927773296	0.2939421836985820	T	T	T
0.0831305031143316	0.4153325770389041	0.2048755372609383	T	T	T
0.2500000000000000	0.2484235322000004	0.1155260000000027	F	F	F
0.2522835006218786	0.2508686347244561	0.3838605351791677	T	T	T
0.4166669999999968	0.3317565322000036	0.0259050000000016	F	F	F
0.4173809400108299	0.3319490994498821	0.2943832725638501	T	T	T
0.3336528684992109	0.4153080114890997	0.2052461510871900	T	T	T
0.5000000000000000	0.2484235322000004	0.1155260000000027	F	F	F
0.4989500022356992	0.2476479729666095	0.3836277436131643	T	T	T
0.6666669999999968	0.3317565322000036	0.0259050000000016	F	F	F
0.6678205288078766	0.3342331841123227	0.2953862721893568	T	T	T
0.5836194494358550	0.4154528834228004	0.2050126663386666	T	T	T
0.7500000000000000	0.2484235322000004	0.1155260000000027	F	F	F
0.7471024970376802	0.2443311685824581	0.3836205481226174	T	T	T
0.9166669999999968	0.3317565322000036	0.0259050000000016	F	F	F
0.9159890878375097	0.3325987784721429	0.2942562481307823	T	T	T
0.8334072971986115	0.4152347406651359	0.2049292074482430	T	T	T
0.0000000000000000	0.4984235322000004	0.1155260000000027	F	F	F
0.0040865487318631	0.5012627670015881	0.3836040666024883	T	T	T
0.1666669999999968	0.5817565322000036	0.0259050000000016	F	F	F
0.1663672116731673	0.5816611604044200	0.2943189374902458	T	T	T
0.0828024555680121	0.6649305030125120	0.2054442592077350	T	T	T
0.2500000000000000	0.4984235322000004	0.1155260000000027	F	F	F
0.2499509163017352	0.4983117649972615	0.3837998782466368	T	T	T
0.4166669999999968	0.5817565322000036	0.0259050000000016	F	F	F
0.4169649723491629	0.5814271297256076	0.2940403078051104	T	T	T
0.3332907675526556	0.6651315447971060	0.2049425877680001	T	T	T
0.5000000000000000	0.4984235322000004	0.1155260000000027	F	F	F
0.4955257222383322	0.4949882789936458	0.3837116515884556	T	T	T
0.6666669999999968	0.5817565322000036	0.0259050000000016	F	F	F
0.6677056594873955	0.5807878599052542	0.2957482665433328	T	T	T
0.5838849902128521	0.6647716892561560	0.2050731707969338	T	T	T
0.7500000000000000	0.4984235322000004	0.1155260000000027	F	F	F
0.9166669999999968	0.5817565322000036	0.0259050000000016	F	F	F
0.9143084432538391	0.5807127563323357	0.2953994122439856	T	T	T
0.8331834264761218	0.6650174187133961	0.2050124778739878	T	T	T
0.0000000000000000	0.7484235322000004	0.1155260000000027	F	F	F
0.0007906558029348	0.7494911121562701	0.3836335453898841	T	T	T
0.1666669999999968	0.8317565322000036	0.0259050000000016	F	F	F
0.1659595508730373	0.8308130409414458	0.2939790110866209	T	T	T
0.0831410011248654	0.9149735987021667	0.2048720176842322	T	T	T
0.2500000000000000	0.7484235322000004	0.1155260000000027	F	F	F
0.2474056824071645	0.7458022847712720	0.3838302585751575	T	T	T
0.4166669999999968	0.8317565322000036	0.0259050000000016	F	F	F
0.4162828854673921	0.8323051653706762	0.2940524834568250	T	T	T
0.3335310769766895	0.9151091639709226	0.2048514935635810	T	T	T

	0.5000000000000000	0.7484235322000004	0.1155260000000027	F	F	F
	0.6666669999999968	0.8317565322000036	0.0259050000000016	F	F	F
