

Pathway 1

\$POSCAR 1 Au

1.000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.4900460000000000	0.6390840000000000	0.5000000000000000	T	T	T
0.6311810000000000	0.6345790000000000	0.5000000000000000	T	T	T
0.5658930000000000	0.7480240000000000	0.5000000000000000	T	T	T
0.5610210000000000	0.5192460000000000	0.5000000000000000	T	T	T
0.4270120000000000	0.5180870000000000	0.5000000000000000	T	T	T
0.4943580000000000	0.4024630000000000	0.5000000000000000	T	T	T
0.3573640000000000	0.3976690000000000	0.5000000000000000	T	T	T
0.4296270000000000	0.2838050000000000	0.5000000000000000	T	T	T
0.2914460000000000	0.5136039999999999	0.5000000000000000	T	T	T
0.5656130000000000	0.2875150000000000	0.5000000000000000	T	T	T
0.3552510000000000	0.6325090000000000	0.5000000000000000	T	T	T
0.6324930000000000	0.4027530000000000	0.5000000000000000	T	T	T
0.6986940000000000	0.5206620000000000	0.5000000000000000	T	T	T

Au

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Selective dynamics

Direct

0.4915226179017853	0.6455413375736023	0.5000000000000000	T	T	T
0.6317053151094096	0.6382330079245850	0.5000000000000000	T	T	T
0.5709862217153882	0.7541413110424954	0.5000000000000000	T	T	T
0.5573537881256339	0.5231229768172537	0.5000000000000000	T	T	T
0.4249917901523843	0.5133038921615731	0.5000000000000000	T	T	T
0.4988741966887915	0.4021419081029379	0.5000000000000000	T	T	T
0.3543406689314321	0.3967755599236710	0.5000000000000000	T	T	T
0.4316531338025065	0.2877774821586994	0.5000000000000000	T	T	T
0.2866523975510440	0.5121958296238128	0.5000000000000000	T	T	T
0.5674429149784702	0.2822119097062436	0.5000000000000000	T	T	T
0.3589574960575069	0.6270845547565294	0.5000000000000000	T	T	T
0.6342414327899715	0.3978948653444375	0.5000000000000000	T	T	T

0. 6912775107444802 0. 5195753648642066 0. 5000000000000000 T T T

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Selective dynamics

Direct

0. 4923562480667565 0. 6521658410409605 0. 5000000000000000 T T T

0. 6326351889743835 0. 6403063142932932 0. 5000000000000000 T T T

0. 5744403198852867 0. 7579332494955491 0. 5000000000000000 T T T

0. 5528819729526634 0. 5283069408712863 0. 5000000000000000 T T T

0. 4222244302997132 0. 5069728271158056 0. 5000000000000000 T T T

0. 5049762762263561 0. 4028370679316554 0. 5000000000000000 T T T

0. 3486260713883882 0. 3945849835065331 0. 5000000000000000 T T T

0. 4332521968530197 0. 2922013310102198 0. 5000000000000000 T T T

0. 2838779386348356 0. 5121830653840223 0. 5000000000000000 T T T

0. 5679264610680738 0. 2788922689466848 0. 5000000000000000 T T T

0. 3625954329691652 0. 6231427344295155 0. 5000000000000000 T T T

0. 6390295949012577 0. 3922122665794430 0. 5000000000000000 T T T

0. 6851773681288131 0. 5182611093950752 0. 5000000000000000 T T T

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Selective dynamics

Direct

0. 4928743619417489 0. 6580984301006764 0. 5000000000000000 T T T

0. 6334703172020650 0. 6414183299874424 0. 5000000000000000 T T T

0. 5774585947349300 0. 7605284793231039 0. 5000000000000000 T T T

0. 5481098556007468 0. 5335993437721358 0. 5000000000000000 T T T

0. 4197794738377645 0. 5001652771437552 0. 5000000000000000 T T T

0. 5119263178349220 0. 4041880249738754 0. 5000000000000000 T T T

0. 3420627634789917 0. 3922966822196031 0. 5000000000000000 T T T

0. 4346207808009609 0. 2972325712732130 0. 5000000000000000 T T T

0. 2819057986354011 0. 5126532405538656 0. 5000000000000000 T T T

0. 5677529014487306 0. 2767931159823704 0. 5000000000000000 T T T

0. 3663483646131099 0. 6191768718141042 0. 5000000000000000 T T T

0. 6442902601664906 0. 3869945927005355 0. 5000000000000000 T T T

0. 6793997127012192 0. 5168550401553702 0. 5000000000000000 T T T

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Selective dynamics

Direct

0. 4930951463419148 0. 6635454592374238 0. 5000000000000000 T T T

0. 6338715506279218 0. 6418049800552782 0. 5000000000000000 T T T

0. 5806248392602739 0. 7624895436264153 0. 5000000000000000 T T T

0. 5427182966232073 0. 5386943877236596 0. 5000000000000000 T T T

0. 4179115757466305 0. 4927593989745983 0. 5000000000000000 T T T

0. 5192091089212647 0. 4062054886101392 0. 5000000000000000 T T T

0. 3357325846487015 0. 3899439697104004 0. 5000000000000000 T T T

0. 4357128435163151 0. 3026814739865366 0. 5000000000000000 T T T

0. 2807146636904077 0. 5132591213131427 0. 5000000000000000 T T T

0. 5671222704106745 0. 2758009479662452 0. 5000000000000000 T T T

0. 3705723018020247 0. 6148918548458707 0. 5000000000000000 T T T

0. 6492007701309153 0. 3826875397215357 0. 5000000000000000 T T T

0. 6735135527586701 0. 5152358342288039 0. 5000000000000000 T T T

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Selective dynamics

Direct

0. 4930282196267194 0. 6675760733119021 0. 5000000000000000 T T T

0. 6334970193698648 0. 6414562469576741 0. 5000000000000000 T T T

0. 5832229364945725 0. 7635971614511715 0. 5000000000000000 T T T

0. 5378337181538919 0. 5421796046659192 0. 5000000000000000 T T T

0. 4170968300534850 0. 4865672388430247 0. 5000000000000000 T T T

0. 5248203307811716 0. 4085075641703765 0. 5000000000000000 T T T

0. 3310925868340044 0. 3879830793838769 0. 5000000000000000 T T T

0. 4363123732448939 0. 3075398673085000 0. 5000000000000000 T T T

0. 2808143373580623 0. 5137322749947600 0. 5000000000000000 T T T

0. 5663283995728184 0. 2760987144864688 0. 5000000000000000 T T T

0. 3745385473668350 0. 6113366652326325 0. 5000000000000000 T T T

0. 6529600735729626 0. 3798730960892659 0. 5000000000000000 T T T

0. 6684541325688226 0. 5135524131044791 0. 5000000000000000 T T T

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Selective dynamics

Direct

0. 4929742080696855 0. 6714360385044621 0. 5000000000000000 T T T

0. 6326195383924695 0. 6406981624183044 0. 5000000000000000 T T T

0. 5856735867975789 0. 7645506000150172 0. 5000000000000000 T T T

0. 5329096802326029 0. 5451181938250439 0. 5000000000000000 T T T

0. 4166889198337102 0. 4805335602992702 0. 5000000000000000 T T T

0. 5299683564313870 0. 4110052244923694 0. 5000000000000000 T T T

0. 3266783852221178 0. 3859965586550912 0. 5000000000000000 T T T

0. 4368843866047895 0. 3129767564221641 0. 5000000000000000 T T T

0. 2815705507043815 0. 5140065518026165 0. 5000000000000000 T T T

0. 5655132333925464 0. 2770211182511982 0. 5000000000000000 T T T

0. 3788544952932839 0. 6076710669433654 0. 5000000000000000 T T T

0. 6566830089586451 0. 3774299808506733 0. 5000000000000000 T T T

0. 6629811561014267 0. 5115561875204655 0. 5000000000000000 T T T

Au

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Selective dynamics

Direct

0. 4928989832368413 0. 6752446541019294 0. 5000000000000000 T T T

0. 6311539758483155 0. 6395326804100635 0. 5000000000000000 T T T

0. 5881607152183376 0. 7653154402507329 0. 5000000000000000 T T T

0. 5279866170413755 0. 5476368389313578 0. 5000000000000000 T T T

0. 4165547449576446 0. 4747293870354532 0. 5000000000000000 T T T

0. 5347277851848302 0. 4136276945925699 0. 5000000000000000 T T T

0. 3223916737184255 0. 3839797652108797 0. 5000000000000000 T T T

0. 4374955623278579 0. 3188745875680298 0. 5000000000000000 T T T

0. 2829553774720167 0. 5139673588507079 0. 5000000000000000 T T T

0. 5647345951475575 0. 2784890200485310 0. 5000000000000000 T T T

0. 3833490420247027 0. 6040214470692167 0. 5000000000000000 T T T

0. 6603103065467417 0. 3752250184258324 0. 5000000000000000 T T T

0. 6572801313326023 0. 5093561075047184 0. 5000000000000000 T T T
Au
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Au

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Selective dynamics

Direct

0. 4926807469625065 0. 6793450802872216 0. 5000000000000000 T T T
0. 6286685901032035 0. 6379658550409769 0. 5000000000000000 T T T
0. 5912218104361302 0. 7658865608106776 0. 5000000000000000 T T T
0. 5231365989666074 0. 5496750646506013 0. 5000000000000000 T T T
0. 4165443165295044 0. 4691739743848417 0. 5000000000000000 T T T
0. 5390325878204538 0. 4162907150810025 0. 5000000000000000 T T T
0. 3178594893985902 0. 3816163331319744 0. 5000000000000000 T T T
0. 4379096918106430 0. 3247655610860596 0. 5000000000000000 T T T
0. 2852208247464731 0. 5133625803523397 0. 5000000000000000 T T T
0. 5640055004516555 0. 2808197854266229 0. 5000000000000000 T T T
0. 3876797015367899 0. 6007575995164288 0. 5000000000000000 T T T
0. 6640904511091610 0. 3731504108107919 0. 5000000000000000 T T T
0. 6519492269873721 0. 5071904794204822 0. 5000000000000000 T T T

\$POSCAR 1 Au

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Selective dynamics

Direct

0. 4919560000000000 0. 6842000000000000 0. 5000000000000000 T T T
0. 6246760000000000 0. 6358310000000000 0. 5000000000000000 T T T
0. 5966850000000000 0. 7652960000000000 0. 5000000000000000 T T T
0. 5186600000000000 0. 5512030000000000 0. 5000000000000000 T T T
0. 4159010000000000 0. 4648270000000000 0. 5000000000000000 T T T
0. 5417480000000000 0. 4189640000000000 0. 5000000000000000 T T T
0. 3130620000000000 0. 3771420000000000 0. 5000000000000000 T T T
0. 4374940000000000 0. 3284890000000000 0. 5000000000000000 T T T
0. 2886900000000000 0. 5107520000000000 0. 5000000000000000 T T T
0. 5640530000000000 0. 2856710000000000 0. 5000000000000000 T T T
0. 3900390000000000 0. 5997490000000000 0. 5000000000000000 T T T
0. 6686780000000000 0. 3722690000000000 0. 5000000000000000 T T T
0. 6483580000000000 0. 5056070000000000 0. 5000000000000000 T T T

Pathway 2

\$POSCAR 1 Au

1.000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

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Selective dynamics

Direct

0.4900460000000000	0.6390840000000000	0.5000000000000000	T T T
0.6311810000000000	0.6345790000000000	0.5000000000000000	T T T
0.5658930000000000	0.7480240000000000	0.5000000000000000	T T T
0.5610210000000000	0.5192460000000000	0.5000000000000000	T T T
0.4270120000000000	0.5180870000000000	0.5000000000000000	T T T
0.4943580000000000	0.4024630000000000	0.5000000000000000	T T T
0.3573640000000000	0.3976690000000000	0.5000000000000000	T T T
0.4296270000000000	0.2838050000000000	0.5000000000000000	T T T
0.2914460000000000	0.5136039999999999	0.5000000000000000	T T T
0.5656130000000000	0.2875150000000000	0.5000000000000000	T T T
0.3552510000000000	0.6325090000000000	0.5000000000000000	T T T
0.6324930000000000	0.4027530000000000	0.5000000000000000	T T T
0.6986940000000000	0.5206620000000000	0.5000000000000000	T T T

Au

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20.0000000000000000	0.0000000000000000	0.0000000000000000
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Au

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Selective dynamics

Direct

0.4863554993248179	0.6398267723342675	0.5000000000000000	T T T
0.6432891422611786	0.6357033807183323	0.5000000000000000	T T T
0.5696971525387269	0.7425788277822114	0.5000000000000000	T T T
0.5610918938969113	0.5248728010944412	0.5000000000000000	T T T
0.4245718239826497	0.5184792065197622	0.5000000000000000	T T T
0.4940596671532709	0.4052334633598779	0.5000000000000000	T T T
0.3569535895567874	0.3969043917116817	0.5000000000000000	T T T
0.4309633070773588	0.2850186163265088	0.5000000000000000	T T T
0.2874618345268002	0.5099643956520679	0.5000000000000000	T T T
0.5658025839460894	0.2887011016112642	0.5000000000000000	T T T
0.3496587622200395	0.6296323157578521	0.5000000000000000	T T T
0.6297607389514679	0.4049213339937375	0.5000000000000000	T T T

0. 7003334902529336 0. 5181629074489380 0. 5000000000000000 T T T

Au

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Au

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Selective dynamics

Direct

0. 4827133942999862 0. 6398290359694455 0. 5000000000000000 T T T

0. 6582740997930110 0. 6417705735343175 0. 5000000000000000 T T T

0. 5712704616315443 0. 7376242734152213 0. 5000000000000000 T T T

0. 5604572509139961 0. 5278742413183209 0. 5000000000000000 T T T

0. 4228771877028211 0. 5180341104584359 0. 5000000000000000 T T T

0. 4936923994946165 0. 4057556004829694 0. 5000000000000000 T T T

0. 3564333380700492 0. 3961466230885448 0. 5000000000000000 T T T

0. 4313544292739038 0. 2850379569422796 0. 5000000000000000 T T T

0. 2853306370130170 0. 5080997382761184 0. 5000000000000000 T T T

0. 5656998446410002 0. 2883242208294133 0. 5000000000000000 T T T

0. 3463203540152883 0. 6281023178130674 0. 5000000000000000 T T T

0. 6282452034271645 0. 4050767477608538 0. 5000000000000000 T T T

0. 6973309084753055 0. 5183240513593150 0. 5000000000000000 T T T

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Selective dynamics

Direct

0. 4800023468929104 0. 6395304599815368 0. 5000000000000000 T T T

0. 6728464953000824 0. 6487233434931966 0. 5000000000000000 T T T

0. 5734719295947327 0. 7323344100627489 0. 5000000000000000 T T T

0. 5579599841364660 0. 5280023647460258 0. 5000000000000000 T T T

0. 4210258473282211 0. 5173934949678632 0. 5000000000000000 T T T

0. 4932490813040445 0. 4053331260220178 0. 5000000000000000 T T T

0. 3558695148004488 0. 3954181487866505 0. 5000000000000000 T T T

0. 4315713248430976 0. 2847873704676983 0. 5000000000000000 T T T

0. 2838439197526815 0. 5069672313139071 0. 5000000000000000 T T T

0. 5658634578936129 0. 2881935485874045 0. 5000000000000000 T T T

0. 3442222455822602 0. 6273074434020854 0. 5000000000000000 T T T

0. 6277200455122398 0. 4053395225032743 0. 5000000000000000 T T T

0. 6923533235292773 0. 5206690191955182 0. 5000000000000000 T T T

Au

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Au

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Selective dynamics

Direct

0. 4765947259158439 0. 6397532632596272 0. 5000000000000000 T T T

0. 6865892340534738 0. 6538086841594097 0. 5000000000000000 T T T

0. 5772527240176504 0. 7250950266757494 0. 5000000000000000 T T T

0. 5549988993647941 0. 5286695727156003 0. 5000000000000000 T T T

0. 4188341015549654 0. 5167445038895689 0. 5000000000000000 T T T

0. 4927992995887930 0. 4050309762339689 0. 5000000000000000 T T T

0. 3553948395519859 0. 3944983766371715 0. 5000000000000000 T T T

0. 4318869104854299 0. 2844352684481732 0. 5000000000000000 T T T

0. 2822763726132708 0. 5056504009467777 0. 5000000000000000 T T T

0. 5664695641999464 0. 2888151576374764 0. 5000000000000000 T T T

0. 3418240522164654 0. 6266113515484614 0. 5000000000000000 T T T

0. 6272228586371962 0. 4068445877250658 0. 5000000000000000 T T T

0. 6878559422886258 0. 5240423056344866 0. 5000000000000000 T T T

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Selective dynamics

Direct

0. 4722521771933318 0. 6408085440112030 0. 5000000000000000 T T T

0. 6985881437815852 0. 6567948270788242 0. 5000000000000000 T T T

0. 5815768308432270 0. 7148440472814113 0. 5000000000000000 T T T

0. 5526134657088333 0. 5309746214117903 0. 5000000000000000 T T T

0. 4169073435519501 0. 5162932401416660 0. 5000000000000000 T T T

0. 4923840383177748 0. 4051978958884553 0. 5000000000000000 T T T

0. 3552081711192369 0. 3935044106080636 0. 5000000000000000 T T T

0. 4321344259558457 0. 2840220568077649 0. 5000000000000000 T T T

0. 2809569265489874 0. 5043312155929707 0. 5000000000000000 T T T

0. 5672639972706872 0. 2902381169837244 0. 5000000000000000 T T T

0. 3389885776161917 0. 6260781288798652 0. 5000000000000000 T T T

0. 6263661854867454 0. 4094267841977141 0. 5000000000000000 T T T

0. 6847592495753816 0. 5274855781467473 0. 5000000000000000 T T T

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Selective dynamics

Direct

0. 4686179191159517 0. 6420818968291819 0. 5000000000000000 T T T

0. 7074492406042847 0. 6601915012681794 0. 5000000000000000 T T T

0. 5841283381096041 0. 7011455615128775 0. 5000000000000000 T T T

0. 5496882715307492 0. 5324380198066697 0. 5000000000000000 T T T

0. 4161869175943408 0. 5154908119021272 0. 5000000000000000 T T T

0. 4927073717991638 0. 4062333277557713 0. 5000000000000000 T T T

0. 3543230523450314 0. 3925834552214291 0. 5000000000000000 T T T

0. 4324539039800040 0. 2852682766671261 0. 5000000000000000 T T T

0. 2806139051244586 0. 5043071217345430 0. 5000000000000000 T T T

0. 5677926491685805 0. 2913666583635867 0. 5000000000000000 T T T

0. 3368775765757536 0. 6258374224895821 0. 5000000000000000 T T T

0. 6271042983731347 0. 4120832435314605 0. 5000000000000000 T T T

0. 6820560889517059 0. 5309721696446853 0. 5000000000000000 T T T

Au

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Au

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Selective dynamics

Direct

0. 4654796808463534 0. 6430938846100416 0. 5000000000000000 T T T

0. 7147043621545472 0. 6624409564300567 0. 5000000000000000 T T T

0. 5870372037846626 0. 6862247048802892 0. 5000000000000000 T T T

0. 5479494164176247 0. 5340582260465554 0. 5000000000000000 T T T

0. 4150818026107105 0. 5157586259145575 0. 5000000000000000 T T T

0. 4927059424489531 0. 4075606217639695 0. 5000000000000000 T T T

0. 3540480579156908 0. 3923719738896529 0. 5000000000000000 T T T

0. 4331044851949347 0. 2859905261031552 0. 5000000000000000 T T T

0. 2798630641517380 0. 5035630982083463 0. 5000000000000000 T T T

0. 5681413032554594 0. 2931706182434172 0. 5000000000000000 T T T

0. 3342835498080651 0. 6257038218852009 0. 5000000000000000 T T T

0. 6272806762437300 0. 4149666878549118 0. 5000000000000000 T T T

0.6803199894188166 0.5350957199185390 0.5000000000000000 T T T
Au
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20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000

Au

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Selective dynamics

Direct

0.4633485230758019 0.6441378288370061 0.5000000000000000 T T T
0.7207385893349779 0.6646338273546503 0.5000000000000000 T T T
0.5903535749833363 0.6708092758730461 0.5000000000000000 T T T
0.5464091915171708 0.5345932577948537 0.5000000000000000 T T T
0.4135782481167656 0.5166553284116574 0.5000000000000000 T T T
0.4922541730691628 0.4088397902486549 0.5000000000000000 T T T
0.3540822714460212 0.3924559886515497 0.5000000000000000 T T T
0.4338499986469410 0.2863939020150644 0.5000000000000000 T T T
0.2787774532520309 0.5025159084964995 0.5000000000000000 T T T
0.5686231656578933 0.2956122010776062 0.5000000000000000 T T T
0.3317377813259924 0.6258089005383414 0.5000000000000000 T T T
0.6272537011511503 0.4180209216920436 0.5000000000000000 T T T
0.6789928668158450 0.5395223306159211 0.5000000000000000 T T T

\$POSCAR 1 Au

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20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
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Selective dynamics

Direct

0.4636570000000000 0.6439460000000000 0.5000000000000000 T T T
0.7273970000000000 0.6673930000000000 0.5000000000000000 T T T
0.5952850000000000 0.6578450000000000 0.5000000000000000 T T T
0.5438880000000000 0.5323070000000000 0.5000000000000000 T T T
0.4104940000000000 0.5172720000000000 0.5000000000000000 T T T
0.4898990000000000 0.4094040000000000 0.5000000000000000 T T T
0.3529900000000000 0.3917820000000000 0.5000000000000000 T T T
0.4346750000000000 0.2860550000000000 0.5000000000000000 T T T
0.2763070000000000 0.5011910000000000 0.5000000000000000 T T T
0.5697470000000000 0.3002420000000000 0.5000000000000000 T T T
0.3299850000000000 0.6259470000000000 0.5000000000000000 T T T
0.6266480000000000 0.4225300000000000 0.5000000000000000 T T T
0.6790280000000000 0.5440850000000000 0.5000000000000000 T T T

Pathway 3

\$POSCAR 1 Au

1.000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.4900460000000000	0.6390840000000000	0.5000000000000000	T T T
0.6311810000000000	0.6345790000000000	0.5000000000000000	T T T
0.5658930000000000	0.7480240000000000	0.5000000000000000	T T T
0.5610210000000000	0.5192460000000000	0.5000000000000000	T T T
0.4270120000000000	0.5180870000000000	0.5000000000000000	T T T
0.4943580000000000	0.4024630000000000	0.5000000000000000	T T T
0.3573640000000000	0.3976690000000000	0.5000000000000000	T T T
0.4296270000000000	0.2838050000000000	0.5000000000000000	T T T
0.2914460000000000	0.5136039999999999	0.5000000000000000	T T T
0.5656130000000000	0.2875150000000000	0.5000000000000000	T T T
0.3552510000000000	0.6325090000000000	0.5000000000000000	T T T
0.6324930000000000	0.4027530000000000	0.5000000000000000	T T T
0.6986940000000000	0.5206620000000000	0.5000000000000000	T T T

Au

1.0000000000000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Au

13

Selective dynamics

Direct

0.4868326293819808	0.6432441585405543	0.5000000000000000	T T T
0.6355835397456356	0.6342901396381111	0.5000000000000000	T T T
0.5695583918815410	0.7469147113437956	0.5000000000000000	T T T
0.5592664426183632	0.5236498652524461	0.5000000000000000	T T T
0.4253111110843063	0.5206821523593891	0.5000000000000000	T T T
0.4969366169218244	0.4055041224797072	0.5000000000000000	T T T
0.3597176937654983	0.3999020288908933	0.5000000000000000	T T T
0.4344031078798878	0.2877690016220918	0.5000000000000000	T T T
0.2880912904507112	0.5122663580956296	0.5000000000000000	T T T
0.5681816218537096	0.2809826586637432	0.5000000000000000	T T T
0.3506921821464310	0.6318738414470024	0.5000000000000000	T T T
0.6309027965235963	0.3976208661040931	0.5000000000000000	T T T