	0.6671140443426287	0.8315894105651240	0.2940366054145350	T	T	T
	0.5835055272358867	0.9153494221138412	0.2049421872407279	T	T	T
	0.7500000000000000	0.7484235322000004	0.1155260000000027	F	F	F
	0.7533596209864873	0.7528578196801743	0.3836857004001287	T	T	T
	0.9166669999999968	0.8317565322000036	0.0259050000000016	F	F	F
	0.9166009189762169	0.8311408375221676	0.2943894555570823	T	T	T
	0.8333529021307712	0.9150060350856569	0.2052475679928251	T	T	T
	0.0000000000000000	0.9984235322000004	0.1155260000000027	F	F	F
	0.9974819961637769	0.9960548636563336	0.3838926262468721	T	T	T
	0.1666669999999968	0.0817565322000036	0.0259050000000016	F	F	F
	0.1662848669036741	0.0822808250860453	0.2940432109787451	T	T	T
	0.0835602202019996	0.1650729967406230	0.2047692510416992	T	T	T
	0.2500000000000000	0.9984235322000004	0.1155260000000027	F	F	F
	0.4166669999999968	0.0817565322000036	0.0259050000000016	F	F	F
	0.4177124894451403	0.0826105228151497	0.2939777499489967	T	T	T
	0.3336533246287390	0.1654810990875786	0.2048709817009267	T	T	T
	0.5000000000000000	0.9984235322000004	0.1155260000000027	F	F	F
	0.5025741117036785	0.0009552648879158	0.3837884216113994	T	T	T
	0.6666669999999968	0.0817565322000036	0.0259050000000016	F	F	F
	0.6669330237640245	0.0822336381551494	0.2943137988018782	T	T	T
	0.5837231173355049	0.1658402277298376	0.2054444042996166	T	T	T
	0.7500000000000000	0.9984235322000004	0.1155260000000027	F	F	F
	0.7499998529742877	0.9983827715491987	0.3837944190041935	T	T	T
	0.9166669999999968	0.0817565322000036	0.0259050000000016	F	F	F
	0.9163816510296510	0.0814164076460805	0.2939463225333164	T	T	T
	0.8333048799268138	0.1654938284466772	0.2048788440143615	T	T	T
	0.7506874909510606	0.4979093244425375	0.5272163711422024	T	T	T
2Pt/Cu(111) ^{s2}	1.0000000000000000					
	8.8905908144889398	-5.1329849999999997	0.0000000000000000			
	0.0000000000000000	10.2659699999999994	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.3821300000000001			
	C Pt Cu O					
	1 2 78 1					
	Selective dynamics					
	Direct					
	0.4995636118365108	0.2516512563683406	0.4747699574867343	T	T	T
	0.4999281630667736	0.2501706745059784	0.3947351112319890	T	T	T
	0.5002609611927691	0.7502510128111395	0.3840402142454640	T	T	T
	0.0000000000000000	0.0000000000000000	0.1155260000000027	F	F	F
	0.9993552961884354	0.9997643427917425	0.3831086448575352	T	T	T
	0.1666669999999968	0.0833330000000032	0.0259050000000016	F	F	F
	0.1668912289966941	0.0835005669079640	0.2943985038042399	T	T	T
	0.0835762934612242	0.1667525263171417	0.2050726555135433	T	T	T
	0.2500000000000000	0.0000000000000000	0.1155260000000027	F	F	F
	0.2446592913229321	0.9958376168543619	0.3839635914558123	T	T	T
	0.4166669999999968	0.0833330000000032	0.0259050000000016	F	F	F
	0.4179700536615337	0.0857263253998325	0.2959295280704375	T	T	T
	0.3334738098689066	0.1667691750908783	0.2049907711776592	T	T	T
	0.5000000000000000	0.0000000000000000	0.1155260000000027	F	F	F

0.5001761052329629	0.9984548920245460	0.3854684835394123	T	T	T
0.6666669999999968	0.0833330000000032	0.0259050000000016	F	F	F