0.6945226091284116 0.5153006122534184 0.5000000000000000 T T T

Au

1.0000000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

Au

13

Selective dynamics

Direct

0.4830431863901787 0.6467186195868787 0.5000000000000000 T T T

0.6404283625289516 0.6346489400267300 0.5000000000000000 T T T

0.5708198815307959 0.7455141366106426 0.5000000000000000 T T T

0.5573898871434039 0.5293633592918114 0.5000000000000000 T T T

0.4236908951289676 0.5226512052270407 0.5000000000000000 T T T

0.4991539942203631 0.4097208154078011 0.5000000000000000 T T T

0.3614596862058723 0.4010647684025017 0.5000000000000000 T T T

0.4392487220689792 0.2914156815825103 0.5000000000000000 T T T

0.2861822999661252 0.5111971690965119 0.5000000000000000 T T T

0.5707357394469363 0.2736550502635225 0.5000000000000000 T T T

0.3470394353480944 0.6317023331348910 0.5000000000000000 T T T

0.6308195966785459 0.3912923043994677 0.5000000000000000 T T T

0.6899883392905002 0.5110561299435009 0.5000000000000000 T T T

Au

1.0000000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

Au

13

Selective dynamics

Direct

0.4791967034693016 0.6500702898060123 0.5000000000000000 T T T

0.6452824532480103 0.6346582457824043 0.5000000000000000 T T T

0.5717699645350404 0.7439034558288293 0.5000000000000000 T T T

0.5554880715119848 0.5356981611856206 0.5000000000000000 T T T

0.4221850908406437 0.5242863338188626 0.5000000000000000 T T T

0.5012662775490140 0.4144355617081828 0.5000000000000000 T T T

0.3630707682905069 0.4017930741548176 0.5000000000000000 T T T

0.4440957864658201 0.2950169478420661 0.5000000000000000 T T T

0.2848818028742724 0.5101375680736854 0.5000000000000000 T T T

0.5728700049240044 0.2663117805955856 0.5000000000000000 T T T

0.3439687220442426 0.6315614973734114 0.5000000000000000 T T T

0.6307807526017635 0.3850445553514497 0.5000000000000000 T T T

0. 6851436232553468 0. 5070830392840124 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4753927472377634 0. 6534539010981271 0. 5000000000000000 T T T

0. 6500199914729025 0. 6341856964533347 0. 5000000000000000 T T T

0. 5726277100972695 0. 7420128905139941 0. 5000000000000000 T T T

0. 5537219621598086 0. 5423243453930170 0. 5000000000000000 T T T

0. 4209661170752487 0. 5257278035187976 0. 5000000000000000 T T T

0. 5036115103252292 0. 4193388022405931 0. 5000000000000000 T T T

0. 3648340542792781 0. 4023607092173070 0. 5000000000000000 T T T

0. 4491139931263260 0. 2987344416543038 0. 5000000000000000 T T T

0. 2839602071946637 0. 5090460495919816 0. 5000000000000000 T T T

0. 5744240835243064 0. 2591604192637256 0. 5000000000000000 T T T

0. 3412629806568371 0. 6313559170966160 0. 5000000000000000 T T T

0. 6303449146062168 0. 3792112415351480 0. 5000000000000000 T T T

0. 6797197464038283 0. 5030882915028578 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4713931136317796 0. 6568690698420357 0. 5000000000000000 T T T

0. 6545022858761498 0. 6332260332420515 0. 5000000000000000 T T T

0. 5733375900688299 0. 7395728481892462 0. 5000000000000000 T T T

0. 5519895478805805 0. 5490919858294365 0. 5000000000000000 T T T

0. 4200358876044997 0. 5270200362857345 0. 5000000000000000 T T T

0. 5063630993147311 0. 4243476772416140 0. 5000000000000000 T T T

0. 3668888774916519 0. 4027218538512884 0. 5000000000000000 T T T

0. 4545731598190406 0. 3025181122998338 0. 5000000000000000 T T T

0. 2834161334902389 0. 5078591858895777 0. 5000000000000000 T T T

0. 5756209902980405 0. 2524385629795706 0. 5000000000000000 T T T

0. 3387392165561834 0. 6311192724132200 0. 5000000000000000 T T T

0. 6293926019815929 0. 3740450336777175 0. 5000000000000000 T T T

0. 6737475109101332 0. 4991708357203591 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4657862299709195 0. 6610293273014362 0. 5000000000000000 T T T

0. 6601528451416975 0. 6309450392310006 0. 5000000000000000 T T T

0. 5744829671281231 0. 7343534344269826 0. 5000000000000000 T T T

0. 5500770397640447 0. 5575040749906822 0. 5000000000000000 T T T

0. 4192430185778169 0. 5288157362498139 0. 5000000000000000 T T T

0. 5097907476726087 0. 4305792939119122 0. 5000000000000000 T T T

0. 3699644358377575 0. 4032053247568831 0. 5000000000000000 T T T

0. 4615446462089267 0. 3071248681049676 0. 5000000000000000 T T T

0. 2833619605841072 0. 5063144249680379 0. 5000000000000000 T T T

0. 5768618620248602 0. 2454708017185333 0. 5000000000000000 T T T

0. 3352161060837918 0. 6310975455032251 0. 5000000000000000 T T T

0. 6271085539543015 0. 3688130857623870 0. 5000000000000000 T T T

0. 6664096000964764 0. 4947475495968361 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4597971376990249 0. 6650783821008012 0. 5000000000000000 T T T

0. 6657829462037501 0. 6277793771714792 0. 5000000000000000 T T T

0. 5753848016496911 0. 7268927487369491 0. 5000000000000000 T T T

0. 5485969493463526 0. 5658884131602192 0. 5000000000000000 T T T

0. 4188568023182842 0. 5310669763401218 0. 5000000000000000 T T T

0. 5130028525024493 0. 4367289743919441 0. 5000000000000000 T T T

0. 3736397877909699 0. 4038927118073051 0. 5000000000000000 T T T

0. 4683976520855552 0. 3113144261277545 0. 5000000000000000 T T T

0. 2839082508218741 0. 5046490762270331 0. 5000000000000000 T T T

0. 5780421034204262 0. 2398736811664241 0. 5000000000000000 T T T

0. 3312464999637418 0. 6311980009391435 0. 5000000000000000 T T T

0. 6240010561144308 0. 3644225252074486 0. 5000000000000000 T T T

```

0. 6593431696368327 0. 4912152114000337 0. 5000000000000000 T T T
Au
1. 0000000000000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

```

Au

13

Selective dynamics

Direct

```

0. 4535801377374781 0. 6693051777568489 0. 5000000000000000 T T T
0. 6711538016764586 0. 6236916986125104 0. 5000000000000000 T T T
0. 5757658078121096 0. 7179912892724185 0. 5000000000000000 T T T
0. 5475213888213255 0. 5736117428128437 0. 5000000000000000 T T T
0. 4186913552667366 0. 5342271873049139 0. 5000000000000000 T T T
0. 5153398103406551 0. 4426805151847672 0. 5000000000000000 T T T
0. 3782188209417222 0. 4049063100552677 0. 5000000000000000 T T T
0. 4751378832403050 0. 3148529409976776 0. 5000000000000000 T T T
0. 2852741599993816 0. 5029071355943552 0. 5000000000000000 T T T
0. 5793385411838824 0. 2349729743048370 0. 5000000000000000 T T T
0. 3266052717091425 0. 6315254822306128 0. 5000000000000000 T T T
0. 6204139210301778 0. 3607303616052994 0. 5000000000000000 T T T
0. 6529591019335845 0. 4885976851140656 0. 5000000000000000 T T T

```

\$POSCAR 1 Au

```

1. 000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

```

13

Selective dynamics

Direct

```

0. 4475120000000000 0. 6748370000000000 0. 5000000000000000 T T T
0. 6757790000000000 0. 6177680000000000 0. 5000000000000000 T T T
0. 5763350000000000 0. 7102690000000000 0. 5000000000000000 T T T
0. 5463620000000000 0. 5784880000000000 0. 5000000000000000 T T T
0. 4180750000000000 0. 5399750000000000 0. 5000000000000000 T T T
0. 5156700000000000 0. 4478040000000000 0. 5000000000000000 T T T
0. 3844570000000000 0. 4067740000000000 0. 5000000000000000 T T T
0. 4813230000000000 0. 3165730000000000 0. 5000000000000000 T T T
0. 2884210000000000 0. 5014800000000000 0. 5000000000000000 T T T
0. 5811890000000000 0. 2295590000000000 0. 5000000000000000 T T T
0. 3204760000000000 0. 6334580000000000 0. 5000000000000000 T T T
0. 6166170000000000 0. 3571890000000000 0. 5000000000000000 T T T
0. 6477850000000001 0. 4858270000000000 0. 5000000000000000 T T T

```

Pathway 4

\$POSCAR 1 Au

1.000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.4900460000000000	0.6390840000000000	0.5000000000000000	T T T
0.6311810000000000	0.6345790000000000	0.5000000000000000	T T T
0.5658930000000000	0.7480240000000000	0.5000000000000000	T T T
0.5610210000000000	0.5192460000000000	0.5000000000000000	T T T
0.4270120000000000	0.5180870000000000	0.5000000000000000	T T T
0.4943580000000000	0.4024630000000000	0.5000000000000000	T T T
0.3573640000000000	0.3976690000000000	0.5000000000000000	T T T
0.4296270000000000	0.2838050000000000	0.5000000000000000	T T T
0.2914460000000000	0.5136039999999999	0.5000000000000000	T T T
0.5656130000000000	0.2875150000000000	0.5000000000000000	T T T
0.3552510000000000	0.6325090000000000	0.5000000000000000	T T T
0.6324930000000000	0.4027530000000000	0.5000000000000000	T T T
0.6986940000000000	0.5206620000000000	0.5000000000000000	T T T

Au

1.0000000000000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Au

13

Selective dynamics

Direct

0.4790291334153737	0.6445235748234164	0.5000000000000000	T T T
0.6345667327819806	0.6305385155726394	0.5000000000000000	T T T
0.5672362959118922	0.7417356360942364	0.5000000000000000	T T T
0.5622000721941619	0.5199562021350583	0.5000000000000000	T T T
0.4282661232819311	0.5213482840902031	0.5000000000000000	T T T
0.4957100365657243	0.4037790575604928	0.5000000000000000	T T T
0.3604040582952264	0.3977289626777814	0.5000000000000000	T T T
0.4308902490554358	0.2831683002495811	0.5000000000000000	T T T
0.2947196598134340	0.5129088092968868	0.5000000000000000	T T T
0.5657867584489977	0.2882776974538831	0.5000000000000000	T T T
0.3441765149611657	0.6364998514704536	0.5000000000000000	T T T
0.6342304871208594	0.4020516710263614	0.5000000000000000	T T T

0. 7027833702006357 0. 5174834375490374 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4671224475236771 0. 6507026947956062 0. 5000000000000000 T T T

0. 6384729848832368 0. 6282134117727464 0. 5000000000000000 T T T

0. 5660427079031991 0. 7360288763724440 0. 5000000000000000 T T T

0. 5652357086873652 0. 5186827194470197 0. 5000000000000000 T T T

0. 4317962862473422 0. 5227985690785155 0. 5000000000000000 T T T

0. 4969830976475242 0. 4037127654046573 0. 5000000000000000 T T T

0. 3622130060357282 0. 3983053877842747 0. 5000000000000000 T T T

0. 4308824151035395 0. 2828506603029729 0. 5000000000000000 T T T

0. 2991449901480325 0. 5142724218200760 0. 5000000000000000 T T T

0. 5655133076288623 0. 2878813727388720 0. 5000000000000000 T T T

0. 3344647825711316 0. 6414738403364425 0. 5000000000000000 T T T

0. 6362821149538935 0. 4000340649839194 0. 5000000000000000 T T T

0. 7058456466795016 0. 5150432151624953 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4559582594166680 0. 6554092919457850 0. 5000000000000000 T T T

0. 6417475889091724 0. 6263701235274628 0. 5000000000000000 T T T

0. 5634236605072059 0. 7299894436096732 0. 5000000000000000 T T T

0. 5688942987036492 0. 5168454733978770 0. 5000000000000000 T T T

0. 4363249000810355 0. 5234181659648967 0. 5000000000000000 T T T

0. 4983228349440452 0. 4032778869088224 0. 5000000000000000 T T T

0. 3635905842227720 0. 3995808919192659 0. 5000000000000000 T T T

0. 4306433204115868 0. 2830748971987100 0. 5000000000000000 T T T

0. 3039896865199744 0. 5168792155623978 0. 5000000000000000 T T T

0. 5654400239141747 0. 2872755253151285 0. 5000000000000000 T T T

0. 3245217111911456 0. 6469960486353200 0. 5000000000000000 T T T

0. 6384158774903301 0. 3979183871277412 0. 5000000000000000 T T T

0. 7087267525092712 0. 5129646488869626 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4455525727435325 0. 6580870708794846 0. 5000000000000000 T T T

0. 6446263725479248 0. 6248609007836595 0. 5000000000000000 T T T

0. 5594899039057109 0. 7230967249072582 0. 5000000000000000 T T T

0. 5727097803326641 0. 5150409606547035 0. 5000000000000000 T T T

0. 4411877425057595 0. 5238303308433117 0. 5000000000000000 T T T

0. 4999342628392704 0. 4028342556619163 0. 5000000000000000 T T T

0. 3649219778989042 0. 4018231717597409 0. 5000000000000000 T T T

0. 4303374398223537 0. 2840485515908672 0. 5000000000000000 T T T

0. 3088794264276044 0. 5206244986596418 0. 5000000000000000 T T T

0. 5656028246948932 0. 2865612574713153 0. 5000000000000000 T T T

0. 3145763098805092 0. 6523010705201355 0. 5000000000000000 T T T

0. 6406566619552602 0. 3958060744435704 0. 5000000000000000 T T T

0. 7115242262588677 0. 5110851318244387 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4359096208851913 0. 6584671319909843 0. 5000000000000000 T T T

0. 6475423103537584 0. 6237451434927400 0. 5000000000000000 T T T

0. 5545073290633147 0. 7150173584470108 0. 5000000000000000 T T T

0. 5764443224857999 0. 5136685620264682 0. 5000000000000000 T T T

0. 4458839564812755 0. 5244459257612882 0. 5000000000000000 T T T

0. 5017858062404184 0. 4027318322548765 0. 5000000000000000 T T T

0. 3663524090985653 0. 4049332376762634 0. 5000000000000000 T T T

0. 4300424700514023 0. 2858469231861956 0. 5000000000000000 T T T

0. 3135519405398007 0. 5252862709371203 0. 5000000000000000 T T T

0. 5658740033153901 0. 2858493515414961 0. 5000000000000000 T T T

0. 3051099562880694 0. 6569677945670298 0. 5000000000000000 T T T

0. 6427883406753329 0. 3938207324806472 0. 5000000000000000 T T T

0. 7142070398961766 0. 5092197356379262 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4250125286593297 0. 6561389306509542 0. 5000000000000000 T T T

0. 6519454711473723 0. 6229474545705296 0. 5000000000000000 T T T

0. 5477471511422852 0. 7024176703808435 0. 5000000000000000 T T T

0. 5805789695255087 0. 5133734319085259 0. 5000000000000000 T T T

0. 4508709911608635 0. 5255990210711081 0. 5000000000000000 T T T

0. 5044010461242338 0. 4034027610812051 0. 5000000000000000 T T T

0. 3683403236605289 0. 4096679120856331 0. 5000000000000000 T T T

0. 4299057426707889 0. 2892159387712484 0. 5000000000000000 T T T

0. 3183757832546146 0. 5317278182483506 0. 5000000000000000 T T T

0. 5662801101945015 0. 2851066528320549 0. 5000000000000000 T T T

0. 2944541027595314 0. 6616432083626504 0. 5000000000000000 T T T

0. 6447684605481215 0. 3920857417635035 0. 5000000000000000 T T T

0. 7173188326748443 0. 5066734582734418 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4158698927947984 0. 6545772360339271 0. 5000000000000000 T T T

0. 6589219396001261 0. 6231780445118373 0. 5000000000000000 T T T

0. 5426624710521337 0. 6853417772376019 0. 5000000000000000 T T T

0. 5836419785328006 0. 5159206099775110 0. 5000000000000000 T T T

0. 4539575344281189 0. 5282022579965336 0. 5000000000000000 T T T

0. 5067818124833051 0. 4056853434451542 0. 5000000000000000 T T T

0. 3705099776935732 0. 4138295844613882 0. 5000000000000000 T T T

0. 4303910869139689 0. 2927960713209058 0. 5000000000000000 T T T

0. 3205481889099282 0. 5361730694638276 0. 5000000000000000 T T T

0. 5663172329729826 0. 2850893984930086 0. 5000000000000000 T T T

0. 2854149439608987 0. 6637633281681790 0. 5000000000000000 T T T

0. 6452105723502402 0. 3918518775526079 0. 5000000000000000 T T T

0. 7197718885649048 0. 5035914013375749 0. 5000000000000000 T T T
Au
1. 0000000000000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4099398437489995 0. 6559702838793949 0. 5000000000000000 T T T
0. 6661798077418027 0. 6254144739252697 0. 5000000000000000 T T T
0. 5396687158893652 0. 6641790129646169 0. 5000000000000000 T T T
0. 5855185321483424 0. 5194978914797778 0. 5000000000000000 T T T
0. 4552135194087621 0. 5312739171389417 0. 5000000000000000 T T T
0. 5082316846562167 0. 4081363371017354 0. 5000000000000000 T T T
0. 3722159843259306 0. 4167552940625990 0. 5000000000000000 T T T
0. 4310003313499586 0. 2953287451435756 0. 5000000000000000 T T T
0. 3210761265815476 0. 5386506611256519 0. 5000000000000000 T T T
0. 5661269035862104 0. 2855801766065344 0. 5000000000000000 T T T
0. 2793451557281109 0. 6642304641755160 0. 5000000000000000 T T T
0. 6448479659047642 0. 3927825352101749 0. 5000000000000000 T T T
0. 7206349528734391 0. 5022002071862712 0. 5000000000000000 T T T

\$POSCAR 1 Au

1. 000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

13

Selective dynamics

Direct

0. 4034420000000000 0. 6570700000000000 0. 5000000000000000 T T T
0. 6689910000000000 0. 6273180000000000 0. 5000000000000000 T T T
0. 5351780000000000 0. 6442360000000000 0. 5000000000000000 T T T
0. 5893640000000000 0. 5179950000000000 0. 5000000000000000 T T T
0. 4558520000000000 0. 5319520000000000 0. 5000000000000000 T T T
0. 5108330000000000 0. 4094880000000000 0. 5000000000000000 T T T
0. 3739820000000000 0. 4215080000000000 0. 5000000000000000 T T T
0. 4318710000000000 0. 2996850000000000 0. 5000000000000000 T T T
0. 3206220000000000 0. 5426360000000000 0. 5000000000000000 T T T
0. 5670520000000000 0. 2865900000000000 0. 5000000000000000 T T T
0. 2712570000000000 0. 6655489999999999 0. 5000000000000000 T T T
0. 6478800000000000 0. 3929740000000000 0. 5000000000000000 T T T
0. 7236760000000000 0. 5029990000000000 0. 5000000000000000 T T T

Pathway 5

\$POSCAR 1 Au

1.000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.4900460000000000	0.6390840000000000	0.5000000000000000	T T T
0.6311810000000000	0.6345790000000000	0.5000000000000000	T T T
0.5658930000000000	0.7480240000000000	0.5000000000000000	T T T
0.5610210000000000	0.5192460000000000	0.5000000000000000	T T T
0.4270120000000000	0.5180870000000000	0.5000000000000000	T T T
0.4943580000000000	0.4024630000000000	0.5000000000000000	T T T
0.3573640000000000	0.3976690000000000	0.5000000000000000	T T T
0.4296270000000000	0.2838050000000000	0.5000000000000000	T T T
0.2914460000000000	0.5136039999999999	0.5000000000000000	T T T
0.5656130000000000	0.2875150000000000	0.5000000000000000	T T T
0.3552510000000000	0.6325090000000000	0.5000000000000000	T T T
0.6324930000000000	0.4027530000000000	0.5000000000000000	T T T
0.6986940000000000	0.5206620000000000	0.5000000000000000	T T T

Au

1.0000000000000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Au

13

Selective dynamics

Direct

0.4885815303031479	0.6381183056959074	0.5000000000000000	T T T
0.6353029949895743	0.6361431437108122	0.5000000000000000	T T T
0.5643268324024417	0.7463477665781707	0.5000000000000000	T T T
0.5636730124176709	0.5215202008458226	0.5000000000000000	T T T
0.4276920615431927	0.5166451738385379	0.5000000000000000	T T T
0.5002279699121035	0.4047663209018096	0.5000000000000000	T T T
0.3556859133993837	0.4034706335657925	0.5000000000000000	T T T
0.4296270804153317	0.2925509245379669	0.5000000000000000	T T T
0.2810766695362755	0.5128209043151633	0.5000000000000000	T T T
0.5656701965919007	0.2849363162162303	0.5000000000000000	T T T
0.3526320609671639	0.6257375167358159	0.5000000000000000	T T T
0.6368919018496559	0.3983251000805063	0.5000000000000000	T T T

0. 6986117595584745 0. 5186176929774327 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4856799553520557 0. 6386197410286337 0. 5000000000000000 T T T

0. 6400410670182491 0. 6375967046544213 0. 5000000000000000 T T T

0. 5635886939182059 0. 7446060439630399 0. 5000000000000000 T T T

0. 5646737515326913 0. 5259481677063383 0. 5000000000000000 T T T

0. 4291921933171155 0. 5146578700582359 0. 5000000000000000 T T T

0. 5075276390218780 0. 4068895323868881 0. 5000000000000000 T T T

0. 3514958822678487 0. 4070225297021327 0. 5000000000000000 T T T

0. 4304518351814338 0. 3004822573262010 0. 5000000000000000 T T T

0. 2722762045268075 0. 5127716412835358 0. 5000000000000000 T T T

0. 5651359722027067 0. 2824769764599753 0. 5000000000000000 T T T

0. 3504728218009427 0. 6202476977282276 0. 5000000000000000 T T T

0. 6423981692597078 0. 3925784072593408 0. 5000000000000000 T T T

0. 6970657988250243 0. 5161024304429768 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4821753485429857 0. 6393519443796843 0. 5000000000000000 T T T

0. 6447013093572878 0. 6385251645937668 0. 5000000000000000 T T T

0. 5630278507557415 0. 7426087824032510 0. 5000000000000000 T T T

0. 5644380778201777 0. 5312568658704661 0. 5000000000000000 T T T

0. 4304279982917845 0. 5120976359912748 0. 5000000000000000 T T T

0. 5156358716478102 0. 4089282774684019 0. 5000000000000000 T T T

0. 3465125306448775 0. 4093564619559591 0. 5000000000000000 T T T

0. 4317434513586926 0. 3083866428822868 0. 5000000000000000 T T T

0. 2651293130856519 0. 5132390916232451 0. 5000000000000000 T T T

0. 5643242345500619 0. 2806647353690370 0. 5000000000000000 T T T

0. 3487878506697407 0. 6156107953572321 0. 5000000000000000 T T T

0. 6484374364632730 0. 3865535633565479 0. 5000000000000000 T T T

0. 6946587111529136 0. 5134200387487985 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4784562555144125 0. 6400975476196723 0. 5000000000000000 T T T