0.6666152654520187	0.0838253501497297	0.2948382094701558	T	T	T
0.5832999584638178	0.1667244719422385	0.2050462369550037	T	T	T
0.7500000000000000	0.0000000000000000	0.1155260000000027	F	F	F
0.7534575024058500	0.0020338802416661	0.3843848997110604	T	T	T
0.9166669999999968	0.0833330000000032	0.0259050000000016	F	F	F
0.9165204840448176	0.0835268479586370	0.2943031769327000	T	T	T
0.8329162309917115	0.1667365056288317	0.2051349803385724	T	T	T
0.0000000000000000	0.2500000000000000	0.1155260000000027	F	F	F
0.0000026174517599	0.2501373511285430	0.3828154825280901	T	T	T
0.1666669999999968	0.3333330000000032	0.0259050000000016	F	F	F
0.1670958403944015	0.3334383401810504	0.2943914862214665	T	T	T
0.0831517612877827	0.4165111623714244	0.2050072607901217	T	T	T
0.2500000000000000	0.2500000000000000	0.1155260000000027	F	F	F
0.2445975979418125	0.2490005885724981	0.3839181099391107	T	T	T
0.4166669999999968	0.3333330000000032	0.0259050000000016	F	F	F
0.4179283014672824	0.3324288899450085	0.2958634830674299	T	T	T
0.3338157154086288	0.4162398524459617	0.2053897401462344	T	T	T
0.5000000000000000	0.2500000000000000	0.1155260000000027	F	F	F
0.6666669999999968	0.3333330000000032	0.0259050000000016	F	F	F
0.6643010324761184	0.3322194266704344	0.2956828863019358	T	T	T
0.5833066601905122	0.4166521048672666	0.2050349218476255	T	T	T
0.7500000000000000	0.2500000000000000	0.1155260000000027	F	F	F
0.7548559489796778	0.2503626116662658	0.3839584049487589	T	T	T
0.9166669999999968	0.3333330000000032	0.0259050000000016	F	F	F
0.9160284886483822	0.3333672812264533	0.2943173733638723	T	T	T
0.8322541538320479	0.4161632889646014	0.2053869537208619	T	T	T
0.0000000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.0007910873008787	0.5004911162683117	0.3829819486724609	T	T	T
0.1666669999999968	0.5833330000000032	0.0259050000000016	F	F	F
0.1663446310310197	0.5832514804973411	0.2940738727927390	T	T	T
0.0831618465264543	0.6667347129727015	0.2050034846600417	T	T	T
0.2500000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.2470196671344107	0.4981356949951922	0.3841275443685182	T	T	T
0.4166669999999968	0.5833330000000032	0.0259050000000016	F	F	F
0.4157517659094069	0.5810412997575620	0.2935904282567956	T	T	T
0.3331598290303645	0.6666296593007974	0.2046934159698877	T	T	T
0.5000000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.5001762612149567	0.5020437863393262	0.3854033919477687	T	T	T
0.6666669999999968	0.5833330000000032	0.0259050000000016	F	F	F
0.6666249932331425	0.5829369248098722	0.2948056231366283	T	T	T
0.5834026121609874	0.6661774595329131	0.2048483212730439	T	T	T
0.7500000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.7549163316646285	0.5047568160758533	0.3839230376655649	T	T	T
0.9166669999999968	0.5833330000000032	0.0259050000000016	F	F	F
0.9160483870356596	0.5828064278418044	0.2943060044473944	T	T	T
0.8329266845154764	0.6662644002258410	0.2051238892714716	T	T	T
0.0000000000000000	0.7500000000000000	0.1155260000000027	F	F	F
0.0000268338091934	0.7500758122280736	0.3828177179697473	T	T	T