0. 6490536527708355 0. 6387258494320570 0. 5000000000000000 T T T

0. 5628387051755134 0. 7402627115707225 0. 5000000000000000 T T T

0. 5636803757439806 0. 5366076341999917 0. 5000000000000000 T T T

0. 4316974337482459 0. 5090845273861064 0. 5000000000000000 T T T

0. 5239367243961407 0. 4111004442514838 0. 5000000000000000 T T T

0. 3416852243576577 0. 4113660777313638 0. 5000000000000000 T T T

0. 4332304867411558 0. 3168008824087359 0. 5000000000000000 T T T

0. 2584808294294528 0. 5138084716542534 0. 5000000000000000 T T T

0. 5633600974596642 0. 2798017589257768 0. 5000000000000000 T T T

0. 3473544292190454 0. 6108539842937138 0. 5000000000000000 T T T

0. 6543566278880791 0. 3810632628736982 0. 5000000000000000 T T T

0. 6918691419834435 0. 5104268476523733 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4744905385004791 0. 6408270236396897 0. 5000000000000000 T T T

0. 6530370003300286 0. 6383081460406471 0. 5000000000000000 T T T

0. 5630234392784378 0. 7373604229731312 0. 5000000000000000 T T T

0. 5626943409202150 0. 5417599850073516 0. 5000000000000000 T T T

0. 4332560230674738 0. 5056867560619215 0. 5000000000000000 T T T

0. 5320810836296836 0. 4135804768926634 0. 5000000000000000 T T T

0. 3374953699192070 0. 4135150081672649 0. 5000000000000000 T T T

0. 4347032012002162 0. 3257326766893573 0. 5000000000000000 T T T

0. 2520084494005274 0. 5143348631128271 0. 5000000000000000 T T T

0. 5623109956102077 0. 2800481963087104 0. 5000000000000000 T T T

0. 3460880253153379 0. 6056069921426739 0. 5000000000000000 T T T

0. 6598782827695353 0. 3762381571195891 0. 5000000000000000 T T T

0. 6889332345650264 0. 5070012958441409 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4682302710805428 0. 6420016948343851 0. 5000000000000000 T T T

0. 6588213759737654 0. 6367758754893513 0. 5000000000000000 T T T

0. 5644848015724786 0. 7313711617620442 0. 5000000000000000 T T T

0. 5611554856537221 0. 5485810139597551 0. 5000000000000000 T T T

0. 4359300176842978 0. 5014031710515008 0. 5000000000000000 T T T

0. 5416350478200269 0. 4176180328874301 0. 5000000000000000 T T T

0. 3335160764691562 0. 4170094101545861 0. 5000000000000000 T T T

0. 4364292546127342 0. 3369268798255257 0. 5000000000000000 T T T

0. 2436338547826917 0. 5143316415631203 0. 5000000000000000 T T T

0. 5611019994665265 0. 2825525674056862 0. 5000000000000000 T T T

0. 3441117395977581 0. 5977403080869996 0. 5000000000000000 T T T

0. 6659111980977040 0. 3711150600730433 0. 5000000000000000 T T T

0. 6850388619380915 0. 5025731829065299 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4614731703475723 0. 6425314524646171 0. 5000000000000000 T T T

0. 6651237408239344 0. 6342676316705069 0. 5000000000000000 T T T

0. 5658706308649184 0. 7230540327676772 0. 5000000000000000 T T T

0. 5598088300647078 0. 5552517766963270 0. 5000000000000000 T T T

0. 4392177264448215 0. 4981549726074490 0. 5000000000000000 T T T

0. 5501524696609321 0. 4220485815848450 0. 5000000000000000 T T T

0. 3306572140745174 0. 4217642579526142 0. 5000000000000000 T T T

0. 4379122779678712 0. 3471938034388800 0. 5000000000000000 T T T

0. 2354780560170676 0. 5139858096560902 0. 5000000000000000 T T T

0. 5599289432957062 0. 2866729638716007 0. 5000000000000000 T T T

0. 3417450881415386 0. 5894454147168524 0. 5000000000000000 T T T

0. 6711744312681361 0. 3667458921213204 0. 5000000000000000 T T T


```
0.6814574061539673 0.4988834104511708 0.5000000000000000 T T T
Au
1.0000000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
```

Au

13

Selective dynamics

Direct

```
0.4541770140191160 0.6414149010701254 0.5000000000000000 T T T
0.6731480786078711 0.6313866415561848 0.5000000000000000 T T T
0.5667251591108874 0.7116065474530842 0.5000000000000000 T T T
0.5601595117050668 0.5617812971401075 0.5000000000000000 T T T
0.4429451438197318 0.4980554498271687 0.5000000000000000 T T T
0.5560690916674608 0.4268664147799072 0.5000000000000000 T T T
0.3291296310325795 0.4279888930792456 0.5000000000000000 T T T
0.4390389523723757 0.3554681123740213 0.5000000000000000 T T T
0.2270319507105660 0.5123664870391134 0.5000000000000000 T T T
0.5589698375836256 0.2915984320352967 0.5000000000000000 T T T
0.3380127282735376 0.5812137436584428 0.5000000000000000 T T T
0.6746493038775371 0.3636375764835447 0.5000000000000000 T T T
0.6799435833507075 0.4966155035037035 0.5000000000000000 T T T
```

\$POSCAR 1 Au

```
1.000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
```

13

Selective dynamics

Direct

```
0.4474140000000000 0.6388390000000000 0.5000000000000000 T T T
0.6827490000000001 0.6290070000000000 0.5000000000000000 T T T
0.5673280000000001 0.7005860000000000 0.5000000000000000 T T T
0.5635110000000000 0.5653920000000000 0.5000000000000000 T T T
0.4455200000000000 0.5013730000000000 0.5000000000000000 T T T
0.5601360000000000 0.4314910000000000 0.5000000000000000 T T T
0.3279640000000000 0.4336840000000000 0.5000000000000000 T T T
0.4404870000000000 0.3639870000000000 0.5000000000000000 T T T
0.2177250000000000 0.5071140000000000 0.5000000000000000 T T T
0.5571380000000000 0.2962770000000000 0.5000000000000000 T T T
0.3315230000000000 0.5748980000000000 0.5000000000000000 T T T
0.6760180000000000 0.3619510000000000 0.5000000000000000 T T T
0.6824880000000000 0.4954010000000000 0.5000000000000000 T T T
```

Pathway 6

\$POSCAR 1 Au

1.000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.4900460000000000	0.6390840000000000	0.5000000000000000	T T T
0.6311810000000000	0.6345790000000000	0.5000000000000000	T T T
0.5658930000000000	0.7480240000000000	0.5000000000000000	T T T
0.5610210000000000	0.5192460000000000	0.5000000000000000	T T T
0.4270120000000000	0.5180870000000000	0.5000000000000000	T T T
0.4943580000000000	0.4024630000000000	0.5000000000000000	T T T
0.3573640000000000	0.3976690000000000	0.5000000000000000	T T T
0.4296270000000000	0.2838050000000000	0.5000000000000000	T T T
0.2914460000000000	0.5136039999999999	0.5000000000000000	T T T
0.5656130000000000	0.2875150000000000	0.5000000000000000	T T T
0.3552510000000000	0.6325090000000000	0.5000000000000000	T T T
0.6324930000000000	0.4027530000000000	0.5000000000000000	T T T
0.6986940000000000	0.5206620000000000	0.5000000000000000	T T T

Au

1.0000000000000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Au

13

Selective dynamics

Direct

0.4902053341163297	0.6431338554228327	0.5000000000000000	T T T
0.6287710932235843	0.6338788241447467	0.5000000000000000	T T T
0.5885644938013020	0.7553758548336764	0.5000000000000000	T T T
0.5572143581699940	0.5199384820046272	0.5000000000000000	T T T
0.4244347857320234	0.5171433976321254	0.5000000000000000	T T T
0.4923180099056132	0.4012055959541992	0.5000000000000000	T T T
0.3560103751522258	0.3952994048346140	0.5000000000000000	T T T
0.4292778377069183	0.2818608266587471	0.5000000000000000	T T T
0.2888267865328091	0.5107979924781053	0.5000000000000000	T T T
0.5656897389412775	0.2868679658342433	0.5000000000000000	T T T
0.3543571513716683	0.6304898187454454	0.5000000000000000	T T T
0.6292256985243461	0.4036633630720264	0.5000000000000000	T T T

0. 6951037562249488 0. 5203446183846071 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4861182832210960 0. 6388639256044591 0. 5000000000000000 T T T

0. 6236070456018343 0. 6370172734961769 0. 5000000000000000 T T T

0. 6101635236262416 0. 7637846785277659 0. 5000000000000000 T T T

0. 5555526029885188 0. 5198255745914494 0. 5000000000000000 T T T

0. 4222450568823214 0. 5148519469215013 0. 5000000000000000 T T T

0. 4921585458464147 0. 4001747178941019 0. 5000000000000000 T T T

0. 3555104645182113 0. 3936227403028082 0. 5000000000000000 T T T

0. 4295709602667652 0. 2808534514440141 0. 5000000000000000 T T T

0. 2866672241718360 0. 5083498893210683 0. 5000000000000000 T T T

0. 5665309741127251 0. 2869829727827582 0. 5000000000000000 T T T

0. 3510607938814352 0. 6283110071103500 0. 5000000000000000 T T T

0. 6290463366155347 0. 4046030030555193 0. 5000000000000000 T T T

0. 6917676171731457 0. 5227588189480212 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4817613072849682 0. 6363636704996101 0. 5000000000000000 T T T

0. 6182338561255915 0. 6407127754343768 0. 5000000000000000 T T T

0. 6328984616023814 0. 7674593256749700 0. 5000000000000000 T T T

0. 5537286771354168 0. 5203368678642508 0. 5000000000000000 T T T

0. 4200404304349170 0. 5130960507017100 0. 5000000000000000 T T T

0. 4919730009560940 0. 3996391149616725 0. 5000000000000000 T T T

0. 3550455451034775 0. 3919295974776090 0. 5000000000000000 T T T

0. 4300506999581365 0. 2800208137915384 0. 5000000000000000 T T T

0. 2844125173211832 0. 5055737879965133 0. 5000000000000000 T T T

0. 5674091144680725 0. 2875097439665112 0. 5000000000000000 T T T

0. 3472633767663393 0. 6260815747848615 0. 5000000000000000 T T T

0. 6288496191465669 0. 4058690217384577 0. 5000000000000000 T T T

0. 6883328367198411 0. 5254076551079105 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4773410374921159 0. 6358061772287964 0. 5000000000000000 T T T

0. 6127428811577511 0. 6443452997416121 0. 5000000000000000 T T T

0. 6556091081765089 0. 7645636132699302 0. 5000000000000000 T T T

0. 5516481400571265 0. 5216417765526065 0. 5000000000000000 T T T

0. 4178839777539060 0. 5122492236591445 0. 5000000000000000 T T T

0. 4916627970685201 0. 3998228663798881 0. 5000000000000000 T T T

0. 3548570436215510 0. 3902314305486934 0. 5000000000000000 T T T

0. 4308614967448198 0. 2793261282059539 0. 5000000000000000 T T T

0. 2824195529618755 0. 5026023166431072 0. 5000000000000000 T T T

0. 5682510683370670 0. 2888162172189170 0. 5000000000000000 T T T

0. 3431343486538360 0. 6241865053058010 0. 5000000000000000 T T T

0. 6285197896593681 0. 4078541579071942 0. 5000000000000000 T T T

0. 6850682295443530 0. 5285542873383625 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4725574702976691 0. 6360693667340624 0. 5000000000000000 T T T

0. 6070004133457677 0. 6480386627904388 0. 5000000000000000 T T T

0. 6757287460725403 0. 7555982363345999 0. 5000000000000000 T T T

0. 5494425054317574 0. 5236026788876260 0. 5000000000000000 T T T

0. 4157809598572396 0. 5118086950304245 0. 5000000000000000 T T T

0. 4916029469405527 0. 4007099680766154 0. 5000000000000000 T T T

0. 3551975018367437 0. 3882939610570246 0. 5000000000000000 T T T

0. 4327692250831177 0. 2787438081510579 0. 5000000000000000 T T T

0. 2808618537782092 0. 4994093944370016 0. 5000000000000000 T T T

0. 5697284750280389 0. 2911910340830623 0. 5000000000000000 T T T

0. 3385655737253189 0. 6224688983030764 0. 5000000000000000 T T T

0. 6285269433921366 0. 4111152353916541 0. 5000000000000000 T T T

0. 6822369003784046 0. 5329500607233308 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4680047540041871 0. 6368462384542208 0. 5000000000000000 T T T

0. 6012855713046743 0. 6513700870689801 0. 5000000000000000 T T T

0. 6931785354875248 0. 7400146974271867 0. 5000000000000000 T T T

0. 5473406599827358 0. 5258317930411889 0. 5000000000000000 T T T

0. 4139253696961079 0. 5118347574128453 0. 5000000000000000 T T T

0. 4916506987923447 0. 4021541543175412 0. 5000000000000000 T T T

0. 3556150791375639 0. 3869234731219018 0. 5000000000000000 T T T

0. 4347982445678186 0. 2787761106942594 0. 5000000000000000 T T T

0. 2797731768538302 0. 4971257867332749 0. 5000000000000000 T T T

0. 5712466525995362 0. 2942403298345474 0. 5000000000000000 T T T

0. 3343126798553639 0. 6215060856990209 0. 5000000000000000 T T T

0. 6287706745018118 0. 4152033396707800 0. 5000000000000000 T T T

0. 6800974575567067 0. 5381731465242426 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4637914830218877 0. 6376429684908074 0. 5000000000000000 T T T

0. 5952676820182335 0. 6544675376165840 0. 5000000000000000 T T T

0. 7049058379022035 0. 7201417995784367 0. 5000000000000000 T T T

0. 5458946590390669 0. 5279643661292877 0. 5000000000000000 T T T

0. 4126969667495739 0. 5119100741084255 0. 5000000000000000 T T T

0. 4921617586321702 0. 4037149234751500 0. 5000000000000000 T T T

0. 3562334271480170 0. 3859576098432565 0. 5000000000000000 T T T

0. 4369784678352211 0. 2792502116395605 0. 5000000000000000 T T T

0. 2792663857648351 0. 4955277812781642 0. 5000000000000000 T T T

0. 5731426647625066 0. 2975844368538757 0. 5000000000000000 T T T

0. 3306788461039122 0. 6209183509830443 0. 5000000000000000 T T T

0. 6297541721979472 0. 4200829087086985 0. 5000000000000000 T T T

```
0. 6792272193236276 0. 5448370312947002 0. 5000000000000000 T T T
Au
1. 0000000000000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000
```

Au

13

Selective dynamics

Direct

```
0. 4603079399501079 0. 6385739806675483 0. 5000000000000000 T T T
0. 5898789350833865 0. 6577013298793020 0. 5000000000000000 T T T
0. 7119852073007248 0. 6980090045507881 0. 5000000000000000 T T T
0. 5450346933792951 0. 5299842317996487 0. 5000000000000000 T T T
0. 4118889560630075 0. 5120161439365057 0. 5000000000000000 T T T
0. 4928696609118794 0. 4053900573501855 0. 5000000000000000 T T T
0. 3567016150329072 0. 3854084174847944 0. 5000000000000000 T T T
0. 4391379553033539 0. 2802302998086196 0. 5000000000000000 T T T
0. 2788093255258838 0. 4943287741117569 0. 5000000000000000 T T T
0. 5749622776659222 0. 3006195933367495 0. 5000000000000000 T T T
0. 3279381180573975 0. 6203427776248864 0. 5000000000000000 T T T
0. 6310158387981957 0. 4251078837602132 0. 5000000000000000 T T T
0. 6794690572242587 0. 5522875056889931 0. 5000000000000000 T T T
```

\$POSCAR 1 Au

```
1. 000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000
```

13

Selective dynamics

Direct

```
0. 4581840000000000 0. 6424530000000001 0. 5000000000000000 T T T
0. 5891860000000000 0. 6613700000000000 0. 5000000000000000 T T T
0. 7208360000000000 0. 6759579999999999 0. 5000000000000000 T T T
0. 5426220000000000 0. 5339600000000000 0. 5000000000000000 T T T
0. 4098990000000000 0. 5138400000000000 0. 5000000000000000 T T T
0. 4933670000000000 0. 4090840000000000 0. 5000000000000000 T T T
0. 3572320000000000 0. 3862450000000000 0. 5000000000000000 T T T
0. 4428960000000000 0. 2837150000000000 0. 5000000000000000 T T T
0. 2764250000000000 0. 4926440000000000 0. 5000000000000000 T T T
0. 5773270000000000 0. 3030530000000000 0. 5000000000000000 T T T
0. 3252980000000000 0. 6193610000000001 0. 5000000000000000 T T T
0. 6295150000000000 0. 4274250000000000 0. 5000000000000000 T T T
0. 6772130000000000 0. 5508920000000000 0. 5000000000000000 T T T
```

Pathway 7

\$POSCAR 1 Au

1.000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.4900460000000000	0.6390840000000000	0.5000000000000000	T T T
0.6311810000000000	0.6345790000000000	0.5000000000000000	T T T
0.5658930000000000	0.7480240000000000	0.5000000000000000	T T T
0.5610210000000000	0.5192460000000000	0.5000000000000000	T T T
0.4270120000000000	0.5180870000000000	0.5000000000000000	T T T
0.4943580000000000	0.4024630000000000	0.5000000000000000	T T T
0.3573640000000000	0.3976690000000000	0.5000000000000000	T T T
0.4296270000000000	0.2838050000000000	0.5000000000000000	T T T
0.2914460000000000	0.5136039999999999	0.5000000000000000	T T T
0.5656130000000000	0.2875150000000000	0.5000000000000000	T T T
0.3552510000000000	0.6325090000000000	0.5000000000000000	T T T
0.6324930000000000	0.4027530000000000	0.5000000000000000	T T T
0.6986940000000000	0.5206620000000000	0.5000000000000000	T T T

Au

1.0000000000000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Au

13

Selective dynamics

Direct

0.4882201850245226	0.6461404425828292	0.5000000000000000	T T T
0.6316950734837400	0.6349581504640566	0.5000000000000000	T T T
0.5708981522048067	0.7504492190320333	0.5000000000000000	T T T
0.5619861070053811	0.5214595240823195	0.5000000000000000	T T T
0.4300642995910223	0.5225957396130729	0.5000000000000000	T T T
0.4910731216063161	0.4045273811971634	0.5000000000000000	T T T
0.3584198145438015	0.3892990943939959	0.5000000000000000	T T T
0.4270203253159393	0.2744251740866289	0.5000000000000000	T T T
0.2987654101899727	0.5077554541763432	0.5000000000000000	T T T
0.5598199975091773	0.2903057721109029	0.5000000000000000	T T T
0.3523791778520992	0.6332200770674180	0.5000000000000000	T T T
0.6298797689626033	0.4039486281861107	0.5000000000000000	T T T

0. 6997780832420895 0. 5209153430071767 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4853090923144900 0. 6532105060509203 0. 5000000000000000 T T T

0. 6326779343196197 0. 6353658700541820 0. 5000000000000000 T T T

0. 5737028197378247 0. 7516569725747066 0. 5000000000000000 T T T

0. 5644816109699721 0. 5226389919381143 0. 5000000000000000 T T T

0. 4335785292040928 0. 5286071685369880 0. 5000000000000000 T T T

0. 4890918276882638 0. 4087720587912345 0. 5000000000000000 T T T

0. 3594427843958262 0. 3814697382422056 0. 5000000000000000 T T T

0. 4237460743676576 0. 2646550584798166 0. 5000000000000000 T T T

0. 3054221189562727 0. 5026460082933181 0. 5000000000000000 T T T

0. 5534200357834265 0. 2932408520907777 0. 5000000000000000 T T T

0. 3493060090445077 0. 6334509677137770 0. 5000000000000000 T T T

0. 6286755159022394 0. 4035747699344882 0. 5000000000000000 T T T

0. 7011451639898728 0. 5207110372994820 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4803481657861052 0. 6614092913219877 0. 5000000000000000 T T T

0. 6344769484583626 0. 6353962963265308 0. 5000000000000000 T T T

0. 5757729074941005 0. 7517437906350829 0. 5000000000000000 T T T

0. 5672080821316982 0. 5231316479249133 0. 5000000000000000 T T T

0. 4371352336257876 0. 5351082344756970 0. 5000000000000000 T T T

0. 4874651888753960 0. 4134274632389718 0. 5000000000000000 T T T

0. 3609173031062282 0. 3745980495209327 0. 5000000000000000 T T T

0. 4211385952547095 0. 2558906734032433 0. 5000000000000000 T T T

0. 3121594857749246 0. 4979297794817583 0. 5000000000000000 T T T

0. 5473436392315500 0. 2960255923554807 0. 5000000000000000 T T T

0. 3459316652917160 0. 6331015875418757 0. 5000000000000000 T T T

0. 6275307948028133 0. 4024863769208805 0. 5000000000000000 T T T

0. 7025715069140818 0. 5197512168526652 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4736677853015038 0. 6702036145883608 0. 5000000000000000 T T T

0. 6374250070046049 0. 6349109335539870 0. 5000000000000000 T T T

0. 5770957197007104 0. 7505277671068836 0. 5000000000000000 T T T

0. 5697550397177042 0. 5232701020342386 0. 5000000000000000 T T T

0. 4407724572073192 0. 5419075085155183 0. 5000000000000000 T T T

0. 4854492796192827 0. 4179012786285347 0. 5000000000000000 T T T

0. 3625383113393871 0. 3686643616189318 0. 5000000000000000 T T T

0. 4194255273893096 0. 2486921041277274 0. 5000000000000000 T T T

0. 3194302341322091 0. 4937088487476163 0. 5000000000000000 T T T

0. 5417732740493728 0. 2986914961410801 0. 5000000000000000 T T T

0. 3424037397291120 0. 6322329740240408 0. 5000000000000000 T T T

0. 6261265901463090 0. 4012748553225052 0. 5000000000000000 T T T

0. 7041365514714495 0. 5180141555905728 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4668694751125673 0. 6785804335483691 0. 5000000000000000 T T T

0. 6407831002142308 0. 6341713448881505 0. 5000000000000000 T T T

0. 5776048649816431 0. 7486415785159233 0. 5000000000000000 T T T

0. 5718361855050770 0. 5233965091354881 0. 5000000000000000 T T T

0. 4443796477764776 0. 5489844314181329 0. 5000000000000000 T T T

0. 4828868412270843 0. 4225392550393491 0. 5000000000000000 T T T

0. 3646052403674215 0. 3632624314769261 0. 5000000000000000 T T T

0. 4182695043573089 0. 2422946021275175 0. 5000000000000000 T T T

0. 3274810406413346 0. 4897747523381582 0. 5000000000000000 T T T

0. 5361404113682532 0. 3015169869511930 0. 5000000000000000 T T T

0. 3392262632575079 0. 6308567735191888 0. 5000000000000000 T T T

0. 6243504983638123 0. 4002414072313297 0. 5000000000000000 T T T

0. 7055664436961430 0. 5157394938103268 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4555542699163079 0. 6902224678981145 0. 5000000000000000 T T T

0. 6480633663560103 0. 6328615854031668 0. 5000000000000000 T T T

0. 5761513924084274 0. 7431334321862904 0. 5000000000000000 T T T

0. 5745342448815721 0. 5252039075105617 0. 5000000000000000 T T T

0. 4498293302260332 0. 5600739024622655 0. 5000000000000000 T T T

0. 4798074339715184 0. 4307999464647064 0. 5000000000000000 T T T

0. 3703633393268259 0. 3563342414175628 0. 5000000000000000 T T T

0. 4167640432731112 0. 2330686693592280 0. 5000000000000000 T T T

0. 3404899982391494 0. 4848112455703424 0. 5000000000000000 T T T

0. 5261958667000055 0. 3063398294434379 0. 5000000000000000 T T T

0. 3346896104067179 0. 6270400465012561 0. 5000000000000000 T T T

0. 6201395241323546 0. 3993955944816000 0. 5000000000000000 T T T

0. 7074170988383170 0. 5107151313015406 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4421830500157594 0. 6982549215894790 0. 5000000000000000 T T T

0. 6605405573302873 0. 6307608496444929 0. 5000000000000000 T T T

0. 5709722726283051 0. 7279030876424166 0. 5000000000000000 T T T

0. 5773326801604526 0. 5309952292880292 0. 5000000000000000 T T T

0. 4532757020007595 0. 5689170026656510 0. 5000000000000000 T T T

0. 4810157689252505 0. 4386446937833032 0. 5000000000000000 T T T

0. 3767519586464919 0. 3549377997893574 0. 5000000000000000 T T T

0. 4158674773592613 0. 2290331507293311 0. 5000000000000000 T T T

0. 3476175665931350 0. 4839789535891889 0. 5000000000000000 T T T

0. 5196051911204165 0. 3104437575886946 0. 5000000000000000 T T T

0. 3293898755594941 0. 6216236475504682 0. 5000000000000000 T T T

0. 6161547764506640 0. 4009292454705173 0. 5000000000000000 T T T

0. 7092926492703699 0. 5035776606690980 0. 5000000000000000 T T T
Au
1. 0000000000000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4319330521498424 0. 7045935517590526 0. 5000000000000000 T T T
0. 6723209720334770 0. 6300091568524981 0. 5000000000000000 T T T
0. 5632945667783646 0. 7032891984669931 0. 5000000000000000 T T T
0. 5797907342306341 0. 5371643440910058 0. 5000000000000000 T T T
0. 4551121002140774 0. 5756578200851197 0. 5000000000000000 T T T
0. 4826859596422634 0. 4443169452511233 0. 5000000000000000 T T T
0. 3798273485717615 0. 3561338883095391 0. 5000000000000000 T T T
0. 4157520298586591 0. 2289519794584530 0. 5000000000000000 T T T
0. 3508605279310028 0. 4850605456643219 0. 5000000000000000 T T T
0. 5175296335545293 0. 3132977406884819 0. 5000000000000000 T T T
0. 3265220373203136 0. 6187081481420036 0. 5000000000000000 T T T
0. 6142596439375602 0. 4033155860700503 0. 5000000000000000 T T T
0. 7101109224670470 0. 4995010951614316 0. 5000000000000000 T T T

\$POSCAR 1 Au

1. 000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

13

Selective dynamics

Direct

0. 4252030000000000 0. 7108210000000000 0. 5000000000000000 T T T
0. 6804950000000000 0. 6321430000000000 0. 5000000000000000 T T T
0. 5537630000000000 0. 6744490000000000 0. 5000000000000000 T T T
0. 5822150000000000 0. 5393750000000000 0. 5000000000000000 T T T
0. 4542130000000000 0. 5788240000000000 0. 5000000000000000 T T T
0. 4839490000000000 0. 4479200000000000 0. 5000000000000000 T T T
0. 3823430000000000 0. 3580450000000000 0. 5000000000000000 T T T
0. 4168380000000000 0. 2301600000000000 0. 5000000000000000 T T T
0. 3521150000000000 0. 4869070000000000 0. 5000000000000000 T T T
0. 5173370000000000 0. 3164410000000000 0. 5000000000000000 T T T
0. 3250860000000000 0. 6190490000000000 0. 5000000000000000 T T T
0. 6148590000000000 0. 4059320000000000 0. 5000000000000000 T T T
0. 7115840000000000 0. 4999340000000000 0. 5000000000000000 T T T

Pathway 8

\$POSCAR 1 Au

1.000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.4900460000000000	0.6390840000000000	0.5000000000000000	T T T
0.6311810000000000	0.6345790000000000	0.5000000000000000	T T T
0.5658930000000000	0.7480240000000000	0.5000000000000000	T T T
0.5610210000000000	0.5192460000000000	0.5000000000000000	T T T
0.4270120000000000	0.5180870000000000	0.5000000000000000	T T T
0.4943580000000000	0.4024630000000000	0.5000000000000000	T T T
0.3573640000000000	0.3976690000000000	0.5000000000000000	T T T
0.4296270000000000	0.2838050000000000	0.5000000000000000	T T T
0.2914460000000000	0.5136039999999999	0.5000000000000000	T T T
0.5656130000000000	0.2875150000000000	0.5000000000000000	T T T
0.3552510000000000	0.6325090000000000	0.5000000000000000	T T T
0.6324930000000000	0.4027530000000000	0.5000000000000000	T T T
0.6986940000000000	0.5206620000000000	0.5000000000000000	T T T

Au

1.0000000000000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Au

13

Selective dynamics

Direct

0.4891330732568904	0.6409235651296579	0.5000000000000000	T T T
0.6281284803352043	0.6375757665907492	0.5000000000000000	T T T
0.5622188161798415	0.7515489955632650	0.5000000000000000	T T T
0.5669712118481494	0.5168428745152679	0.5000000000000000	T T T
0.4331347818422521	0.5179562554177758	0.5000000000000000	T T T
0.4984396185687785	0.4012183152629211	0.5000000000000000	T T T
0.3600435143683253	0.4046245096228963	0.5000000000000000	T T T
0.4249154675620488	0.2879626531200051	0.5000000000000000	T T T
0.2841545408269806	0.5123595309706913	0.5000000000000000	T T T
0.5614924675552245	0.2825894244690350	0.5000000000000000	T T T
0.3550582828012693	0.6251054387855798	0.5000000000000000	T T T
0.6356860157044820	0.3965108614398628	0.5000000000000000	T T T

0. 7006232843159530 0. 5247818091122171 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4865896644473932 0. 6448183996250214 0. 5000000000000000 T T T

0. 6247005756111097 0. 6386871386544354 0. 5000000000000000 T T T

0. 5612063011152630 0. 7539208031351254 0. 5000000000000000 T T T

0. 5737793321621735 0. 5130782159353156 0. 5000000000000000 T T T

0. 4405563783151129 0. 5191741882506163 0. 5000000000000000 T T T

0. 5000239751527501 0. 4000278341537859 0. 5000000000000000 T T T

0. 3618557305521908 0. 4102440056895258 0. 5000000000000000 T T T

0. 4214924150376650 0. 2906005415406654 0. 5000000000000000 T T T

0. 2770345522214900 0. 5109373524591014 0. 5000000000000000 T T T

0. 5574992850400630 0. 2784456964062780 0. 5000000000000000 T T T

0. 3544739612723182 0. 6186941672458479 0. 5000000000000000 T T T

0. 6358979768645088 0. 3894504392508998 0. 5000000000000000 T T T

0. 7048894241449982 0. 5319212176533055 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4831460769212592 0. 6491578581894669 0. 5000000000000000 T T T

0. 6208086851805850 0. 6389422431448816 0. 5000000000000000 T T T

0. 5606188937609959 0. 7557846168690900 0. 5000000000000000 T T T

0. 5809153007344705 0. 5088155777978313 0. 5000000000000000 T T T

0. 4478930408054442 0. 5207999140580897 0. 5000000000000000 T T T

0. 5010702846636446 0. 3992490583001513 0. 5000000000000000 T T T

0. 3637152979769498 0. 4154039977658477 0. 5000000000000000 T T T

0. 4185789281576427 0. 2931613189122401 0. 5000000000000000 T T T

0. 2714599606491045 0. 5094290000079628 0. 5000000000000000 T T T

0. 5533801152389994 0. 2746144250541374 0. 5000000000000000 T T T

0. 3541289253776447 0. 6127556305539675 0. 5000000000000000 T T T

0. 6352369999586422 0. 3818379505689791 0. 5000000000000000 T T T

0. 7090470743823919 0. 5400484087772784 0. 5000000000000000 T T T
Au

1. 0000000000000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4789516757764858 0. 6535571502957019 0. 5000000000000000 T T T
0. 6164455068756062 0. 6382393347479661 0. 5000000000000000 T T T
0. 5601466678842675 0. 7570716970051208 0. 5000000000000000 T T T
0. 5880805022222105 0. 5046094311868209 0. 5000000000000000 T T T
0. 4555210201292865 0. 5227057990234425 0. 5000000000000000 T T T
0. 5023184807607379 0. 3989333612686546 0. 5000000000000000 T T T
0. 3660590965659227 0. 4211420421622283 0. 5000000000000000 T T T
0. 4156703277664728 0. 2964310648916265 0. 5000000000000000 T T T
0. 2666084112734585 0. 5074843992911368 0. 5000000000000000 T T T
0. 5489762646087555 0. 2712836589880993 0. 5000000000000000 T T T
0. 3541609559002346 0. 6063021954770890 0. 5000000000000000 T T T
0. 6346979640129123 0. 3746680795123765 0. 5000000000000000 T T T
0. 7123627248184193 0. 5475717861496489 0. 5000000000000000 T T T

Au

1. 0000000000000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4742117458735250 0. 6574559146679873 0. 5000000000000000 T T T
0. 6119417435535646 0. 6365865888969692 0. 5000000000000000 T T T
0. 5595687828109572 0. 7574030335368334 0. 5000000000000000 T T T
0. 5950445697950733 0. 5006192747919849 0. 5000000000000000 T T T
0. 4633887152694284 0. 5248952746558970 0. 5000000000000000 T T T
0. 5038642281048612 0. 3991888346509069 0. 5000000000000000 T T T
0. 3689356893445526 0. 4279418336545806 0. 5000000000000000 T T T
0. 4127767700168566 0. 3007913621341455 0. 5000000000000000 T T T
0. 2622054919022224 0. 5048152015041212 0. 5000000000000000 T T T
0. 5445173677506542 0. 2687043871878391 0. 5000000000000000 T T T
0. 3544525817366223 0. 5992405801330886 0. 5000000000000000 T T T
0. 6342849467197638 0. 3682014556881593 0. 5000000000000000 T T T

0. 7148069827118589 0. 5541562584973833 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4708192220885197 0. 6621758571509891 0. 5000000000000000 T T T

0. 6057222832752145 0. 6319047326831267 0. 5000000000000000 T T T

0. 5631216926172030 0. 7564016788960176 0. 5000000000000000 T T T

0. 5986000640059941 0. 4963843432869072 0. 5000000000000000 T T T

0. 4693155458322825 0. 5283347712843068 0. 5000000000000000 T T T

0. 5028271165801307 0. 3995524610843930 0. 5000000000000000 T T T

0. 3698105082869776 0. 4301350713326907 0. 5000000000000000 T T T

0. 4102060468370319 0. 3014653599785503 0. 5000000000000000 T T T

0. 2604608672103170 0. 5029266148947531 0. 5000000000000000 T T T

0. 5428156299013680 0. 2710701378254024 0. 5000000000000000 T T T

0. 3557438125064797 0. 5938690121970158 0. 5000000000000000 T T T

0. 6356643195639869 0. 3676645235554556 0. 5000000000000000 T T T

0. 7148925063885372 0. 5581154358303010 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4670843009123127 0. 6652094964585809 0. 5000000000000000 T T T

0. 5996274223577857 0. 6277280426279248 0. 5000000000000000 T T T

0. 5646194734348169 0. 7547613767139685 0. 5000000000000000 T T T

0. 6028926081648416 0. 4928346566350502 0. 5000000000000000 T T T

0. 4751817173430835 0. 5311133338565638 0. 5000000000000000 T T T

0. 5034110183185894 0. 4006423202857822 0. 5000000000000000 T T T

0. 3718932035856853 0. 4343057233878840 0. 5000000000000000 T T T

0. 4082291644064996 0. 3040319565059780 0. 5000000000000000 T T T

0. 2588476413778009 0. 5013182183982918 0. 5000000000000000 T T T

0. 5401323090651320 0. 2718809702986843 0. 5000000000000000 T T T

0. 3569223888453606 0. 5887960775456140 0. 5000000000000000 T T T

0. 6366226301562243 0. 3645125484118367 0. 5000000000000000 T T T

0. 7145357374783583 0. 5628652788737468 0. 5000000000000000 T T T
Au
1. 0000000000000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4634138386500984 0. 6671904486232756 0. 5000000000000000 T T T
0. 5941802714349234 0. 6241514296788105 0. 5000000000000000 T T T
0. 5648335784679805 0. 7527699731972617 0. 5000000000000000 T T T
0. 6076944457373961 0. 4894052438500971 0. 5000000000000000 T T T
0. 4803753259626678 0. 5333474942155134 0. 5000000000000000 T T T
0. 5050369914227246 0. 4018005240967327 0. 5000000000000000 T T T
0. 3746435948676268 0. 4388744344601726 0. 5000000000000000 T T T
0. 4063463325344419 0. 3077602154183361 0. 5000000000000000 T T T
0. 2578312581547044 0. 4996434812003996 0. 5000000000000000 T T T
0. 5367477012025238 0. 2719445181036076 0. 5000000000000000 T T T
0. 3580089576906307 0. 5846857394392475 0. 5000000000000000 T T T
0. 6373248159816226 0. 3601153071479090 0. 5000000000000000 T T T
0. 7135625022252116 0. 5683111905685448 0. 5000000000000000 T T T

\$POSCAR 1 Au

1. 000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

13

Selective dynamics

Direct

0. 4601700000000000 0. 6674410000000000 0. 5000000000000000 T T T
0. 5911740000000000 0. 6226030000000000 0. 5000000000000000 T T T
0. 5628100000000000 0. 7513540000000000 0. 5000000000000000 T T T
0. 6134120000000000 0. 4868340000000000 0. 5000000000000000 T T T
0. 4846730000000000 0. 5343680000000000 0. 5000000000000000 T T T
0. 5077390000000001 0. 4027070000000000 0. 5000000000000000 T T T
0. 3782210000000000 0. 4430750000000000 0. 5000000000000000 T T T
0. 4038120000000000 0. 3124470000000000 0. 5000000000000000 T T T
0. 2577010000000000 0. 4967320000000000 0. 5000000000000000 T T T
0. 5317670000000000 0. 2713120000000000 0. 5000000000000000 T T T
0. 3584730000000000 0. 5816150000000000 0. 5000000000000000 T T T
0. 6369930000000000 0. 3549050000000000 0. 5000000000000000 T T T
0. 7130550000000000 0. 5746070000000000 0. 5000000000000000 T T T

Pathway 9

\$POSCAR 1 Au

1.000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.4900460000000000	0.6390840000000000	0.5000000000000000	T T T
0.6311810000000000	0.6345790000000000	0.5000000000000000	T T T
0.5658930000000000	0.7480240000000000	0.5000000000000000	T T T
0.5610210000000000	0.5192460000000000	0.5000000000000000	T T T
0.4270120000000000	0.5180870000000000	0.5000000000000000	T T T
0.4943580000000000	0.4024630000000000	0.5000000000000000	T T T
0.3573640000000000	0.3976690000000000	0.5000000000000000	T T T
0.4296270000000000	0.2838050000000000	0.5000000000000000	T T T
0.2914460000000000	0.5136039999999999	0.5000000000000000	T T T
0.5656130000000000	0.2875150000000000	0.5000000000000000	T T T
0.3552510000000000	0.6325090000000000	0.5000000000000000	T T T
0.6324930000000000	0.4027530000000000	0.5000000000000000	T T T
0.6986940000000000	0.5206620000000000	0.5000000000000000	T T T

Au

1.0000000000000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Au

13

Selective dynamics

Direct

0.4837494831129033	0.6371590629789359	0.5000000000000000	T T T
0.6375934425027283	0.6348521047948873	0.5000000000000000	T T T
0.5638033327923812	0.7418303377441134	0.5000000000000000	T T T
0.5621649530927424	0.5235197966917576	0.5000000000000000	T T T
0.4291476894854301	0.5149690029492512	0.5000000000000000	T T T
0.4930003782580136	0.3976248998957405	0.5000000000000000	T T T
0.3550804225759990	0.3960869053484472	0.5000000000000000	T T T
0.4246072130767368	0.2805601898730063	0.5000000000000000	T T T
0.2971300601585620	0.5163866322403677	0.5000000000000000	T T T
0.5707479791115336	0.2887647972208847	0.5000000000000000	T T T
0.3494407703362171	0.6390795959603679	0.5000000000000000	T T T
0.6298704637810817	0.4082082084163413	0.5000000000000000	T T T

0. 7036633064893586 0. 5209579711122196 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4783876086487154 0. 6358028066750536 0. 5000000000000000 T T T

0. 6431426520635734 0. 6367173270245262 0. 5000000000000000 T T T

0. 5624435743768982 0. 7380806142576205 0. 5000000000000000 T T T

0. 5639282811376867 0. 5289955703300979 0. 5000000000000000 T T T

0. 4328128186787569 0. 5102245744162778 0. 5000000000000000 T T T

0. 4920554874151493 0. 3903600506938616 0. 5000000000000000 T T T

0. 3533345201110543 0. 3961356068798099 0. 5000000000000000 T T T

0. 4166694276577397 0. 2785007567718905 0. 5000000000000000 T T T

0. 3017853101374925 0. 5188213569472153 0. 5000000000000000 T T T

0. 5781788740260091 0. 2888533369109133 0. 5000000000000000 T T T

0. 3449127082022085 0. 6447525525364363 0. 5000000000000000 T T T

0. 6267190966553643 0. 4119807867159883 0. 5000000000000000 T T T

0. 7056291368290916 0. 5207741639005818 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4731984031475079 0. 6342228065693670 0. 5000000000000000 T T T

0. 6487355400337893 0. 6388574450228263 0. 5000000000000000 T T T

0. 5608473454804054 0. 7342017907629028 0. 5000000000000000 T T T

0. 5657535355015165 0. 5352138057318766 0. 5000000000000000 T T T

0. 4371189549021647 0. 5053527840392267 0. 5000000000000000 T T T

0. 4910411447874707 0. 3827210484123796 0. 5000000000000000 T T T

0. 3520271035411105 0. 3965291663863582 0. 5000000000000000 T T T

0. 4091623468563559 0. 2767226574562058 0. 5000000000000000 T T T

0. 3067440405932284 0. 5212151413345393 0. 5000000000000000 T T T

0. 5851347935432664 0. 2892834833165446 0. 5000000000000000 T T T

0. 3408606234616512 0. 6497838453440753 0. 5000000000000000 T T T

0. 6227027086195143 0. 4155921898544717 0. 5000000000000000 T T T

0. 7066729562151377 0. 5203033390861191 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4678378925909856 0. 6324116448249594 0. 5000000000000000 T T T

0. 6546047994182191 0. 6411277281128059 0. 5000000000000000 T T T

0. 5589153580709618 0. 7294803839757045 0. 5000000000000000 T T T

0. 5675675772166289 0. 5419014316419641 0. 5000000000000000 T T T

0. 4421102825446732 0. 5006412538485824 0. 5000000000000000 T T T

0. 4899376659985328 0. 3753314741317433 0. 5000000000000000 T T T

0. 3513681335980148 0. 3971292990099516 0. 5000000000000000 T T T

0. 4026775310238787 0. 2750422138891068 0. 5000000000000000 T T T

0. 3124533246594464 0. 5237419341573054 0. 5000000000000000 T T T

0. 5908760352147031 0. 2902195084034059 0. 5000000000000000 T T T

0. 3369616027156471 0. 6540872771773386 0. 5000000000000000 T T T

0. 6176155056746148 0. 4192882689550089 0. 5000000000000000 T T T

0. 7070737887958879 0. 5195970843499420 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4633188108720651 0. 6310953370809262 0. 5000000000000000 T T T

0. 6597718972707294 0. 6427886218844568 0. 5000000000000000 T T T

0. 5578142048127086 0. 7246554072298531 0. 5000000000000000 T T T

0. 5688771649676762 0. 5479261567840558 0. 5000000000000000 T T T

0. 4466555042022568 0. 4971717779017595 0. 5000000000000000 T T T

0. 4887212205808845 0. 3700114423279975 0. 5000000000000000 T T T

0. 3516093500134294 0. 3975610083861393 0. 5000000000000000 T T T

0. 3984155259942022 0. 2735305766388578 0. 5000000000000000 T T T

0. 3175659943856765 0. 5255692046981605 0. 5000000000000000 T T T

0. 5943308420183491 0. 2916957303443471 0. 5000000000000000 T T T

0. 3338310400873379 0. 6566494841066602 0. 5000000000000000 T T T

0. 6122941773863716 0. 4227247162337780 0. 5000000000000000 T T T

0. 7067937665348977 0. 5186200372564351 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4587517497169133 0. 6297285223482375 0. 5000000000000000 T T T

0. 6647240676177250 0. 6442089868204061 0. 5000000000000000 T T T

0. 5569212184879607 0. 7191021710351081 0. 5000000000000000 T T T

0. 5698138168714163 0. 5539577368775793 0. 5000000000000000 T T T

0. 4515283424632803 0. 4938641566075329 0. 5000000000000000 T T T

0. 4874737064908784 0. 3651691251336855 0. 5000000000000000 T T T

0. 3523586317048749 0. 3980916745880652 0. 5000000000000000 T T T

0. 3946395684351527 0. 2721106296895383 0. 5000000000000000 T T T

0. 3230986798889670 0. 5274478612785697 0. 5000000000000000 T T T

0. 5972094972331565 0. 2936450692318643 0. 5000000000000000 T T T

0. 3307704394674273 0. 6588383025161691 0. 5000000000000000 T T T

0. 6067964589093141 0. 4262757701475693 0. 5000000000000000 T T T

0. 7059133234957133 0. 5175594929429104 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4542625018109921 0. 6280396327133877 0. 5000000000000000 T T T

0. 6693480379243059 0. 6455677197612683 0. 5000000000000000 T T T

0. 5561190461200332 0. 7130804882265138 0. 5000000000000000 T T T

0. 5703962096599263 0. 5596927725964210 0. 5000000000000000 T T T

0. 4566584181567057 0. 4908178861738396 0. 5000000000000000 T T T

0. 4863279189955972 0. 3605239189700950 0. 5000000000000000 T T T

0. 3536484054293331 0. 3988661382611530 0. 5000000000000000 T T T

0. 3909428395283951 0. 2708833758307643 0. 5000000000000000 T T T

0. 3290243397790992 0. 5293885857508392 0. 5000000000000000 T T T

0. 5998354428483650 0. 2959934934755401 0. 5000000000000000 T T T

0. 3277256096708233 0. 6607576458712767 0. 5000000000000000 T T T

0. 6013613206577746 0. 4297690441933665 0. 5000000000000000 T T T

0. 7043494123122673 0. 5166187952819389 0. 5000000000000000 T T T
Au
1. 0000000000000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4501623095756542 0. 6258465424766416 0. 5000000000000000 T T T
0. 6736974774802634 0. 6470970153013803 0. 5000000000000000 T T T
0. 5552411075338303 0. 7073477627675657 0. 5000000000000000 T T T
0. 5707967714554949 0. 5645700335649471 0. 5000000000000000 T T T
0. 4617438452466409 0. 4879350307718818 0. 5000000000000000 T T T
0. 4855150395060182 0. 3553743204749703 0. 5000000000000000 T T T
0. 3555970981644718 0. 4000340147041531 0. 5000000000000000 T T T
0. 3863742332688661 0. 2700798240630611 0. 5000000000000000 T T T
0. 3351683005444508 0. 5314941858799289 0. 5000000000000000 T T T
0. 6029150837553267 0. 2988790081680107 0. 5000000000000000 T T T
0. 3245806112421742 0. 6625113014782140 0. 5000000000000000 T T T
0. 5962703919385418 0. 4328027550620756 0. 5000000000000000 T T T
0. 7019372388253523 0. 5160276967501221 0. 5000000000000000 T T T

\$POSCAR 1 Au

1. 000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

13

Selective dynamics

Direct

0. 4473830000000000 0. 6237009999999999 0. 5000000000000000 T T T
0. 6763800000000000 0. 6489880000000000 0. 5000000000000000 T T T
0. 5536740000000000 0. 7038310000000000 0. 5000000000000000 T T T
0. 5707400000000000 0. 5672430000000001 0. 5000000000000000 T T T
0. 4656390000000000 0. 4846570000000000 0. 5000000000000000 T T T
0. 4859740000000000 0. 3478570000000000 0. 5000000000000000 T T T
0. 3585250000000000 0. 4019810000000000 0. 5000000000000000 T T T
0. 3788720000000000 0. 2709760000000000 0. 5000000000000000 T T T
0. 3401570000000000 0. 5337809999999999 0. 5000000000000000 T T T
0. 6087410000000000 0. 3021770000000000 0. 5000000000000000 T T T
0. 3218470000000000 0. 6642600000000000 0. 5000000000000000 T T T
0. 5932020000000000 0. 4340540000000000 0. 5000000000000000 T T T
0. 6988660000000000 0. 5164930000000000 0. 5000000000000000 T T T