0.1666669999999968	0.8333330000000032	0.0259050000000016	F	F	F

	0.1671148019297860	0.8338196726230342	0.2943993441466898	T	T	T
	0.0835809961293731	0.9169083649675291	0.2050718926503631	T	T	T
	0.2500000000000000	0.7500000000000000	0.1155260000000027	F	F	F
	0.2470393737094589	0.7491220482521329	0.3841399629735833	T	T	T
	0.4166669999999968	0.8333330000000032	0.0259050000000016	F	F	F
	0.4157530831570057	0.8348970309314078	0.2936001132706672	T	T	T
	0.3338320466840284	0.9176895769238078	0.2054059375607364	T	T	T
	0.5000000000000000	0.7500000000000000	0.1155260000000027	F	F	F
	0.6666669999999968	0.8333330000000032	0.0259050000000016	F	F	F
	0.6683972225158917	0.8342731914876612	0.2934947650207411	T	T	T
	0.5834048942404170	0.9173240221830020	0.2048568949079025	T	T	T
	0.7500000000000000	0.7500000000000000	0.1155260000000027	F	F	F
	0.7534494398261996	0.7516513528619824	0.3843680607013051	T	T	T
	0.9166669999999968	0.8333330000000032	0.0259050000000016	F	F	F
	0.9165236073626968	0.8331153749283069	0.2942971376450855	T	T	T
	0.8331835426013688	0.9166312407842564	0.2049269653877104	T	T	T
	0.4992598361202553	0.2528474233696433	0.5244778454334272	T	T	T
3Pt/Cu(111) ^{s2}	1.0000000000000000					
	8.8905908144889398	-5.1329849999999997	0.0000000000000000			
	0.0000000000000000	10.2659699999999994	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.3821300000000001			
	C Pt Cu O					
	1 3 77 1					
	Selective dynamics					
	Direct					
	0.2520688788991159	0.2499867263003400	0.4748953068665585	T	T	T
	0.2503150934979775	0.2501002261534613	0.3948382243120014	T	T	T
	0.7501396923997846	0.2498469851528328	0.3839864252870886	T	T	T
	0.7500892229229038	0.7501749369316320	0.3839637785687720	T	T	T
	0.0000000000000000	0.0000000000000000	0.1155260000000027	F	F	F
	-0.0012790077162007	0.9980159409939628	0.3854748820905412	T	T	T
	0.1666669999999968	0.0833330000000032	0.0259050000000016	F	F	F
	0.1677819665626190	0.0857277723872008	0.2959197074641105	T	T	T
	0.0833826675308028	0.1666876957143610	0.2051620601301045	T	T	T
	0.2500000000000000	0.0000000000000000	0.1155260000000027	F	F	F
	0.2506436555487635	0.9954727611533662	0.3839071532346908	T	T	T
	0.4166669999999968	0.0833330000000032	0.0259050000000016	F	F	F
	0.4162353747828921	0.0833227904420573	0.2945897862901170	T	T	T
	0.3332687666992006	0.1667233002641240	0.2050751596286389	T	T	T
	0.5000000000000000	0.0000000000000000	0.1155260000000027	F	F	F
	0.4978840533618678	0.9970027117678408	0.3842564843131728	T	T	T
	0.6666669999999968	0.0833330000000032	0.0259050000000016	F	F	F
	0.6660269153422765	0.0816876351719290	0.2935501489744387	T	T	T
	0.5828021456257503	0.1665592045868942	0.2048089634632549	T	T	T
	0.7500000000000000	0.0000000000000000	0.1155260000000027	F	F	F
	0.7482799807767695	0.9991039069365991	0.3857969192582838	T	T	T
	0.9166669999999968	0.0833330000000032	0.0259050000000016	F	F	F
	0.9174153776114011	0.0836912889044012	0.2951198063534956	T	T	T
	0.8339813201710772	0.1665684097817189	0.2049113370451147	T	T	T
	0.0000000000000000	0.2500000000000000	0.1155260000000027	F	F	F
	-0.0012384844623542	0.2506536097964009	0.3855085442387368	T	T	T

0.1666669999999968	0.3333330000000032	0.0259050000000016	F	F	F
0.1678074111182898	0.3319966617702350	0.2959637577718999	T	T	T
0.0838659303407579	0.4161399500929202	0.2054135949829027	T	T	T
0.2500000000000000	0.2500000000000000	0.1155260000000027	F	F	F
0.4166669999999968	0.3333330000000032	0.0259050000000016	F	F	F
0.4144111077529049	0.3321806103896132	0.2961108933992427	T	T	T
0.3332679859586617	0.4165281550023787	0.2050817662406434	T	T	T
0.5000000000000000	0.2500000000000000	0.1155260000000027	F	F	F
0.5014810246626750	0.2488640808392302	0.3853875557060737	T	T	T
0.6666669999999968	0.3333330000000032	0.0259050000000016	F	F	F
0.6653724420508346	0.3342070530778461	0.2936682692674313	T	T	T
0.5824263756903423	0.4161981105871086	0.2054256643957504	T	T	T
0.7500000000000000	0.2500000000000000	0.1155260000000027	F	F	F
0.9166669999999968	0.3333330000000032	0.0259050000000016	F	F	F
0.9191864047883914	0.3342239523620116	0.2935897571876885	T	T	T
0.8335512491655549	0.4169019033079516	0.2047469554464517	T	T	T
0.0000000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.0024082165525335	0.5028172352347066	0.3840953369677539	T	T	T
0.1666669999999968	0.5833330000000032	0.0259050000000016	F	F	F
0.1667107540129460	0.5828630959520225	0.2943794658621262	T	T	T
0.0834927631096208	0.6667309541889087	0.2050589153561505	T	T	T
0.2500000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.2506664214534558	0.5050783973541090	0.3839503381738675	T	T	T
0.4166669999999968	0.5833330000000032	0.0259050000000016	F	F	F
0.4162304906527084	0.5828666872295918	0.2946028489217837	T	T	T
0.3333168647706254	0.6663322202943678	0.2051094692592989	T	T	T
0.5000000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.5014366242152629	0.5025060167360751	0.3853983162938366	T	T	T
0.6666669999999968	0.5833330000000032	0.0259050000000016	F	F	F
0.6653412907945204	0.5810867656003653	0.2936657328515477	T	T	T
0.5827972527017721	0.6662116547190894	0.2048126745106828	T	T	T
0.7500000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.7509356707561404	0.5004287401573074	0.3855100769946262	T	T	T
0.9166669999999968	0.5833330000000032	0.0259050000000016	F	F	F
0.9170346541272243	0.5834859283056848	0.2942580334619774	T	T	T
0.8335377064406069	0.6666208877409107	0.2047468423541896	T	T	T
0.0000000000000000	0.7500000000000000	0.1155260000000027	F	F	F
0.0023677605314207	0.7495157166156532	0.3840877449147470	T	T	T
0.1666669999999968	0.8333330000000032	0.0259050000000016	F	F	F
0.1666947731860500	0.8337847050815868	0.2943695149943539	T	T	T
0.0838544855112201	0.9176923070308810	0.2054062948227764	T	T	T
0.2500000000000000	0.7500000000000000	0.1155260000000027	F	F	F
0.2500676779451437	0.7500037755730901	0.3826802722098437	T	T	T
0.4166669999999968	0.8333330000000032	0.0259050000000016	F	F	F
0.4165397857815835	0.8332530313764739	0.2943449026614437	T	T	T
0.3333167962629096	0.9169635974900321	0.2051052020198752	T	T	T
0.5000000000000000	0.7500000000000000	0.1155260000000027	F	F	F