Pathway 10

\$POSCAR 1 Au

1.000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.4900460000000000	0.6390840000000000	0.5000000000000000	T T T
0.6311810000000000	0.6345790000000000	0.5000000000000000	T T T
0.5658930000000000	0.7480240000000000	0.5000000000000000	T T T
0.5610210000000000	0.5192460000000000	0.5000000000000000	T T T
0.4270120000000000	0.5180870000000000	0.5000000000000000	T T T
0.4943580000000000	0.4024630000000000	0.5000000000000000	T T T
0.3573640000000000	0.3976690000000000	0.5000000000000000	T T T
0.4296270000000000	0.2838050000000000	0.5000000000000000	T T T
0.2914460000000000	0.5136039999999999	0.5000000000000000	T T T
0.5656130000000000	0.2875150000000000	0.5000000000000000	T T T
0.3552510000000000	0.6325090000000000	0.5000000000000000	T T T
0.6324930000000000	0.4027530000000000	0.5000000000000000	T T T
0.6986940000000000	0.5206620000000000	0.5000000000000000	T T T

Au

1.0000000000000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Au

13

Selective dynamics

Direct

0.4888966779182945	0.6361213921105170	0.5000000000000000	T T T
0.6308732650007975	0.6289470297388220	0.5000000000000000	T T T
0.5673888245148877	0.7427229552814095	0.5000000000000000	T T T
0.5590346520437506	0.5163149596974139	0.5000000000000000	T T T
0.4232550810634828	0.5179426416237001	0.5000000000000000	T T T
0.4900595175593996	0.4027763723712283	0.5000000000000000	T T T
0.3528247823027913	0.3964056471225213	0.5000000000000000	T T T
0.4316225426978407	0.2823702924820997	0.5000000000000000	T T T
0.2892762901123037	0.5153408459344208	0.5000000000000000	T T T
0.5689640434852709	0.2956252099974372	0.5000000000000000	T T T
0.3535164937232937	0.6347736533502553	0.5000000000000000	T T T
0.6376405292921731	0.4082045504030422	0.5000000000000000	T T T

0. 7066463002856570 0. 5224544498871442 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4887657382224306 0. 6339576414847393 0. 5000000000000000 T T T

0. 6299431023423794 0. 6241875721963236 0. 5000000000000000 T T T

0. 5683878272420844 0. 7392164934698217 0. 5000000000000000 T T T

0. 5560632275332898 0. 5123154269267458 0. 5000000000000000 T T T

0. 4203469877712473 0. 5182539819240002 0. 5000000000000000 T T T

0. 4837366063898151 0. 4013508169455675 0. 5000000000000000 T T T

0. 3479080163223118 0. 3970919554336589 0. 5000000000000000 T T T

0. 4353202152952532 0. 2779552764475506 0. 5000000000000000 T T T

0. 2873650559252248 0. 5186486006710932 0. 5000000000000000 T T T

0. 5713916023604975 0. 3026953903918376 0. 5000000000000000 T T T

0. 3533783448493134 0. 6372785097861463 0. 5000000000000000 T T T

0. 6436847081511057 0. 4122566037668726 0. 5000000000000000 T T T

0. 7137075675949941 0. 5247917305556598 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4890126019529541 0. 6321543017423568 0. 5000000000000000 T T T

0. 6291516469564540 0. 6203517251497692 0. 5000000000000000 T T T

0. 5691917018273400 0. 7365853778482082 0. 5000000000000000 T T T

0. 5532225643793438 0. 5083920921351474 0. 5000000000000000 T T T

0. 4182500005911173 0. 5184940537754136 0. 5000000000000000 T T T

0. 4769959246205132 0. 3988326979370262 0. 5000000000000000 T T T

0. 3424503361463053 0. 3999542252581171 0. 5000000000000000 T T T

0. 4414974116840497 0. 2716596607178952 0. 5000000000000000 T T T

0. 2854891418949150 0. 5226657576304083 0. 5000000000000000 T T T

0. 5730888145866024 0. 3088481777950226 0. 5000000000000000 T T T

0. 3538717123147148 0. 6393585131538708 0. 5000000000000000 T T T

0. 6485536992221635 0. 4156146094513971 0. 5000000000000000 T T T

0. 7192234438234801 0. 5270888074053937 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4894279742517120 0. 6301626079140754 0. 5000000000000000 T T T

0. 6285729347800042 0. 6166559943260213 0. 5000000000000000 T T T

0. 5699979479899216 0. 7340055910336752 0. 5000000000000000 T T T

0. 5505253934580797 0. 5044401408973102 0. 5000000000000000 T T T

0. 4164034736210483 0. 5183570529715177 0. 5000000000000000 T T T

0. 4702223369565506 0. 3958893007256341 0. 5000000000000000 T T T

0. 3368922201401877 0. 4030126907956160 0. 5000000000000000 T T T

0. 4482476908020036 0. 2657911507576537 0. 5000000000000000 T T T

0. 2837437442532533 0. 5266245313400257 0. 5000000000000000 T T T

0. 5741548178202783 0. 3151787296158566 0. 5000000000000000 T T T

0. 3547237260039650 0. 6410765670117800 0. 5000000000000000 T T T

0. 6526093383205499 0. 4192381544616884 0. 5000000000000000 T T T

0. 7244774016024059 0. 5295674881491543 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4899811677019740 0. 6277885118459251 0. 5000000000000000 T T T

0. 6282404017148339 0. 6124355957946287 0. 5000000000000000 T T T

0. 5711639168349203 0. 7310007347476344 0. 5000000000000000 T T T

0. 5479053883704884 0. 5002883000554285 0. 5000000000000000 T T T

0. 4145257508743306 0. 5178049397674290 0. 5000000000000000 T T T

0. 4634918516858571 0. 3931522775531974 0. 5000000000000000 T T T

0. 3314332129284002 0. 4050920075202762 0. 5000000000000000 T T T

0. 4544446023090333 0. 2616631804520299 0. 5000000000000000 T T T

0. 2821613712504708 0. 5298935369620058 0. 5000000000000000 T T T

0. 5744632398709104 0. 3223908461708895 0. 5000000000000000 T T T

0. 3557739280284162 0. 6422591834304505 0. 5000000000000000 T T T

0. 6561121800153624 0. 4237733103019642 0. 5000000000000000 T T T

0. 7303019884149726 0. 5324575753981451 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4907451739553430 0. 6245542710263228 0. 5000000000000000 T T T

0. 6280036438969941 0. 6062814311511636 0. 5000000000000000 T T T

0. 5735011531506490 0. 7265922399550061 0. 5000000000000000 T T T

0. 5447188605094071 0. 4951452234404916 0. 5000000000000000 T T T

0. 4121044697380841 0. 5167824253619935 0. 5000000000000000 T T T

0. 4559395723910630 0. 3903948222445883 0. 5000000000000000 T T T

0. 3251745152211421 0. 4068179070070920 0. 5000000000000000 T T T

0. 4614844702219963 0. 2589938966675950 0. 5000000000000000 T T T

0. 2801913903789132 0. 5330512950214767 0. 5000000000000000 T T T

0. 5741764970306735 0. 3317490633632861 0. 5000000000000000 T T T

0. 3571025485846167 0. 6429940101772195 0. 5000000000000000 T T T

0. 6593197266009594 0. 4304734037672888 0. 5000000000000000 T T T

0. 7375369783201194 0. 5361700108164735 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4914482638051705 0. 6211183559997300 0. 5000000000000000 T T T

0. 6277522415148762 0. 5992349841495369 0. 5000000000000000 T T T

0. 5765224918879616 0. 7214855249142481 0. 5000000000000000 T T T

0. 5413629977573924 0. 4902891103442710 0. 5000000000000000 T T T

0. 4095137889066542 0. 5155386101241790 0. 5000000000000000 T T T

0. 4493076153563240 0. 3879055071430906 0. 5000000000000000 T T T

0. 3194020606918383 0. 4081631837880824 0. 5000000000000000 T T T

0. 4685009293588360 0. 2580110310427386 0. 5000000000000000 T T T

0. 2781788551079658 0. 5356684539484607 0. 5000000000000000 T T T

0. 5737281119928648 0. 3409157803127223 0. 5000000000000000 T T T

0. 3584108451862942 0. 6433024173942882 0. 5000000000000000 T T T

0. 6616122923827810 0. 4381968983553323 0. 5000000000000000 T T T

```
0.7442585060510086 0.5401701424833167 0.5000000000000000 T T T
Au
1.0000000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
```

Au

13

Selective dynamics

Direct

```
0.4919613923443409 0.6176253839046961 0.5000000000000000 T T T
0.6276175439454178 0.5917509578071987 0.5000000000000000 T T T
0.5804372933220951 0.7155132378341041 0.5000000000000000 T T T
0.5375272542004309 0.4864506954286648 0.5000000000000000 T T T
0.4065298951677938 0.5141443345791049 0.5000000000000000 T T T
0.4433526375518855 0.3851171451673403 0.5000000000000000 T T T
0.3139192251551737 0.4098153915374084 0.5000000000000000 T T T
0.4760859446610279 0.2579050341689804 0.5000000000000000 T T T
0.2758308805977992 0.5384226270749392 0.5000000000000000 T T T
0.5735998484802730 0.3488758022448071 0.5000000000000000 T T T
0.3597669797745082 0.6434730538300625 0.5000000000000000 T T T
0.6631758611108403 0.4462582908999325 0.5000000000000000 T T T
0.7501942436883603 0.5446480455227618 0.5000000000000000 T T T
```

\$POSCAR 1 Au

```
1.000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
```

13

Selective dynamics

Direct

```
0.4922130000000000 0.6139070000000000 0.5000000000000000 T T T
0.6267779999999999 0.5852730000000000 0.5000000000000000 T T T
0.5846020000000000 0.7092870000000000 0.5000000000000000 T T T
0.5336050000000000 0.4830650000000000 0.5000000000000000 T T T
0.4031820000000000 0.5123330000000000 0.5000000000000000 T T T
0.4373780000000000 0.3810500000000000 0.5000000000000000 T T T
0.3081070000000000 0.4127920000000000 0.5000000000000000 T T T
0.4852740000000000 0.2581270000000000 0.5000000000000000 T T T
0.2730710000000000 0.5425489999999999 0.5000000000000000 T T T
0.5748280000000000 0.3547710000000000 0.5000000000000000 T T T
0.3615480000000000 0.6437030000000000 0.5000000000000000 T T T
0.6653690000000000 0.4522940000000000 0.5000000000000000 T T T
0.7540440000000000 0.5508490000000000 0.5000000000000000 T T T
```

Pathway 11

\$POSCAR 1 Au

1.000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.4900460000000000	0.6390840000000000	0.5000000000000000	T T T
0.6311810000000000	0.6345790000000000	0.5000000000000000	T T T
0.5658930000000000	0.7480240000000000	0.5000000000000000	T T T
0.5610210000000000	0.5192460000000000	0.5000000000000000	T T T
0.4270120000000000	0.5180870000000000	0.5000000000000000	T T T
0.4943580000000000	0.4024630000000000	0.5000000000000000	T T T
0.3573640000000000	0.3976690000000000	0.5000000000000000	T T T
0.4296270000000000	0.2838050000000000	0.5000000000000000	T T T
0.2914460000000000	0.5136039999999999	0.5000000000000000	T T T
0.5656130000000000	0.2875150000000000	0.5000000000000000	T T T
0.3552510000000000	0.6325090000000000	0.5000000000000000	T T T
0.6324930000000000	0.4027530000000000	0.5000000000000000	T T T
0.6986940000000000	0.5206620000000000	0.5000000000000000	T T T

Au

1.0000000000000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Au

13

Selective dynamics

Direct

0.4884863610401484	0.6392452147644478	0.5000000000000000	T T T
0.6273848740282000	0.6321446509103354	0.5000000000000000	T T T
0.5659395237473668	0.7475108100640820	0.5000000000000000	T T T
0.5642079893069504	0.5141034748489611	0.5000000000000000	T T T
0.4294365241345472	0.5173364567752029	0.5000000000000000	T T T
0.4957392921301664	0.4005899531551725	0.5000000000000000	T T T
0.3556820814874515	0.4041791325251337	0.5000000000000000	T T T
0.4232893433888077	0.2885300257575786	0.5000000000000000	T T T
0.2829062200731758	0.5143159010291050	0.5000000000000000	T T T
0.5694304888811690	0.2901197414274782	0.5000000000000000	T T T
0.3539826636933713	0.6273051096878953	0.5000000000000000	T T T
0.6412071333662422	0.4018984829298506	0.5000000000000000	T T T

0. 7023065047224371 0. 5227215048879592 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4860596347501833 0. 6423400245783525 0. 5000000000000000 T T T

0. 6235598153525799 0. 6296156726381167 0. 5000000000000000 T T T

0. 5674363464916132 0. 7475410660672873 0. 5000000000000000 T T T

0. 5672211531308308 0. 5085224014895342 0. 5000000000000000 T T T

0. 4337525376640697 0. 5178455500525174 0. 5000000000000000 T T T

0. 4949477406573253 0. 3976669434692449 0. 5000000000000000 T T T

0. 3544204197576282 0. 4094767900795382 0. 5000000000000000 T T T

0. 4150820155655005 0. 2911613191416441 0. 5000000000000000 T T T

0. 275553607477676 0. 5144274797841165 0. 5000000000000000 T T T

0. 5753593163638024 0. 2926036491525999 0. 5000000000000000 T T T

0. 3529310443459240 0. 6228080302566528 0. 5000000000000000 T T T

0. 6488860777448112 0. 4015862637619250 0. 5000000000000000 T T T

0. 7047875374279929 0. 5244052956073160 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4828104369677151 0. 6462957520397413 0. 5000000000000000 T T T

0. 6195494611830353 0. 6267436208898526 0. 5000000000000000 T T T

0. 5691222436636638 0. 7471078677960553 0. 5000000000000000 T T T

0. 5703182433419334 0. 5024451922190692 0. 5000000000000000 T T T

0. 4385603998197708 0. 5189144269848611 0. 5000000000000000 T T T

0. 4932458368784822 0. 3950041727216319 0. 5000000000000000 T T T

0. 3536048246098416 0. 4143947014707886 0. 5000000000000000 T T T

0. 4073786307135194 0. 2934785821474031 0. 5000000000000000 T T T

0. 2691066377280139 0. 5143611464931718 0. 5000000000000000 T T T

0. 5806525802660254 0. 2953673606250894 0. 5000000000000000 T T T

0. 3518697375792993 0. 6184616461038002 0. 5000000000000000 T T T

0. 6569989478906416 0. 4012995150815424 0. 5000000000000000 T T T

0. 7067810193580930 0. 5261265178471268 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4790394142204127 0. 6505708837137384 0. 5000000000000000 T T T

0. 6152836318641083 0. 6234018937745308 0. 5000000000000000 T T T

0. 5708978862050312 0. 7460416950640850 0. 5000000000000000 T T T

0. 5735017699981093 0. 4960319324436798 0. 5000000000000000 T T T

0. 4438692181774054 0. 5204715325297631 0. 5000000000000000 T T T

0. 4910464975698564 0. 3928804520799332 0. 5000000000000000 T T T

0. 3533517926042310 0. 4193440890119996 0. 5000000000000000 T T T

0. 4005026017172459 0. 2958546520009973 0. 5000000000000000 T T T

0. 2632816646339138 0. 5141004385492003 0. 5000000000000000 T T T

0. 5847283159897788 0. 2986163345140704 0. 5000000000000000 T T T

0. 3509072270199073 0. 6138194415942068 0. 5000000000000000 T T T

0. 6652791863016289 0. 4010117315908781 0. 5000000000000000 T T T

0. 7083097936984005 0. 5278554400188558 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4751065883408152 0. 6547688838668168 0. 5000000000000000 T T T

0. 6105665103329022 0. 6196524582967619 0. 5000000000000000 T T T

0. 5725785289181369 0. 7443933822174741 0. 5000000000000000 T T T

0. 5767650306562826 0. 4896237831119828 0. 5000000000000000 T T T

0. 4496629837558676 0. 5223239629405613 0. 5000000000000000 T T T

0. 4887134790610317 0. 3912400931503346 0. 5000000000000000 T T T

0. 3537578460928489 0. 4245718518397890 0. 5000000000000000 T T T

0. 3941615447363061 0. 2985559970636929 0. 5000000000000000 T T T

0. 2580714106282349 0. 5136468563237517 0. 5000000000000000 T T T

0. 5877580978267763 0. 3022796647102299 0. 5000000000000000 T T T

0. 3503680858092448 0. 6086616732912871 0. 5000000000000000 T T T

0. 6732812199567237 0. 4007362968517980 0. 5000000000000000 T T T

0. 7092076738848632 0. 5295456261989530 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4712576969067685 0. 6584133489301761 0. 5000000000000000 T T T

0. 6043834016898572 0. 6149536069568620 0. 5000000000000000 T T T

0. 5739047336018099 0. 7420243906800725 0. 5000000000000000 T T T

0. 5803915251519104 0. 4827770736801054 0. 5000000000000000 T T T

0. 4562436636674237 0. 5241847922685933 0. 5000000000000000 T T T

0. 4860519260225951 0. 3900879050302857 0. 5000000000000000 T T T

0. 3547835897111211 0. 4304619539938394 0. 5000000000000000 T T T

0. 3877899411473906 0. 3018730076828716 0. 5000000000000000 T T T

0. 2533393873537857 0. 5130127157622741 0. 5000000000000000 T T T

0. 5899973380370029 0. 3073809922346875 0. 5000000000000000 T T T

0. 3506174496573005 0. 6024930748316397 0. 5000000000000000 T T T

0. 6819104879455522 0. 4006293487410205 0. 5000000000000000 T T T

0. 7093278591075181 0. 5317083311674029 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4681287473745908 0. 6605927003213236 0. 5000000000000000 T T T

0. 5980082245099170 0. 6097077808332062 0. 5000000000000000 T T T

0. 5747656223890365 0. 7389798318322911 0. 5000000000000000 T T T

0. 5838416112985552 0. 4758433068949651 0. 5000000000000000 T T T

0. 4624917427487089 0. 5256098206115846 0. 5000000000000000 T T T

0. 4832645064109425 0. 3895740964362501 0. 5000000000000000 T T T

0. 3556365607933987 0. 4362978315052530 0. 5000000000000000 T T T

0. 3818165567902050 0. 3056479052488905 0. 5000000000000000 T T T

0. 2493847459478720 0. 5126512119257336 0. 5000000000000000 T T T

0. 5918220721552531 0. 3140074072603695 0. 5000000000000000 T T T

0. 3513370950319850 0. 5964308120785971 0. 5000000000000000 T T T

0. 6906939790734353 0. 4007613603733892 0. 5000000000000000 T T T

```

0. 7088075354761426 0. 5338964920972651 0. 5000000000000000 T T T
Au
1. 0000000000000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

```

Au

13

Selective dynamics

Direct

```

0. 4653502099312936 0. 6611918480181824 0. 5000000000000000 T T T
0. 5926787383237518 0. 6044541708712369 0. 5000000000000000 T T T
0. 5748838867675746 0. 7352463848928437 0. 5000000000000000 T T T
0. 5872825941683414 0. 4691507640420409 0. 5000000000000000 T T T
0. 4680665244517865 0. 5261835333836294 0. 5000000000000000 T T T
0. 4808898026403848 0. 3893110417933203 0. 5000000000000000 T T T
0. 3561345726518317 0. 4423386515118793 0. 5000000000000000 T T T
0. 3754526988892095 0. 3106460027302774 0. 5000000000000000 T T T
0. 2454789782679867 0. 5126153589725382 0. 5000000000000000 T T T
0. 5942619753104327 0. 3211864336606637 0. 5000000000000000 T T T
0. 3519711799864277 0. 5905717737907260 0. 5000000000000000 T T T
0. 6997477882589289 0. 4013036795552888 0. 5000000000000000 T T T
0. 7078000503520970 0. 5358009494081449 0. 5000000000000000 T T T

```

\$POSCAR 1 Au

```

1. 000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

```

13

Selective dynamics

Direct

```

0. 4630320000000000 0. 6591360000000001 0. 5000000000000000 T T T
0. 5898550000000000 0. 5999830000000000 0. 5000000000000000 T T T
0. 5735340000000000 0. 7308950000000000 0. 5000000000000000 T T T
0. 5908460000000000 0. 4643240000000000 0. 5000000000000000 T T T
0. 4715680000000000 0. 5246520000000000 0. 5000000000000000 T T T
0. 4796430000000000 0. 3876560000000000 0. 5000000000000000 T T T
0. 3561940000000000 0. 4483860000000000 0. 5000000000000000 T T T
0. 3667030000000000 0. 3178180000000000 0. 5000000000000000 T T T
0. 2412410000000000 0. 5129390000000000 0. 5000000000000000 T T T
0. 5990259999999999 0. 3267560000000000 0. 5000000000000000 T T T
0. 3513580000000000 0. 5867660000000000 0. 5000000000000000 T T T
0. 7095890000000000 0. 4031520000000000 0. 5000000000000000 T T T
0. 7074100000000000 0. 5375380000000000 0. 5000000000000000 T T T

```

Pathway 12

\$POSCAR 1 Au

1.000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.4900460000000000	0.6390840000000000	0.5000000000000000	T T T
0.6311810000000000	0.6345790000000000	0.5000000000000000	T T T
0.5658930000000000	0.7480240000000000	0.5000000000000000	T T T
0.5610210000000000	0.5192460000000000	0.5000000000000000	T T T
0.4270120000000000	0.5180870000000000	0.5000000000000000	T T T
0.4943580000000000	0.4024630000000000	0.5000000000000000	T T T
0.3573640000000000	0.3976690000000000	0.5000000000000000	T T T
0.4296270000000000	0.2838050000000000	0.5000000000000000	T T T
0.2914460000000000	0.5136039999999999	0.5000000000000000	T T T
0.5656130000000000	0.2875150000000000	0.5000000000000000	T T T
0.3552510000000000	0.6325090000000000	0.5000000000000000	T T T
0.6324930000000000	0.4027530000000000	0.5000000000000000	T T T
0.6986940000000000	0.5206620000000000	0.5000000000000000	T T T

Au

1.0000000000000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Au

13

Selective dynamics

Direct

0.4877522593755091	0.6393243845567517	0.5000000000000000	T T T
0.6287842344471720	0.6341753867434369	0.5000000000000000	T T T
0.5629425592591766	0.7479527861701653	0.5000000000000000	T T T
0.5596973049606356	0.5177163131714014	0.5000000000000000	T T T
0.4249474256472716	0.5193520447644421	0.5000000000000000	T T T
0.4940565612271645	0.4048273861966137	0.5000000000000000	T T T
0.3555160290842887	0.3994074291361440	0.5000000000000000	T T T
0.4300441066546167	0.2859802291955207	0.5000000000000000	T T T
0.2891215671628741	0.5150897672464578	0.5000000000000000	T T T
0.5660777793639112	0.2941454899939310	0.5000000000000000	T T T
0.3529139635024982	0.6345017715930137	0.5000000000000000	T T T
0.6550667061428026	0.3900826536601292	0.5000000000000000	T T T