0.4978787210914977	0.7508056571016045	0.3842596727926466	T	T	T
0.6666669999999968	0.8333330000000032	0.0259050000000016	F	F	F
0.6660182349275823	0.8343052918281755	0.2935475133210517	T	T	T
0.5834906834437407	0.9167409239160259	0.2049221597681130	T	T	T

	0.7500000000000000	0.7500000000000000	0.1155260000000027	F	F	F
	0.9166669999999968	0.8333330000000032	0.0259050000000016	F	F	F
	0.9191621909711337	0.8349008850411525	0.2935773713019745	T	T	T
	0.8339877087053158	0.9174036716041337	0.2049097430731851	T	T	T
	0.2537310488564060	0.2499318234364835	0.5245972724215825	T	T	T
4Pt/Cu(111) ^{S2}	1.0000000000000000					
	8.8905908144889398	-5.1329849999999997	0.0000000000000000			
	0.0000000000000000	10.2659699999999994	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	23.3821300000000001			
	C	Pt	Cu	O		
	1	4	76	1		
	Selective dynamics					
	Direct					
	0.7474816812383289	0.7492991279871259	0.4745250110641917	T	T	T
	0.2497010921677332	0.2498918051832159	0.3837582001453200	T	T	T
	0.7498660170322182	0.2499169862438494	0.3837613936003839	T	T	T
	0.2497023093146035	0.7497676157232561	0.3837505605888912	T	T	T
	0.7497095853812452	0.7498430229226308	0.3944700891867539	T	T	T
	0.0000000000000000	0.0000000000000000	0.1155260000000027	F	F	F
	0.0014036597477439	0.0018489777803471	0.3854311790227255	T	T	T
	0.1666669999999968	0.0833330000000032	0.0259050000000016	F	F	F
	0.1651339378981180	0.0809462761321916	0.2935866878153486	T	T	T
	0.0826190376775382	0.1660860625413222	0.2048604048775366	T	T	T
	0.2500000000000000	0.0000000000000000	0.1155260000000027	F	F	F
	0.2500102559817097	-0.0000101828005388	0.3855060132364709	T	T	T
	0.4166669999999968	0.0833330000000032	0.0259050000000016	F	F	F
	0.4165733372393842	0.0832889286415980	0.2945189941883057	T	T	T
	0.3334196749622527	0.1665310954020485	0.2048133330289445	T	T	T
	0.5000000000000000	0.0000000000000000	0.1155260000000027	F	F	F
	0.4996719847621710	-0.0000166468560798	0.3855003478386231	T	T	T
	0.6666669999999968	0.0833330000000032	0.0259050000000016	F	F	F
	0.6656808702558862	0.0809712113531369	0.2935852092537601	T	T	T
	0.5830379593816779	0.1665276630545299	0.2048155293894426	T	T	T
	0.7500000000000000	0.0000000000000000	0.1155260000000027	F	F	F
	0.7502005590847081	0.0019090846662100	0.3853874056217400	T	T	T
	0.9166669999999968	0.0833330000000032	0.0259050000000016	F	F	F
	0.9162442590654646	0.0825991538716597	0.2948713884972350	T	T	T
	0.8334106525443374	0.1661041735945075	0.2048614543829119	T	T	T
	0.0000000000000000	0.2500000000000000	0.1155260000000027	F	F	F
	0.0002857572466972	0.2508870090344467	0.3857183279112933	T	T	T
	0.1666669999999968	0.3333330000000032	0.0259050000000016	F	F	F
	0.1657491361322431	0.3341211756500131	0.2935663401074706	T	T	T
	0.0832934385574244	0.4166599674458628	0.2048871172474304	T	T	T
	0.2500000000000000	0.2500000000000000	0.1155260000000027	F	F	F
	0.4166669999999968	0.3333330000000032	0.0259050000000016	F	F	F
	0.4188661191476772	0.3346904780961203	0.2935932111871928	T	T	T
	0.3338644137481344	0.4173310320909009	0.2048548292851577	T	T	T