0. 6930799565481839 0. 5174448420306230 0. 5000000000000000 T T T
Au

1. 0000000000000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4864109297020745 0. 6407619730649277 0. 5000000000000000 T T T
0. 6297123245896513 0. 6330690497474655 0. 5000000000000000 T T T
0. 5633583701149539 0. 7472479089326484 0. 5000000000000000 T T T
0. 5551791903553791 0. 5201149849871950 0. 5000000000000000 T T T
0. 4215622155776169 0. 5210740179701676 0. 5000000000000000 T T T
0. 4902961780356319 0. 4075814308450892 0. 5000000000000000 T T T
0. 3530427443956737 0. 3994093634289239 0. 5000000000000000 T T T
0. 4324570583452548 0. 2864937407685169 0. 5000000000000000 T T T
0. 2870028649797482 0. 5157257789675050 0. 5000000000000000 T T T
0. 5682806074504720 0. 3024981411417635 0. 5000000000000000 T T T
0. 3513924466058819 0. 6363391783571686 0. 5000000000000000 T T T
0. 6756280279476095 0. 3780623911874565 0. 5000000000000000 T T T
0. 6856774976278129 0. 5116225258437250 0. 5000000000000000 T T T

Au

1. 0000000000000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4851385742263005 0. 6410445502082274 0. 5000000000000000 T T T
0. 6302397044976951 0. 6287488663662926 0. 5000000000000000 T T T
0. 5654438981790022 0. 7443765162599032 0. 5000000000000000 T T T
0. 5498968456854039 0. 5204116501363870 0. 5000000000000000 T T T
0. 4167767125204487 0. 5228642846796566 0. 5000000000000000 T T T
0. 4842509601741396 0. 4087823754591077 0. 5000000000000000 T T T
0. 3483052619622466 0. 4008972669371755 0. 5000000000000000 T T T
0. 4406263099488520 0. 2843968183512706 0. 5000000000000000 T T T
0. 2832013664366824 0. 5191874298345095 0. 5000000000000000 T T T
0. 5744835311757166 0. 3135177568769935 0. 5000000000000000 T T T
0. 3500063369919045 0. 6397348721099928 0. 5000000000000000 T T T
0. 6921799680418239 0. 3713561086758668 0. 5000000000000000 T T T

0. 6794509911632839 0. 5046819911058097 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4862420826549536 0. 6386327617111396 0. 5000000000000000 T T T

0. 6276212132983594 0. 6257198601276395 0. 5000000000000000 T T T

0. 5654762206505695 0. 7429581325314693 0. 5000000000000000 T T T

0. 5470541453455222 0. 5152795276362778 0. 5000000000000000 T T T

0. 4140494786621483 0. 5239354038157038 0. 5000000000000000 T T T

0. 4754035817764015 0. 4049266061260817 0. 5000000000000000 T T T

0. 3404281289640355 0. 4073215506966364 0. 5000000000000000 T T T

0. 4547421987492763 0. 2751690411803823 0. 5000000000000000 T T T

0. 2797507884181734 0. 5266519160326717 0. 5000000000000000 T T T

0. 5797494316400665 0. 3224826792430633 0. 5000000000000000 T T T

0. 3518006785073056 0. 6436530719822735 0. 5000000000000000 T T T

0. 7006303333979472 0. 3712338319364473 0. 5000000000000000 T T T

0. 6770521797549132 0. 5020361042534245 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4867442149757882 0. 6375631062529958 0. 5000000000000000 T T T

0. 6249789189518768 0. 6230612700793619 0. 5000000000000000 T T T

0. 5666826647889357 0. 7419508485747943 0. 5000000000000000 T T T

0. 5463092250149056 0. 5099196973902030 0. 5000000000000000 T T T

0. 4134488691894125 0. 5249420776506950 0. 5000000000000000 T T T

0. 4679437128320248 0. 4025898824812309 0. 5000000000000000 T T T

0. 3352391906876136 0. 4096428015064906 0. 5000000000000000 T T T

0. 4636376227146530 0. 2709808369197988 0. 5000000000000000 T T T

0. 2799722198829644 0. 5302361625397457 0. 5000000000000000 T T T

0. 5813074823814238 0. 3314554806836008 0. 5000000000000000 T T T

0. 3528653654151035 0. 6462894619200485 0. 5000000000000000 T T T

0. 7047182892222541 0. 3711741950076624 0. 5000000000000000 T T T

0. 6761526857789968 0. 5001946662720061 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4870283509970429 0. 6358517595423455 0. 5000000000000000 T T T

0. 6238071168813905 0. 6198987798504869 0. 5000000000000000 T T T

0. 5675777508194636 0. 7399475266494465 0. 5000000000000000 T T T

0. 5445609722508460 0. 5060971548066610 0. 5000000000000000 T T T

0. 4120531793946694 0. 5246420360326430 0. 5000000000000000 T T T

0. 4621586360281598 0. 4003392899354506 0. 5000000000000000 T T T

0. 3300687471788227 0. 4118721423506351 0. 5000000000000000 T T T

0. 4726006325527156 0. 2692951289223444 0. 5000000000000000 T T T

0. 2790283891316662 0. 5343328053184566 0. 5000000000000000 T T T

0. 5831130254146293 0. 3420559795525525 0. 5000000000000000 T T T

0. 3538172655387198 0. 6481054432421277 0. 5000000000000000 T T T

0. 7095199323797801 0. 3702746127555194 0. 5000000000000000 T T T

0. 6746664633731823 0. 4972878283550580 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4870215888439538 0. 6341095999695765 0. 5000000000000000 T T T

0. 6231515232532606 0. 6165681778249879 0. 5000000000000000 T T T

0. 5684512428721795 0. 7375843228370840 0. 5000000000000000 T T T

0. 5427831730736737 0. 5033369399755171 0. 5000000000000000 T T T

0. 4104551697707337 0. 5240831445022952 0. 5000000000000000 T T T

0. 4573961232516548 0. 3986766834049973 0. 5000000000000000 T T T

0. 3257084002934896 0. 4133674978672773 0. 5000000000000000 T T T

0. 4815536079946907 0. 2696976172543921 0. 5000000000000000 T T T

0. 2779283989366293 0. 5374730792659643 0. 5000000000000000 T T T

0. 5843801982465342 0. 3542775473316095 0. 5000000000000000 T T T

0. 3543783261492199 0. 6493013633105603 0. 5000000000000000 T T T

0. 7136885425285369 0. 3681991912951311 0. 5000000000000000 T T T

```

0. 6731041669703923 0. 4933253225556426 0. 5000000000000000 T T T
Au
1. 0000000000000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

```

Au

13

Selective dynamics

Direct

```

0. 4864570622558320 0. 6329617284515097 0. 5000000000000000 T T T
0. 6226919492007258 0. 6128148434299276 0. 5000000000000000 T T T
0. 5700794137576267 0. 7347132747895314 0. 5000000000000000 T T T
0. 5404103247992009 0. 5024998467016830 0. 5000000000000000 T T T
0. 4083182381666622 0. 5235046081618449 0. 5000000000000000 T T T
0. 4537705014702560 0. 3973984613355638 0. 5000000000000000 T T T
0. 3219219238365356 0. 4146105760950702 0. 5000000000000000 T T T
0. 4916404092469992 0. 2715368425414275 0. 5000000000000000 T T T
0. 2763284372428694 0. 5402012152777081 0. 5000000000000000 T T T
0. 5857303697215053 0. 3658924439054070 0. 5000000000000000 T T T
0. 3543835526633778 0. 6502099300159091 0. 5000000000000000 T T T
0. 7167742509266071 0. 3650248869199104 0. 5000000000000000 T T T
0. 6714940301749330 0. 4886318301956423 0. 5000000000000000 T T T

```

\$POSCAR 1 Au

```

1. 000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

```

13

Selective dynamics

Direct

```

0. 4844250000000000 0. 6335210000000000 0. 5000000000000000 T T T
0. 6221150000000000 0. 6085310000000000 0. 5000000000000000 T T T
0. 5733800000000000 0. 7309440000000000 0. 5000000000000000 T T T
0. 5374490000000000 0. 5036950000000000 0. 5000000000000000 T T T
0. 4052380000000000 0. 5233670000000000 0. 5000000000000000 T T T
0. 4517090000000000 0. 3965420000000000 0. 5000000000000000 T T T
0. 3190820000000000 0. 4158090000000000 0. 5000000000000000 T T T
0. 5035430000000000 0. 2742880000000000 0. 5000000000000000 T T T
0. 2729770000000000 0. 5420420000000000 0. 5000000000000000 T T T
0. 5875560000000000 0. 3747880000000000 0. 5000000000000000 T T T
0. 3523970000000000 0. 6504710000000000 0. 5000000000000000 T T T
0. 7186780000000000 0. 3610620000000000 0. 5000000000000000 T T T
0. 6714530000000000 0. 4849410000000000 0. 5000000000000000 T T T

```

Pathway 13

\$POSCAR 1 Au

1.000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.4900460000000000	0.6390840000000000	0.5000000000000000	T T T
0.6311810000000000	0.6345790000000000	0.5000000000000000	T T T
0.5658930000000000	0.7480240000000000	0.5000000000000000	T T T
0.5610210000000000	0.5192460000000000	0.5000000000000000	T T T
0.4270120000000000	0.5180870000000000	0.5000000000000000	T T T
0.4943580000000000	0.4024630000000000	0.5000000000000000	T T T
0.3573640000000000	0.3976690000000000	0.5000000000000000	T T T
0.4296270000000000	0.2838050000000000	0.5000000000000000	T T T
0.2914460000000000	0.5136039999999999	0.5000000000000000	T T T
0.5656130000000000	0.2875150000000000	0.5000000000000000	T T T
0.3552510000000000	0.6325090000000000	0.5000000000000000	T T T
0.6324930000000000	0.4027530000000000	0.5000000000000000	T T T
0.6986940000000000	0.5206620000000000	0.5000000000000000	T T T

Au

1.0000000000000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Au

13

Selective dynamics

Direct

0.4899504642951710	0.6445819933513446	0.5000000000000000	T T T
0.6337439112816045	0.6296236443511256	0.5000000000000000	T T T
0.5781674579087203	0.7463628245787703	0.5000000000000000	T T T
0.5542744955621980	0.5224847287882736	0.5000000000000000	T T T
0.4211801091487619	0.5161415369302957	0.5000000000000000	T T T
0.4911441063358706	0.4026029686320469	0.5000000000000000	T T T
0.3542148196343814	0.3929409268475824	0.5000000000000000	T T T
0.4333870431474132	0.2817032321833065	0.5000000000000000	T T T
0.2869355479173928	0.5110693418712088	0.5000000000000000	T T T
0.5698974643373432	0.2917611786235335	0.5000000000000000	T T T
0.3554267274876772	0.6309496339133477	0.5000000000000000	T T T
0.6283806910037912	0.4102439999794999	0.5000000000000000	T T T

0. 7032961619396813 0. 5195339899496948 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4913966587731839 0. 6515285353516380 0. 5000000000000000 T T T

0. 6344265916809161 0. 6254595648353170 0. 5000000000000000 T T T

0. 5870497439195766 0. 7456353208221831 0. 5000000000000000 T T T

0. 5455176178658095 0. 5254697026550350 0. 5000000000000000 T T T

0. 4139599760304115 0. 5103670721474628 0. 5000000000000000 T T T

0. 4898988598207831 0. 4013505725244378 0. 5000000000000000 T T T

0. 3522119644944502 0. 3876180669944481 0. 5000000000000000 T T T

0. 4370234653839123 0. 2792781634217837 0. 5000000000000000 T T T

0. 2815237059168457 0. 5131492104644628 0. 5000000000000000 T T T

0. 5739011943853763 0. 2946744299101889 0. 5000000000000000 T T T

0. 3593787528595407 0. 6293039868334296 0. 5000000000000000 T T T

0. 6252313520979655 0. 4169911116246701 0. 5000000000000000 T T T

0. 7084791167712214 0. 5191742624149714 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4930645253988893 0. 6573337242264823 0. 5000000000000000 T T T

0. 6342457373370710 0. 6220247388767968 0. 5000000000000000 T T T

0. 5934523892094400 0. 7447786690469200 0. 5000000000000000 T T T

0. 5373495556300277 0. 5280089744117936 0. 5000000000000000 T T T

0. 4063478794088881 0. 5038760368509232 0. 5000000000000000 T T T

0. 4896358351069556 0. 4004878523599200 0. 5000000000000000 T T T

0. 3525228286438363 0. 3802588781543226 0. 5000000000000000 T T T

0. 4412437667292012 0. 2766372097907978 0. 5000000000000000 T T T

0. 2759221305747538 0. 5210527659006104 0. 5000000000000000 T T T

0. 5772100181863404 0. 2968826197391939 0. 5000000000000000 T T T

0. 3640591825444206 0. 6273817504989398 0. 5000000000000000 T T T

0. 6226520635925550 0. 4225252517544543 0. 5000000000000000 T T T

0. 7122930876376129 0. 5187515283888627 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4949558325434796 0. 6615486953000359 0. 5000000000000000 T T T

0. 6334616831161890 0. 6187380595595333 0. 5000000000000000 T T T

0. 5985653112395947 0. 7436994056528747 0. 5000000000000000 T T T

0. 5295891296633890 0. 5300910732385798 0. 5000000000000000 T T T

0. 3984686609012434 0. 4976614605252627 0. 5000000000000000 T T T

0. 4892153867251459 0. 4002722004637702 0. 5000000000000000 T T T

0. 3535704449448287 0. 3723434493628202 0. 5000000000000000 T T T

0. 4460234238468655 0. 2741031081611517 0. 5000000000000000 T T T

0. 2712200930152496 0. 5311489478247597 0. 5000000000000000 T T T

0. 5802122891533167 0. 2993933397936603 0. 5000000000000000 T T T

0. 3690661956751338 0. 6250348114970036 0. 5000000000000000 T T T

0. 6203484677651767 0. 4277401660086878 0. 5000000000000000 T T T

0. 7153020814103838 0. 5182252826118937 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4970570190510519 0. 6646936905945552 0. 5000000000000000 T T T

0. 6322612619250393 0. 6151376397676943 0. 5000000000000000 T T T

0. 6034302189254035 0. 7422762201255573 0. 5000000000000000 T T T

0. 5222976041820614 0. 5321701388998945 0. 5000000000000000 T T T

0. 3919021388149430 0. 4924234345507867 0. 5000000000000000 T T T

0. 4882259571442478 0. 4006383789647540 0. 5000000000000000 T T T

0. 3536573807650141 0. 3660767986210320 0. 5000000000000000 T T T

0. 4502073612339272 0. 2726830332744162 0. 5000000000000000 T T T

0. 2686548430381190 0. 5381175394132451 0. 5000000000000000 T T T

0. 5826810384746749 0. 3028421005578682 0. 5000000000000000 T T T

0. 3738810891928522 0. 6220457714669689 0. 5000000000000000 T T T

0. 6178035157922106 0. 4333506883425321 0. 5000000000000000 T T T

0. 7179395714604505 0. 5175445654207359 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4993599191937115 0. 6673285463905586 0. 5000000000000000 T T T

0. 6302460508337684 0. 6106398174789321 0. 5000000000000000 T T T

0. 6085305301938733 0. 7401024597640148 0. 5000000000000000 T T T

0. 5147397760730634 0. 5342205110192586 0. 5000000000000000 T T T

0. 3858292560606786 0. 4875989013037125 0. 5000000000000000 T T T

0. 4869223022752525 0. 4012648822217863 0. 5000000000000000 T T T

0. 3535644551097145 0. 3602749884578414 0. 5000000000000000 T T T

0. 4543600716856780 0. 2717406535079542 0. 5000000000000000 T T T

0. 2673043464441431 0. 5442377643686888 0. 5000000000000000 T T T

0. 5850755879089907 0. 3072064964560663 0. 5000000000000000 T T T

0. 3785950281615396 0. 6187650094583753 0. 5000000000000000 T T T

0. 6149353998104465 0. 4397680632676804 0. 5000000000000000 T T T

0. 7205362762491301 0. 5168519063051801 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5015100076439426 0. 6694480246164868 0. 5000000000000000 T T T

0. 6274858849283393 0. 6048992494353707 0. 5000000000000000 T T T

0. 6139800973146894 0. 7366279371013945 0. 5000000000000000 T T T

0. 5073579356276068 0. 5359841849037763 0. 5000000000000000 T T T

0. 3800612821698077 0. 4833967197233300 0. 5000000000000000 T T T

0. 4855323521828983 0. 4022315360160543 0. 5000000000000000 T T T

0. 3537923944410294 0. 3549047276494410 0. 5000000000000000 T T T

0. 4586241570217523 0. 2713889753861019 0. 5000000000000000 T T T

0. 2665795720769790 0. 5495987977933392 0. 5000000000000000 T T T

0. 5874889185856139 0. 3124951989684172 0. 5000000000000000 T T T

0. 3822633052493895 0. 6160217712486609 0. 5000000000000000 T T T

0. 6120736527572431 0. 4468115312897333 0. 5000000000000000 T T T

0. 7232494400007053 0. 5161913458679354 0. 5000000000000000 T T T
Au
1. 0000000000000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5034294493660324 0. 6709093001392411 0. 5000000000000000 T T T
0. 6239547263262254 0. 5985556722230915 0. 5000000000000000 T T T
0. 6199873829577186 0. 7313703065314549 0. 5000000000000000 T T T
0. 5005159853738819 0. 5369903816314513 0. 5000000000000000 T T T
0. 3741314777752474 0. 4800423480850390 0. 5000000000000000 T T T
0. 4840133230955226 0. 4034006397889899 0. 5000000000000000 T T T
0. 3550118694851966 0. 3498682054842345 0. 5000000000000000 T T T
0. 4636129663220256 0. 2714422709115150 0. 5000000000000000 T T T
0. 2658801352786562 0. 5548151079399983 0. 5000000000000000 T T T
0. 5903412993179358 0. 3184307151747713 0. 5000000000000000 T T T
0. 3841615288010304 0. 6148857629074583 0. 5000000000000000 T T T
0. 6094335689002401 0. 4533235387257737 0. 5000000000000000 T T T
0. 7255252870002800 0. 5159657504570379 0. 5000000000000000 T T T

\$POSCAR 1 Au

1. 000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

13

Selective dynamics

Direct

0. 5057830000000000 0. 6720159999999999 0. 5000000000000000 T T T
0. 6203040000000000 0. 5941860000000000 0. 5000000000000000 T T T
0. 6269330000000000 0. 7258580000000000 0. 5000000000000000 T T T
0. 4942890000000000 0. 5371950000000000 0. 5000000000000000 T T T
0. 3675140000000000 0. 4772410000000000 0. 5000000000000000 T T T
0. 4817810000000000 0. 4041150000000000 0. 5000000000000000 T T T
0. 3577150000000000 0. 3444910000000000 0. 5000000000000000 T T T
0. 4702720000000000 0. 2710390000000000 0. 5000000000000000 T T T
0. 2654330000000000 0. 5608090000000000 0. 5000000000000000 T T T
0. 5938330000000001 0. 3238890000000000 0. 5000000000000000 T T T
0. 3850370000000000 0. 6160790000000000 0. 5000000000000000 T T T
0. 6059130000000000 0. 4573630000000000 0. 5000000000000000 T T T
0. 7251919999999999 0. 5157190000000000 0. 5000000000000000 T T T

Pathway 14

\$POSCAR 1 Au

1.000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.4900460000000000	0.6390840000000000	0.5000000000000000	T T T
0.6311810000000000	0.6345790000000000	0.5000000000000000	T T T
0.5658930000000000	0.7480240000000000	0.5000000000000000	T T T
0.5610210000000000	0.5192460000000000	0.5000000000000000	T T T
0.4270120000000000	0.5180870000000000	0.5000000000000000	T T T
0.4943580000000000	0.4024630000000000	0.5000000000000000	T T T
0.3573640000000000	0.3976690000000000	0.5000000000000000	T T T
0.4296270000000000	0.2838050000000000	0.5000000000000000	T T T
0.2914460000000000	0.5136039999999999	0.5000000000000000	T T T
0.5656130000000000	0.2875150000000000	0.5000000000000000	T T T
0.3552510000000000	0.6325090000000000	0.5000000000000000	T T T
0.6324930000000000	0.4027530000000000	0.5000000000000000	T T T
0.6986940000000000	0.5206620000000000	0.5000000000000000	T T T

Au

1.0000000000000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Au

13

Selective dynamics

Direct

0.4863287618848486	0.6387221335964784	0.5000000000000000	T T T
0.6239138785745078	0.6301712512749497	0.5000000000000000	T T T
0.5633883391773591	0.7463661161765366	0.5000000000000000	T T T
0.5626428579178868	0.5117882545673867	0.5000000000000000	T T T
0.4288426186603373	0.5182634000817601	0.5000000000000000	T T T
0.4924515738681481	0.3997049027014297	0.5000000000000000	T T T
0.3551684473309428	0.3985440872070813	0.5000000000000000	T T T
0.4263923121511929	0.2828122340358497	0.5000000000000000	T T T
0.2954544448297017	0.5179299073766179	0.5000000000000000	T T T
0.5684779331292735	0.2917435157670760	0.5000000000000000	T T T
0.3528654272086956	0.6385311491599081	0.5000000000000000	T T T
0.6423027921043365	0.4021113076793899	0.5000000000000000	T T T

0. 7017701133087169 0. 5233112402294900 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4820623170847044 0. 6409130654688698 0. 5000000000000000 T T T

0. 6177780680928229 0. 6261510606894274 0. 5000000000000000 T T T

0. 5632107139966054 0. 7453168507053541 0. 5000000000000000 T T T

0. 5645249626851753 0. 5044257134025190 0. 5000000000000000 T T T

0. 4316000088007561 0. 5179789283999046 0. 5000000000000000 T T T

0. 4897522039287593 0. 3960881297433902 0. 5000000000000000 T T T

0. 3530197617588273 0. 3995232640158590 0. 5000000000000000 T T T

0. 4206929057903517 0. 2820610933314707 0. 5000000000000000 T T T

0. 2992196808660670 0. 5211001832197206 0. 5000000000000000 T T T

0. 5733068211272644 0. 2953063630181854 0. 5000000000000000 T T T

0. 3495356110759856 0. 6440304681467774 0. 5000000000000000 T T T

0. 6517492947483664 0. 4016761711429193 0. 5000000000000000 T T T

0. 7035471501281865 0. 5254282086316127 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4775426090473202 0. 6435945995026132 0. 5000000000000000 T T T

0. 6117450469630979 0. 6223228736280165 0. 5000000000000000 T T T

0. 5633913911536985 0. 7441334261544595 0. 5000000000000000 T T T

0. 5667167026827907 0. 4972877571648995 0. 5000000000000000 T T T

0. 4349826142408217 0. 5172662234123518 0. 5000000000000000 T T T

0. 4875718353533168 0. 3921231365645956 0. 5000000000000000 T T T

0. 3515401440493462 0. 4007562674437525 0. 5000000000000000 T T T

0. 4142070556142274 0. 2814855200631378 0. 5000000000000000 T T T

0. 3033082639104236 0. 5240661752475055 0. 5000000000000000 T T T

0. 5786811628261399 0. 2984107559307143 0. 5000000000000000 T T T

0. 3456671320975522 0. 6495568437033670 0. 5000000000000000 T T T

0. 6602323122460485 0. 4015599188472874 0. 5000000000000000 T T T

0. 7044132298722103 0. 5274360022801933 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4726934451766710 0. 6465245233305742 0. 5000000000000000 T T T

0. 6052310133756522 0. 6182428894328240 0. 5000000000000000 T T T

0. 5637284849149886 0. 7425405056640815 0. 5000000000000000 T T T

0. 5694675324810484 0. 4901320743005063 0. 5000000000000000 T T T

0. 4390697979968854 0. 5166309146207659 0. 5000000000000000 T T T

0. 4857240779373226 0. 3884848378559294 0. 5000000000000000 T T T

0. 3507283683613701 0. 4022168459858127 0. 5000000000000000 T T T

0. 4082949737905592 0. 2810435675944882 0. 5000000000000000 T T T

0. 3080714991386630 0. 5271436411162086 0. 5000000000000000 T T T

0. 5831062855059889 0. 3013433701417850 0. 5000000000000000 T T T

0. 3413124015086090 0. 6550592521763476 0. 5000000000000000 T T T

0. 6681521173587680 0. 4012666149491154 0. 5000000000000000 T T T

0. 7044195024888493 0. 5293704627960893 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4676182684375480 0. 6496152446599598 0. 5000000000000000 T T T