	0.5000000000000000	0.2500000000000000	0.1155260000000027	F	F	F
	0.4996750108518601	0.2496690425599608	0.3855041838305800	T	T	T
	0.6666669999999968	0.3333330000000032	0.0259050000000016	F	F	F
	0.6656786916554269	0.3347099325247043	0.2935906613518980	T	T	T

0.5837832717605076	0.4176283694600260	0.2053795559897143	T	T	T
0.7500000000000000	0.2500000000000000	0.1155260000000027	F	F	F
0.9166669999999968	0.3333330000000032	0.0259050000000016	F	F	F
0.9182249577814691	0.3341185476624892	0.2935811345911387	T	T	T
0.8334139817079241	0.4173424186565020	0.2048643824747407	T	T	T
0.0000000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.0002792238536970	0.4993780116233127	0.3857015946375295	T	T	T
0.1666669999999968	0.5833330000000032	0.0259050000000016	F	F	F
0.1657512297009776	0.5816404286990849	0.2935622968184627	T	T	T
0.0826149363257032	0.6665498796488367	0.2048599927819680	T	T	T
0.2500000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.2487974037607315	0.4993825652318585	0.3856951003589926	T	T	T
0.4166669999999968	0.5833330000000032	0.0259050000000016	F	F	F
0.4172720988978474	0.5836334121754790	0.2948451271835410	T	T	T
0.3338548236463540	0.6665586408135319	0.2048519319511461	T	T	T
0.5000000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.4977498049893526	0.4982012038080558	0.3853825829804256	T	T	T
0.6666669999999968	0.5833330000000032	0.0259050000000016	F	F	F
0.6677414447018495	0.5856241763494644	0.2959897067859620	T	T	T
0.5833945212755972	0.6667016848932670	0.2051334181825755	T	T	T
0.7500000000000000	0.5000000000000000	0.1155260000000027	F	F	F
0.7501930324561717	0.4982601725595886	0.3854041763040374	T	T	T
0.9166669999999968	0.5833330000000032	0.0259050000000016	F	F	F
0.9162368745391472	0.5836514180967312	0.2948722747093250	T	T	T
0.8332592959650537	0.6667109471735152	0.2051415989843662	T	T	T
0.0000000000000000	0.7500000000000000	0.1155260000000027	F	F	F
0.0014008773716238	0.7495249534929054	0.3854410352710052	T	T	T
0.1666669999999968	0.8333330000000032	0.0259050000000016	F	F	F
0.1651421514333365	0.8341923132656440	0.2935892118074538	T	T	T
0.0823012009488592	0.9161587413438099	0.2053863343107038	T	T	T
0.2500000000000000	0.7500000000000000	0.1155260000000027	F	F	F
0.4166669999999968	0.8333330000000032	0.0259050000000016	F	F	F
0.4188668092516204	0.8341846520264139	0.2935891110047982	T	T	T
0.3334297512242578	0.9169238326711553	0.2048136732247977	T	T	T
0.5000000000000000	0.7500000000000000	0.1155260000000027	F	F	F
0.4977497727285259	0.7495182200073697	0.3853622464605518	T	T	T
0.6666669999999968	0.8333330000000032	0.0259050000000016	F	F	F
0.6677430151034160	0.8321252948469828	0.2959733608918482	T	T	T
0.5837821959195255	0.9161765679148356	0.2053722016651840	T	T	T
0.7500000000000000	0.7500000000000000	0.1155260000000027	F	F	F
0.9166669999999968	0.8333330000000032	0.0259050000000016	F	F	F
0.9141690582572943	0.8320844192711216	0.2960414099057148	T	T	T
0.8332700855492918	0.9165757070709287	0.2051409170259741	T	T	T
0.7456005197608353	0.7488818349010390	0.5242213096920402	T	T	T