0. 5980412925394920 0. 6136258055302457 0. 5000000000000000 T T T

0. 5641757145393403 0. 7403191000833164 0. 5000000000000000 T T T

0. 5725863843927879 0. 4830241174433835 0. 5000000000000000 T T T

0. 4438036694849075 0. 5165105213923662 0. 5000000000000000 T T T

0. 4840138959262940 0. 3854461785223300 0. 5000000000000000 T T T

0. 3505427380180974 0. 4038902328983199 0. 5000000000000000 T T T

0. 4034183066699901 0. 2807830871044971 0. 5000000000000000 T T T

0. 3133149228612734 0. 5302284250323460 0. 5000000000000000 T T T

0. 5864831598358698 0. 3044456680551185 0. 5000000000000000 T T T

0. 3367058701383789 0. 6600848605286457 0. 5000000000000000 T T T

0. 6756948435814947 0. 4008265769463835 0. 5000000000000000 T T T

0. 7036004335898277 0. 5311996817877265 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4611753132209340 0. 6520816198531485 0. 5000000000000000 T T T

0. 5885326020340957 0. 6066243270854251 0. 5000000000000000 T T T

0. 5640394082037365 0. 7358381734964450 0. 5000000000000000 T T T

0. 5766041068940816 0. 4741971202554788 0. 5000000000000000 T T T

0. 4503942847081341 0. 5164578697661218 0. 5000000000000000 T T T

0. 4820892748971815 0. 3821171285853352 0. 5000000000000000 T T T

0. 3507664261656254 0. 4069291801625604 0. 5000000000000000 T T T

0. 3973970918479338 0. 2813519217154917 0. 5000000000000000 T T T

0. 3203804683790982 0. 5347061578586099 0. 5000000000000000 T T T

0. 5904764002640209 0. 3093854588472320 0. 5000000000000000 T T T

0. 3309970211352991 0. 6659365844844497 0. 5000000000000000 T T T

0. 6853107744230994 0. 4008265855782633 0. 5000000000000000 T T T

0. 7018363278700054 0. 5335473722681185 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4549123588343212 0. 6519099294094903 0. 5000000000000000 T T T

0. 5803424032331597 0. 5993991860792549 0. 5000000000000000 T T T

0. 5620153592788770 0. 7301940025068058 0. 5000000000000000 T T T

0. 5804485651360243 0. 4660190127110033 0. 5000000000000000 T T T

0. 4564637539493087 0. 5150991664563358 0. 5000000000000000 T T T

0. 4809101056657528 0. 3787028217140472 0. 5000000000000000 T T T

0. 3515337181880960 0. 4112289228951330 0. 5000000000000000 T T T

0. 3908600917987369 0. 2832095738661212 0. 5000000000000000 T T T

0. 3274392215903606 0. 5403708686724676 0. 5000000000000000 T T T

0. 5948514979302046 0. 3147168483297598 0. 5000000000000000 T T T

0. 3257402988974040 0. 6718176263857427 0. 5000000000000000 T T T

0. 6947825918734881 0. 4016210079551924 0. 5000000000000000 T T T

0. 6996995337169982 0. 5357105329258496 0. 5000000000000000 T T T
Au
1. 0000000000000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4487113193937845 0. 6479565255880094 0. 5000000000000000 T T T
0. 5749525680058446 0. 5936966630245123 0. 5000000000000000 T T T
0. 5566953753194669 0. 7246972284375743 0. 5000000000000000 T T T
0. 5838778046913187 0. 4597697214688767 0. 5000000000000000 T T T
0. 4606028755900212 0. 5109235745687459 0. 5000000000000000 T T T
0. 4816563838508827 0. 3738310731795253 0. 5000000000000000 T T T
0. 3538424731333610 0. 4171919084092858 0. 5000000000000000 T T T
0. 3832729925116548 0. 2870035924325774 0. 5000000000000000 T T T
0. 3339181137200380 0. 5479965376652302 0. 5000000000000000 T T T
0. 6004200544992694 0. 3177852578100778 0. 5000000000000000 T T T
0. 3212928926795590 0. 6788108182912677 0. 5000000000000000 T T T
0. 7031293439671422 0. 4029550673453446 0. 5000000000000000 T T T
0. 6976273031060024 0. 5373815313105811 0. 5000000000000000 T T T

\$POSCAR 1 Au

1. 000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

13

Selective dynamics

Direct

0. 4442620000000000 0. 6422580000000000 0. 5000000000000000 T T T
0. 5712150000000000 0. 5892410000000000 0. 5000000000000000 T T T
0. 5495080000000000 0. 7202440000000000 0. 5000000000000000 T T T
0. 5866350000000000 0. 4550540000000000 0. 5000000000000000 T T T
0. 4627290000000000 0. 5051940000000000 0. 5000000000000000 T T T
0. 4838170000000000 0. 3665510000000000 0. 5000000000000000 T T T
0. 3558320000000000 0. 4231460000000000 0. 5000000000000000 T T T
0. 3744890000000000 0. 2927160000000000 0. 5000000000000000 T T T
0. 3368650000000000 0. 5548610000000000 0. 5000000000000000 T T T
0. 6081839999999999 0. 3191010000000000 0. 5000000000000000 T T T
0. 3200190000000000 0. 6863620000000000 0. 5000000000000000 T T T
0. 7108250000000000 0. 4058720000000000 0. 5000000000000000 T T T
0. 6956200000000000 0. 5393990000000000 0. 5000000000000000 T T T

Pathway 15

\$POSCAR 1 Au

1.000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.4900460000000000	0.6390840000000000	0.5000000000000000	T T T
0.6311810000000000	0.6345790000000000	0.5000000000000000	T T T
0.5658930000000000	0.7480240000000000	0.5000000000000000	T T T
0.5610210000000000	0.5192460000000000	0.5000000000000000	T T T
0.4270120000000000	0.5180870000000000	0.5000000000000000	T T T
0.4943580000000000	0.4024630000000000	0.5000000000000000	T T T
0.3573640000000000	0.3976690000000000	0.5000000000000000	T T T
0.4296270000000000	0.2838050000000000	0.5000000000000000	T T T
0.2914460000000000	0.5136039999999999	0.5000000000000000	T T T
0.5656130000000000	0.2875150000000000	0.5000000000000000	T T T
0.3552510000000000	0.6325090000000000	0.5000000000000000	T T T
0.6324930000000000	0.4027530000000000	0.5000000000000000	T T T
0.6986940000000000	0.5206620000000000	0.5000000000000000	T T T

Au

1.0000000000000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Au

13

Selective dynamics

Direct

0.4881399784939958	0.6402582838103343	0.5000000000000000	T T T
0.6297736235722390	0.6335067693570352	0.5000000000000000	T T T
0.5650676221155236	0.7477965173976485	0.5000000000000000	T T T
0.5591350733966651	0.5181619771118078	0.5000000000000000	T T T
0.4246517157378910	0.5201683276069742	0.5000000000000000	T T T
0.4931255132834135	0.4054771019582633	0.5000000000000000	T T T
0.3549770365090983	0.3994880807197800	0.5000000000000000	T T T
0.4292380619284284	0.2860790562634603	0.5000000000000000	T T T
0.2891556652384573	0.5152637091559198	0.5000000000000000	T T T
0.5648556892333139	0.2948693952786532	0.5000000000000000	T T T
0.3530648440805183	0.6351854486765858	0.5000000000000000	T T T
0.6566026731647293	0.3879037218632496	0.5000000000000000	T T T

0. 6922119599058064 0. 5158420674604313 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4867199204312905 0. 6424494311751118 0. 5000000000000000 T T T

0. 6314645876360043 0. 6319009615843334 0. 5000000000000000 T T T

0. 5665694135689513 0. 7469066541298413 0. 5000000000000000 T T T

0. 5538983683002895 0. 5214128634037615 0. 5000000000000000 T T T

0. 4206410807510197 0. 5224857708641016 0. 5000000000000000 T T T

0. 4886995470835676 0. 4090833431931587 0. 5000000000000000 T T T

0. 3523247900655344 0. 3984752076535396 0. 5000000000000000 T T T

0. 4321819182183100 0. 2867918879058355 0. 5000000000000000 T T T

0. 2869010549147622 0. 5146564161523600 0. 5000000000000000 T T T

0. 5673754331059568 0. 3047318626439969 0. 5000000000000000 T T T

0. 3512160952227440 0. 6373089141492162 0. 5000000000000000 T T T

0. 6781659429564184 0. 3749364112795350 0. 5000000000000000 T T T

0. 6838413047738908 0. 5088607328939719 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4872984536060814 0. 6452385845887820 0. 5000000000000000 T T T

0. 6328316945404625 0. 6275614905932067 0. 5000000000000000 T T T

0. 5721380819903913 0. 7454141103022589 0. 5000000000000000 T T T

0. 5485525470584535 0. 5231717196219997 0. 5000000000000000 T T T

0. 4151798322505322 0. 5273829243203451 0. 5000000000000000 T T T

0. 4803076927617681 0. 4134393601925369 0. 5000000000000000 T T T

0. 3481237680892644 0. 3910958164652433 0. 5000000000000000 T T T

0. 4385223406720352 0. 2859798969249820 0. 5000000000000000 T T T

0. 2848651916448643 0. 5078181665953627 0. 5000000000000000 T T T

0. 5710085370902673 0. 3188488090812433 0. 5000000000000000 T T T

0. 3519032047376728 0. 6441388748375652 0. 5000000000000000 T T T

0. 6920798968815814 0. 3685309180312166 0. 5000000000000000 T T T

0. 6771882165059954 0. 5013797862746774 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4915035302111795 0. 6462081764487463 0. 5000000000000000 T T T

0. 6319366925102422 0. 6256428431713110 0. 5000000000000000 T T T

0. 5762005469056860 0. 7463368040174092 0. 5000000000000000 T T T

0. 5461881841196421 0. 5211524980029556 0. 5000000000000000 T T T

0. 4110915732107090 0. 5345566839046332 0. 5000000000000000 T T T

0. 4701934956700018 0. 4165436574905999 0. 5000000000000000 T T T

0. 3446871857734417 0. 3780034852430659 0. 5000000000000000 T T T

0. 4432080259318268 0. 2836753731428560 0. 5000000000000000 T T T

0. 2848978709364333 0. 4945314978794044 0. 5000000000000000 T T T

0. 5706837068134647 0. 3305141817356607 0. 5000000000000000 T T T

0. 3590241489788797 0. 6568464265912766 0. 5000000000000000 T T T

0. 6957871092805595 0. 3672897288410186 0. 5000000000000000 T T T

0. 6745973876392424 0. 4986991015124253 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4934894960229314 0. 6469243308133524 0. 5000000000000000 T T T

0. 6315601227058920 0. 6235905907589747 0. 5000000000000000 T T T

0. 5793227906760178 0. 7460276378272920 0. 5000000000000000 T T T

0. 5444133272620854 0. 5193874708639807 0. 5000000000000000 T T T

0. 4092400720792058 0. 5396084392435906 0. 5000000000000000 T T T

0. 4625219499886206 0. 4186889847487348 0. 5000000000000000 T T T

0. 3419106777336508 0. 3681988413687101 0. 5000000000000000 T T T

0. 4473626287483662 0. 2832944461890161 0. 5000000000000000 T T T

0. 2875181279461683 0. 4874469605123548 0. 5000000000000000 T T T

0. 5700739958887316 0. 3405419834060265 0. 5000000000000000 T T T

0. 3622740625423516 0. 6637797814286428 0. 5000000000000000 T T T

0. 6974520472010556 0. 3660808832201692 0. 5000000000000000 T T T

0. 6728601597375754 0. 4964301081518269 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4950228318508816 0. 6474830868001552 0. 5000000000000000 T T T

0. 6310096643104172 0. 6212869644488046 0. 5000000000000000 T T T

0. 5821880913014298 0. 7453710688949878 0. 5000000000000000 T T T

0. 5424499201493689 0. 5173511579863935 0. 5000000000000000 T T T

0. 4078712689317656 0. 5441280855653149 0. 5000000000000000 T T T

0. 4546433420995545 0. 4206246687713905 0. 5000000000000000 T T T

0. 3395349760397185 0. 3587723636375213 0. 5000000000000000 T T T

0. 4519756423482127 0. 2840801946843910 0. 5000000000000000 T T T

0. 2916959854816364 0. 4812257417255715 0. 5000000000000000 T T T

0. 5692627806669687 0. 3519780095215903 0. 5000000000000000 T T T

0. 3648362523933938 0. 6693752215587921 0. 5000000000000000 T T T

0. 6985055685240333 0. 3645285812691838 0. 5000000000000000 T T T

0. 6710031350427413 0. 4937953142760644 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4962406191570016 0. 6481475747678702 0. 5000000000000000 T T T

0. 6304466813452910 0. 6188442931545795 0. 5000000000000000 T T T

0. 5851696675691719 0. 7444566556110580 0. 5000000000000000 T T T

0. 5402127727895190 0. 5154407651814642 0. 5000000000000000 T T T

0. 4067643767751142 0. 5480695356144665 0. 5000000000000000 T T T

0. 4468914169027721 0. 4222467775421476 0. 5000000000000000 T T T

0. 3377850374575062 0. 3498733015910599 0. 5000000000000000 T T T

0. 4568454399019012 0. 2860177589769902 0. 5000000000000000 T T T

0. 2968763166162630 0. 4753025621527326 0. 5000000000000000 T T T

0. 5682174597676979 0. 3641742857407158 0. 5000000000000000 T T T

0. 3669606756618898 0. 6740466375072112 0. 5000000000000000 T T T

0. 6986268033170843 0. 3625242960884564 0. 5000000000000000 T T T

0. 6689621925984827 0. 4908560159309538 0. 5000000000000000 T T T
Au
1. 0000000000000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4970992337115393 0. 6496257193128314 0. 5000000000000000 T T T
0. 6300734833725540 0. 6160454565558139 0. 5000000000000000 T T T
0. 5891770502245279 0. 7431056654804543 0. 5000000000000000 T T T
0. 5368952866873695 0. 5157798099822652 0. 5000000000000000 T T T
0. 4045549635670141 0. 5518310786017049 0. 5000000000000000 T T T
0. 4404741177391769 0. 4238131571031796 0. 5000000000000000 T T T
0. 3377456600358743 0. 3408681317599797 0. 5000000000000000 T T T
0. 4624818007051585 0. 2890168259290877 0. 5000000000000000 T T T
0. 3018172813810971 0. 4687322362427892 0. 5000000000000000 T T T
0. 5671517849342591 0. 3750397809098268 0. 5000000000000000 T T T
0. 3689725188134602 0. 6791459497042969 0. 5000000000000000 T T T
0. 6976257502273258 0. 3597161968392811 0. 5000000000000000 T T T
0. 6659305301400675 0. 4872804531179262 0. 5000000000000000 T T T

\$POSCAR 1 Au

1. 000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

13

Selective dynamics

Direct

0. 4962840000000000 0. 6527430000000000 0. 5000000000000000 T T T
0. 6291500000000000 0. 6137680000000000 0. 5000000000000000 T T T
0. 5937450000000000 0. 7415280000000000 0. 5000000000000000 T T T
0. 5323500000000000 0. 5192250000000000 0. 5000000000000000 T T T
0. 3997780000000000 0. 5546900000000000 0. 5000000000000000 T T T
0. 4375370000000000 0. 4250050000000000 0. 5000000000000000 T T T
0. 3420930000000000 0. 3315590000000000 0. 5000000000000000 T T T
0. 4703310000000000 0. 2913190000000000 0. 5000000000000000 T T T
0. 3043900000000000 0. 4605510000000000 0. 5000000000000000 T T T
0. 5666099999999999 0. 3832370000000000 0. 5000000000000000 T T T
0. 3690470000000000 0. 6838740000000000 0. 5000000000000000 T T T
0. 6960030000000000 0. 3575140000000000 0. 5000000000000000 T T T
0. 6626820000000000 0. 4849880000000000 0. 5000000000000000 T T T

Pathway 16

\$POSCAR 1 Au

1.000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.5669720000000000	0.5618430000000000	0.5000000000000000	T	T	T
0.7022180000000000	0.5622530000000000	0.5000000000000000	T	T	T
0.6335700000000000	0.6794410000000000	0.5000000000000000	T	T	T
0.6374700000000000	0.4439330000000000	0.5000000000000000	T	T	T
0.5000000000000000	0.4455030000000000	0.5000000000000000	T	T	T
0.5706300000000000	0.3296890000000000	0.5000000000000000	T	T	T
0.4293700000000000	0.3296890000000000	0.5000000000000000	T	T	T
0.5000000000000000	0.2176350000000000	0.5000000000000000	T	T	T
0.3625300000000000	0.4439330000000000	0.5000000000000000	T	T	T
0.4330280000000000	0.5618430000000000	0.5000000000000000	T	T	T
0.2977820000000000	0.5622530000000000	0.5000000000000000	T	T	T
0.3664300000000000	0.6794410000000000	0.5000000000000000	T	T	T
0.5000000000000000	0.6825460000000000	0.5000000000000000	T	T	T

Au

1.0000000000000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Au

13

Selective dynamics

Direct

0.5622787694395943	0.5590273265354806	0.5000000000000000	T	T	T
0.7116499618810809	0.5587424239908305	0.5000000000000000	T	T	T
0.6350145924092221	0.6685272441641299	0.5000000000000000	T	T	T
0.6370393783146435	0.4491272668960703	0.5000000000000000	T	T	T
0.4956366960251579	0.4444077431385079	0.5000000000000000	T	T	T
0.5733580057071029	0.3346345894956952	0.5000000000000000	T	T	T
0.4276108782504476	0.3281830045561347	0.5000000000000000	T	T	T
0.5080545082842188	0.2215292369892896	0.5000000000000000	T	T	T
0.3591590735713799	0.4427011375209267	0.5000000000000000	T	T	T
0.4280569558545533	0.5633423463402304	0.5000000000000000	T	T	T
0.2952209591877438	0.5635192915446201	0.5000000000000000	T	T	T
0.3665136847478697	0.6843010154093285	0.5000000000000000	T	T	T

0. 5004065363269914 0. 6819583330875176 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5545568988398946 0. 5574213736113904 0. 5000000000000000 T T T

0. 7215083483008005 0. 5562639742301387 0. 5000000000000000 T T T

0. 6359464229874643 0. 6589510876469235 0. 5000000000000000 T T T

0. 6370875412077915 0. 4544323562628620 0. 5000000000000000 T T T

0. 4942800508670251 0. 4410597021753710 0. 5000000000000000 T T T

0. 5784454449796901 0. 3368235438939959 0. 5000000000000000 T T T

0. 4254266641961229 0. 3270267879075122 0. 5000000000000000 T T T

0. 5116559476855466 0. 2250274923217357 0. 5000000000000000 T T T

0. 3587481648511451 0. 4428550927880131 0. 5000000000000000 T T T

0. 4216322951568379 0. 5663532493993628 0. 5000000000000000 T T T

0. 2901926499361789 0. 5608058347367288 0. 5000000000000000 T T T

0. 3686429302732457 0. 6904671174564749 0. 5000000000000000 T T T

0. 5018766407182601 0. 6825133472367010 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5468529931133451 0. 5555948488661623 0. 5000000000000000 T T T

0. 7275271630807283 0. 5548871713043685 0. 5000000000000000 T T T

0. 6354102680560335 0. 6512020641553066 0. 5000000000000000 T T T

0. 6370346984056379 0. 4583915646886855 0. 5000000000000000 T T T

0. 4956231043968129 0. 4359705459495863 0. 5000000000000000 T T T

0. 5851101530179523 0. 3370583492711193 0. 5000000000000000 T T T

0. 4229924350012018 0. 3257841886237634 0. 5000000000000000 T T T

0. 5135320107514740 0. 2279517198299318 0. 5000000000000000 T T T

0. 3606316111042458 0. 4441995241529655 0. 5000000000000000 T T T

0. 4147390302486768 0. 5715404422224448 0. 5000000000000000 T T T

0. 2845861970678930 0. 5556715120190269 0. 5000000000000000 T T T

0. 3720875645076990 0. 6987505990460925 0. 5000000000000000 T T T

0. 5038727712483552 0. 6829984295369753 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5392337430825433 0. 5531362821751028 0. 5000000000000000 T T T

0. 7315719591794217 0. 5539180167342705 0. 5000000000000000 T T T

0. 6341275953307742 0. 6435998579212668 0. 5000000000000000 T T T

0. 6365741716167728 0. 4618441074079380 0. 5000000000000000 T T T

0. 4982786770635965 0. 4297536326737089 0. 5000000000000000 T T T

0. 5930455101994273 0. 3366471194864892 0. 5000000000000000 T T T

0. 4196728765491735 0. 3247119248650668 0. 5000000000000000 T T T

0. 5148039774585683 0. 2314139432429444 0. 5000000000000000 T T T

0. 3638607241572793 0. 4467748680802858 0. 5000000000000000 T T T

0. 4082123537231141 0. 5774348314947264 0. 5000000000000000 T T T

0. 2800593956334399 0. 5515053580990796 0. 5000000000000000 T T T

0. 3751153236197746 0. 7064952951240261 0. 5000000000000000 T T T

0. 5054436923861849 0. 6827657223609244 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5319385006233533 0. 5498928779699096 0. 5000000000000000 T T T

0. 7343067418914901 0. 5531731630847543 0. 5000000000000000 T T T

0. 6321515396762470 0. 6360274671726091 0. 5000000000000000 T T T

0. 6357246602638023 0. 4649731419275426 0. 5000000000000000 T T T

0. 5014761494361053 0. 4227689617036121 0. 5000000000000000 T T T

0. 6016587084867774 0. 3362646142903402 0. 5000000000000000 T T T

0. 4152563470925094 0. 3239594789268257 0. 5000000000000000 T T T

0. 5156711206947520 0. 2361541200905584 0. 5000000000000000 T T T

0. 3687024054326131 0. 4506985646069327 0. 5000000000000000 T T T

0. 4027188396899948 0. 5831715288492131 0. 5000000000000000 T T T

0. 2770082843105267 0. 5483103587717651 0. 5000000000000000 T T T

0. 3773169362944075 0. 7130728985069194 0. 5000000000000000 T T T

0. 5060697661074391 0. 6815337837643808 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5254736305758418 0. 5461087735892876 0. 5000000000000000 T T T

0. 7360040462617922 0. 5527078632050461 0. 5000000000000000 T T T

0. 6295529835120912 0. 6290730663133444 0. 5000000000000000 T T T

0. 6349186436543693 0. 4674757904666558 0. 5000000000000000 T T T

0. 5045393773652701 0. 4157291084739433 0. 5000000000000000 T T T

0. 6097576738421434 0. 3363605552738814 0. 5000000000000000 T T T

0. 4097537000344091 0. 3236730996154608 0. 5000000000000000 T T T

0. 5156500769369258 0. 2429202972225637 0. 5000000000000000 T T T

0. 3754323611635102 0. 4548983008462203 0. 5000000000000000 T T T

0. 3989319035079431 0. 5881308937891097 0. 5000000000000000 T T T

0. 2759811038781478 0. 5451186541308231 0. 5000000000000000 T T T

0. 3782883500151113 0. 7179968541710894 0. 5000000000000000 T T T

0. 5057161492524731 0. 6798077025675985 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5191605965581596 0. 5420947335194746 0. 5000000000000000 T T T

0. 7370847821942214 0. 5520113854464268 0. 5000000000000000 T T T

0. 6265976809748496 0. 6222923231975834 0. 5000000000000000 T T T

0. 6340263926988186 0. 4693144379008111 0. 5000000000000000 T T T

0. 5074897796546427 0. 4092778312092803 0. 5000000000000000 T T T

0. 6175141102990775 0. 3365336981754820 0. 5000000000000000 T T T

0. 4041461388100926 0. 3245477356015542 0. 5000000000000000 T T T

0. 5152312159647010 0. 2515042628473060 0. 5000000000000000 T T T

0. 3825091068753994 0. 4583274555823595 0. 5000000000000000 T T T

0. 3956925334805048 0. 5925191242482419 0. 5000000000000000 T T T

0. 2761464268355118 0. 5413957551566225 0. 5000000000000000 T T T

0. 3792908227168544 0. 7223792986061427 0. 5000000000000000 T T T

0. 5051104129372117 0. 6778029181733112 0. 5000000000000000 T T T
Au
1. 0000000000000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5133670919639099 0. 5381432026959009 0. 5000000000000000 T T T
0. 7374488023445784 0. 5508152889278304 0. 5000000000000000 T T T
0. 6234841050401581 0. 6157760955488794 0. 5000000000000000 T T T
0. 6328124379975696 0. 4701096530147025 0. 5000000000000000 T T T
0. 5102365056368983 0. 4040568596958740 0. 5000000000000000 T T T
0. 6255570849481702 0. 3365542543072380 0. 5000000000000000 T T T
0. 3988135585343596 0. 3265812428742439 0. 5000000000000000 T T T
0. 5151352216925921 0. 2615275107440127 0. 5000000000000000 T T T
0. 3885593897770078 0. 4611623276428237 0. 5000000000000000 T T T
0. 3921046411533868 0. 5964579021601649 0. 5000000000000000 T T T
0. 2767828795896821 0. 5366970516800799 0. 5000000000000000 T T T
0. 3812290363370600 0. 7268176798591792 0. 5000000000000000 T T T
0. 5044692449846838 0. 6753018905122672 0. 5000000000000000 T T T

\$POSCAR 1 Au

1. 000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

13

Selective dynamics

Direct

0. 5078000000000000 0. 5368140000000000 0. 5000000000000000 T T T
0. 7376239999999999 0. 5474820000000000 0. 5000000000000000 T T T
0. 6213270000000000 0. 6094100000000000 0. 5000000000000000 T T T
0. 6309910000000000 0. 4698050000000000 0. 5000000000000000 T T T
0. 5127810000000000 0. 4032400000000000 0. 5000000000000000 T T T
0. 6332870000000000 0. 3367130000000000 0. 5000000000000000 T T T
0. 3963840000000000 0. 3294620000000000 0. 5000000000000000 T T T
0. 5167659999999999 0. 2697260000000000 0. 5000000000000000 T T T
0. 3918510000000000 0. 4634040000000000 0. 5000000000000000 T T T
0. 3852000000000000 0. 6008220000000000 0. 5000000000000000 T T T
0. 2760530000000000 0. 5283960000000000 0. 5000000000000000 T T T
0. 3860080000000000 0. 7326580000000000 0. 5000000000000000 T T T
0. 5039280000000000 0. 6720680000000000 0. 5000000000000000 T T T

Pathway 17

\$POSCAR 1 Au

1.000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.5669720000000000	0.5618430000000000	0.5000000000000000	T T T
0.7022180000000000	0.5622530000000000	0.5000000000000000	T T T
0.6335700000000000	0.6794410000000000	0.5000000000000000	T T T
0.6374700000000000	0.4439330000000000	0.5000000000000000	T T T
0.5000000000000000	0.4455030000000000	0.5000000000000000	T T T
0.5706300000000000	0.3296890000000000	0.5000000000000000	T T T
0.4293700000000000	0.3296890000000000	0.5000000000000000	T T T
0.5000000000000000	0.2176350000000000	0.5000000000000000	T T T
0.3625300000000000	0.4439330000000000	0.5000000000000000	T T T
0.4330280000000000	0.5618430000000000	0.5000000000000000	T T T
0.2977820000000000	0.5622530000000000	0.5000000000000000	T T T
0.3664300000000000	0.6794410000000000	0.5000000000000000	T T T
0.5000000000000000	0.6825460000000000	0.5000000000000000	T T T

Au

1.0000000000000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Au

13

Selective dynamics

Direct

0.5692496337640498	0.5565411309088052	0.5000000000000000	T T T
0.7112451914565568	0.5615583596352870	0.5000000000000000	T T T
0.6358011263367481	0.6725329689293198	0.5000000000000000	T T T
0.6440882190828346	0.4456767502036632	0.5000000000000000	T T T
0.4954193487023643	0.4472314123970078	0.5000000000000000	T T T
0.5705254972866326	0.3373790332435310	0.5000000000000000	T T T
0.4264819670159050	0.3315196059049254	0.5000000000000000	T T T
0.5048870064136781	0.2241485059828859	0.5000000000000000	T T T
0.3556802363073348	0.4432916507957869	0.5000000000000000	T T T
0.4269704116526294	0.5609156886370429	0.5000000000000000	T T T
0.2918427989154868	0.5628035239616083	0.5000000000000000	T T T
0.3667912006956826	0.6816448601987775	0.5000000000000000	T T T

0. 5010178548183429 0. 6747560469604273 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5748607105280098 0. 5526805123778012 0. 5000000000000000 T T T

0. 7179965222363204 0. 5617235035771591 0. 5000000000000000 T T T

0. 6376587802097972 0. 6695372749629562 0. 5000000000000000 T T T

0. 6515890693992984 0. 4452894053936918 0. 5000000000000000 T T T

0. 4913120395660938 0. 4506430319492696 0. 5000000000000000 T T T

0. 5697355664705553 0. 3430830548854114 0. 5000000000000000 T T T

0. 4257715086255787 0. 3332131222392580 0. 5000000000000000 T T T

0. 5076747148233467 0. 2284079274310017 0. 5000000000000000 T T T

0. 3517933761485617 0. 4422602019585591 0. 5000000000000000 T T T

0. 4171966256193247 0. 5620169287662958 0. 5000000000000000 T T T

0. 2826891038014564 0. 5575716566024753 0. 5000000000000000 T T T

0. 3696504699142784 0. 6863751056711600 0. 5000000000000000 T T T

0. 5020720085227030 0. 6671977948586569 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5811788836051422 0. 5490164527187524 0. 5000000000000000 T T T

0. 7216369581277613 0. 5620936088639016 0. 5000000000000000 T T T

0. 6388740432921409 0. 6688370908255485 0. 5000000000000000 T T T

0. 6584329628058367 0. 4432455511165446 0. 5000000000000000 T T T

0. 4879090625931437 0. 4554711243995125 0. 5000000000000000 T T T

0. 5688685118796029 0. 3479603394817530 0. 5000000000000000 T T T

0. 4266112558579201 0. 3350085243701340 0. 5000000000000000 T T T

0. 5090236580983060 0. 2315594172034269 0. 5000000000000000 T T T

0. 3492415448688665 0. 4414032355683059 0. 5000000000000000 T T T

0. 4067040222421280 0. 5640468695793550 0. 5000000000000000 T T T

0. 2733170070262755 0. 5508096092130810 0. 5000000000000000 T T T

0. 3743476831183136 0. 6914907772817561 0. 5000000000000000 T T T

0. 5038549039223531 0. 6590569121892930 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5868195513849217 0. 5444896445329114 0. 5000000000000000 T T T

0. 7239099853022439 0. 5627556854823679 0. 5000000000000000 T T T

0. 6389592933790038 0. 6678607408824059 0. 5000000000000000 T T T

0. 6659337822554477 0. 4402418890983549 0. 5000000000000000 T T T

0. 4843265839421552 0. 4612423758812190 0. 5000000000000000 T T T

0. 5679156309032515 0. 3533645425780534 0. 5000000000000000 T T T

0. 4279373581507810 0. 3372855600891944 0. 5000000000000000 T T T

0. 5107644000922745 0. 2347907781799509 0. 5000000000000000 T T T

0. 3471033796503759 0. 4407442941077266 0. 5000000000000000 T T T

0. 3969452416632621 0. 5667630302882740 0. 5000000000000000 T T T

0. 2655467143753268 0. 5452756059871631 0. 5000000000000000 T T T

0. 3793865798106255 0. 6962636217690473 0. 5000000000000000 T T T

0. 5044519984398875 0. 6489217343758585 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5902255625976250 0. 5395283168163996 0. 5000000000000000 T T T

0. 7247648212986960 0. 5631257889015495 0. 5000000000000000 T T T

0. 6376709762481484 0. 6660675518724852 0. 5000000000000000 T T T

0. 6730302066074121 0. 4372742482422358 0. 5000000000000000 T T T

0. 4808908043222061 0. 4658037920222784 0. 5000000000000000 T T T

0. 5675352442639597 0. 3590326282978240 0. 5000000000000000 T T T

0. 4288344581849153 0. 3395438046182842 0. 5000000000000000 T T T

0. 5129866242757861 0. 2385061520198076 0. 5000000000000000 T T T

0. 3449378486454037 0. 4406263185062415 0. 5000000000000000 T T T

0. 3907111011330916 0. 5684376504836444 0. 5000000000000000 T T T

0. 2608491078990803 0. 5431783220845661 0. 5000000000000000 T T T

0. 3833044783703334 0. 6985088594892200 0. 5000000000000000 T T T

0. 5042592686689802 0. 6403660540676038 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5926416273816801 0. 5337622458135109 0. 5000000000000000 T T T

0. 7247848268255328 0. 5628075815631480 0. 5000000000000000 T T T

0. 6357690827966396 0. 6636140519023919 0. 5000000000000000 T T T

0. 6800332630072151 0. 4340743811911471 0. 5000000000000000 T T T

0. 4773567267771826 0. 4703498777207588 0. 5000000000000000 T T T

0. 5674247460170418 0. 3657281689532728 0. 5000000000000000 T T T

0. 4299208089799590 0. 3420383356539198 0. 5000000000000000 T T T

0. 5160508542275559 0. 2429607371971395 0. 5000000000000000 T T T

0. 3428240879457762 0. 4406656455840167 0. 5000000000000000 T T T

0. 3852256962872776 0. 5698691227750596 0. 5000000000000000 T T T

0. 2566699038400255 0. 5417428834413552 0. 5000000000000000 T T T

0. 3873514721074846 0. 6998876162756198 0. 5000000000000000 T T T

0. 5039474094663150 0. 6324988236305537 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5942601401112320 0. 5276518780283839 0. 5000000000000000 T T T

0. 7244211689282537 0. 5616199355652423 0. 5000000000000000 T T T

0. 6335287924917867 0. 6604302543981559 0. 5000000000000000 T T T

0. 6864066357316119 0. 4310010542338323 0. 5000000000000000 T T T

0. 4740663984838647 0. 4745541063300933 0. 5000000000000000 T T T

0. 5677706487725137 0. 3729134365302625 0. 5000000000000000 T T T

0. 4311809033571222 0. 3447907343120926 0. 5000000000000000 T T T

0. 5196948280383862 0. 2480624791996501 0. 5000000000000000 T T T

0. 3410608801747326 0. 4409643614118393 0. 5000000000000000 T T T

0. 3799914765171795 0. 5715892799509915 0. 5000000000000000 T T T

0. 2526171023532585 0. 5402067939498282 0. 5000000000000000 T T T

0. 3916752607934436 0. 7009676054360315 0. 5000000000000000 T T T

0. 5033262739131891 0. 6252475323210467 0. 5000000000000000 T T T
Au

1. 0000000000000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5953029370614964 0. 5219265742183846 0. 5000000000000000 T T T
0. 7239777023780216 0. 5596109018591914 0. 5000000000000000 T T T
0. 6312303454252516 0. 6564683783308837 0. 5000000000000000 T T T
0. 6922346133749560 0. 4280815293702076 0. 5000000000000000 T T T
0. 4708088359575699 0. 4780916354895430 0. 5000000000000000 T T T
0. 5687064193139847 0. 3797560565867030 0. 5000000000000000 T T T
0. 4325525913102088 0. 3477448474374009 0. 5000000000000000 T T T
0. 5240226438663387 0. 2538103348798665 0. 5000000000000000 T T T
0. 3393434008970573 0. 4414804368548426 0. 5000000000000000 T T T
0. 3745915911737076 0. 5738451144346255 0. 5000000000000000 T T T
0. 2483293492556635 0. 5383353505669082 0. 5000000000000000 T T T
0. 3966010413919386 0. 7020095281989519 0. 5000000000000000 T T T
0. 5022990488371303 0. 6188387105561926 0. 5000000000000000 T T T

\$POSCAR 1 Au

1. 000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

13

Selective dynamics

Direct

0. 5959230000000000 0. 5180150000000000 0. 5000000000000000 T T T
0. 7240280000000000 0. 5558450000000000 0. 5000000000000000 T T T
0. 6297450000000000 0. 6516110000000001 0. 5000000000000000 T T T
0. 6966980000000000 0. 4242490000000000 0. 5000000000000000 T T T
0. 4674510000000000 0. 4811140000000000 0. 5000000000000000 T T T
0. 5695210000000001 0. 3849460000000000 0. 5000000000000000 T T T
0. 4338580000000000 0. 3506140000000000 0. 5000000000000000 T T T
0. 5289509999999999 0. 2594140000000000 0. 5000000000000000 T T T
0. 3377290000000000 0. 4426340000000000 0. 5000000000000000 T T T
0. 3684180000000000 0. 5776550000000000 0. 5000000000000000 T T T
0. 2434020000000000 0. 5357930000000000 0. 5000000000000000 T T T
0. 4032150000000000 0. 7039390000000000 0. 5000000000000000 T T T
0. 5010620000000000 0. 6141680000000000 0. 5000000000000000 T T T

Pathway 18

\$POSCAR 1 Au

1.000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.5669720000000000	0.5618430000000000	0.5000000000000000	T T T
0.7022180000000000	0.5622530000000000	0.5000000000000000	T T T
0.6335700000000000	0.6794410000000000	0.5000000000000000	T T T
0.6374700000000000	0.4439330000000000	0.5000000000000000	T T T
0.5000000000000000	0.4455030000000000	0.5000000000000000	T T T
0.5706300000000000	0.3296890000000000	0.5000000000000000	T T T
0.4293700000000000	0.3296890000000000	0.5000000000000000	T T T
0.5000000000000000	0.2176350000000000	0.5000000000000000	T T T
0.3625300000000000	0.4439330000000000	0.5000000000000000	T T T
0.4330280000000000	0.5618430000000000	0.5000000000000000	T T T
0.2977820000000000	0.5622530000000000	0.5000000000000000	T T T
0.3664300000000000	0.6794410000000000	0.5000000000000000	T T T
0.5000000000000000	0.6825460000000000	0.5000000000000000	T T T

Au

1.0000000000000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Au

13

Selective dynamics

Direct

0.5628757440739447	0.5619932254699175	0.5000000000000000	T T T
0.6939203931989062	0.5568754507730308	0.5000000000000000	T T T
0.6338146817597859	0.6780187732106553	0.5000000000000000	T T T
0.6583465947013484	0.4297930946075945	0.5000000000000000	T T T
0.4999538733945678	0.4473279017178122	0.5000000000000000	T T T
0.5708296657321493	0.3343288204137099	0.5000000000000000	T T T
0.4285349337909877	0.3324556139336867	0.5000000000000000	T T T
0.5031778751540011	0.2223700843121545	0.5000000000000000	T T T
0.3593050381801531	0.4453021002481872	0.5000000000000000	T T T
0.4294857275847341	0.5623973025966692	0.5000000000000000	T T T
0.2936277677265540	0.5636433226903905	0.5000000000000000	T T T
0.3665024459065594	0.6804005127920758	0.5000000000000000	T T T

0. 4996266338117260 0. 6850948805571986 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5562063932803215 0. 5653967343892249 0. 5000000000000000 T T T

0. 6849391150445321 0. 5493747531321579 0. 5000000000000000 T T T

0. 6366593455381632 0. 6751798261027399 0. 5000000000000000 T T T

0. 6769463091773961 0. 4180012600408461 0. 5000000000000000 T T T

0. 4961626265353971 0. 4497759477145032 0. 5000000000000000 T T T

0. 5723903014063014 0. 3406048374102779 0. 5000000000000000 T T T

0. 4288422582101430 0. 3332163819736782 0. 5000000000000000 T T T

0. 5080545917259961 0. 2265450368545727 0. 5000000000000000 T T T

0. 3562089690845979 0. 4442132322256150 0. 5000000000000000 T T T

0. 4245446601001635 0. 5630808749574300 0. 5000000000000000 T T T

0. 2901841512711627 0. 5630040334307876 0. 5000000000000000 T T T

0. 3679598644231784 0. 6819848117972781 0. 5000000000000000 T T T

0. 5009028161816665 0. 6896233353182321 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5473515019819568 0. 5711908031838423 0. 5000000000000000 T T T

0. 6745605338402541 0. 5420108225592626 0. 5000000000000000 T T T

0. 6412594306471389 0. 6714285221760024 0. 5000000000000000 T T T

0. 6853906163335788 0. 4118867506685673 0. 5000000000000000 T T T

0. 4937803905021573 0. 4522578430525502 0. 5000000000000000 T T T

0. 5740630321805671 0. 3444874956477418 0. 5000000000000000 T T T

0. 4315862816307392 0. 3331579134782645 0. 5000000000000000 T T T

0. 5131337701880341 0. 2285629274984557 0. 5000000000000000 T T T

0. 3543439930618993 0. 4406596371655044 0. 5000000000000000 T T T

0. 4165494171741148 0. 5626949464978116 0. 5000000000000000 T T T

0. 2839893267446558 0. 5560576776519498 0. 5000000000000000 T T T

0. 3760876392549711 0. 6865543473463314 0. 5000000000000000 T T T

0. 5079055091867372 0. 6990513512558718 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5388048802497869 0. 5775703910706484 0. 5000000000000000 T T T

0. 6641493969291450 0. 5364111229705755 0. 5000000000000000 T T T

0. 6450342324171805 0. 6678359539923826 0. 5000000000000000 T T T

0. 6890222888076702 0. 4089636921528944 0. 5000000000000000 T T T

0. 4933211708663723 0. 4548081016921849 0. 5000000000000000 T T T

0. 5749353867099346 0. 3466089395000560 0. 5000000000000000 T T T

0. 4348411768440586 0. 3330919003281819 0. 5000000000000000 T T T

0. 5166861875917332 0. 2290326550035159 0. 5000000000000000 T T T

0. 3544856260688019 0. 4374764029492817 0. 5000000000000000 T T T

0. 4081879742607260 0. 5625145602776496 0. 5000000000000000 T T T

0. 2768498106777020 0. 5458272901462358 0. 5000000000000000 T T T

0. 3866948389762457 0. 6914880804219173 0. 5000000000000000 T T T

0. 5169884917598249 0. 7083719347217154 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5321060558249268 0. 5842219926273960 0. 5000000000000000 T T T

0. 6531348233529314 0. 5302058715559497 0. 5000000000000000 T T T

0. 6467379276806445 0. 6631472703442993 0. 5000000000000000 T T T

0. 6922457681498472 0. 4067921923835775 0. 5000000000000000 T T T

0. 4948640631822822 0. 4575415026036947 0. 5000000000000000 T T T

0. 5764388029566342 0. 3480580202549272 0. 5000000000000000 T T T

0. 4378183948876120 0. 3342275967019771 0. 5000000000000000 T T T

0. 5187440495884207 0. 2298441517516036 0. 5000000000000000 T T T

0. 3551590474644228 0. 4360149801836893 0. 5000000000000000 T T T

0. 4027929645607005 0. 5617866986505969 0. 5000000000000000 T T T

0. 2725291705054489 0. 5401503887958624 0. 5000000000000000 T T T

0. 3940361202398670 0. 6921775792498869 0. 5000000000000000 T T T

0. 5233942904320333 0. 7158327690127196 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5262521260708886 0. 5909393075229862 0. 5000000000000000 T T T

0. 6399949040831666 0. 5228465367075189 0. 5000000000000000 T T T

0. 6470930268573116 0. 6574137823443971 0. 5000000000000000 T T T

0. 6956651571505570 0. 4056715481598737 0. 5000000000000000 T T T

0. 4970096034075653 0. 4605291419632240 0. 5000000000000000 T T T

0. 5783935445504739 0. 3498566158548844 0. 5000000000000000 T T T

0. 4407899010748660 0. 3358027614981407 0. 5000000000000000 T T T

0. 5208006412859001 0. 2310719925826012 0. 5000000000000000 T T T

0. 3558798899698787 0. 4349583780580417 0. 5000000000000000 T T T

0. 3987394320993302 0. 5609999919311071 0. 5000000000000000 T T T

0. 2694712795048727 0. 5359878350280717 0. 5000000000000000 T T T

0. 4007877060857312 0. 6915940070963644 0. 5000000000000000 T T T

0. 5291242798386568 0. 7223291066000131 0. 5000000000000000 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5214019455281566 0. 5958028762795486 0. 5000000000000000 T T T

0. 6276325673045466 0. 5149430547863278 0. 5000000000000000 T T T

0. 6468595923234043 0. 6500897527722640 0. 5000000000000000 T T T

0. 6997045309272675 0. 4058830741327250 0. 5000000000000000 T T T

0. 4954520989786384 0. 4630930541428757 0. 5000000000000000 T T T

0. 5802628383324590 0. 3542920180762456 0. 5000000000000000 T T T

0. 4433657043962133 0. 3368784742568901 0. 5000000000000000 T T T

0. 5248195561298377 0. 2336527431096423 0. 5000000000000000 T T T

0. 3559439148617305 0. 4338319895782390 0. 5000000000000000 T T T

0. 3944727642527531 0. 5612831638186598 0. 5000000000000000 T T T

0. 2663279503376080 0. 5317745771279518 0. 5000000000000000 T T T

0. 4079460195543003 0. 6914077669084348 0. 5000000000000000 T T T

0. 5358120327169676 0. 7270684445809433 0. 5000000000000000 T T T
Au
1. 0000000000000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5183875507010283 0. 5967474816426532 0. 5000000000000000 T T T
0. 6198372329895330 0. 5076345625472974 0. 5000000000000000 T T T
0. 6470020759689249 0. 6414752819570725 0. 5000000000000000 T T T
0. 7040981685508242 0. 4062643924865406 0. 5000000000000000 T T T
0. 4890794794296526 0. 4651194646832114 0. 5000000000000000 T T T
0. 5810740060291133 0. 3627271806114132 0. 5000000000000000 T T T
0. 4449476345918270 0. 3370179954786195 0. 5000000000000000 T T T
0. 5322605092038817 0. 2386842329005193 0. 5000000000000000 T T T
0. 3546259023108112 0. 4326826629496973 0. 5000000000000000 T T T
0. 3893758360731578 0. 5635357470442177 0. 5000000000000000 T T T
0. 2627225591014580 0. 5277857678839171 0. 5000000000000000 T T T
0. 4138607589804672 0. 6927331473257784 0. 5000000000000000 T T T
0. 5427298750499083 0. 7275930231686781 0. 5000000000000000 T T T

\$POSCAR 1 Au

1. 000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

13

Selective dynamics

Direct

0. 5158800000000000 0. 5963000000000001 0. 5000000000000000 T T T
0. 6141170000000000 0. 5035990000000000 0. 5000000000000000 T T T
0. 6486910000000000 0. 6330810000000000 0. 5000000000000000 T T T
0. 7060390000000000 0. 4077700000000000 0. 5000000000000000 T T T
0. 4818420000000000 0. 4670400000000000 0. 5000000000000000 T T T
0. 5805600000000000 0. 3701760000000000 0. 5000000000000000 T T T
0. 4462540000000000 0. 3364940000000000 0. 5000000000000000 T T T
0. 5414860000000000 0. 2442610000000000 0. 5000000000000000 T T T
0. 3521210000000000 0. 4305550000000000 0. 5000000000000000 T T T
0. 3834300000000000 0. 5669470000000000 0. 5000000000000000 T T T
0. 2588310000000000 0. 5235980000000000 0. 5000000000000000 T T T
0. 4198980000000000 0. 6949660000000000 0. 5000000000000000 T T T
0. 5508540000000000 0. 7252130000000000 0. 5000000000000000 T T T

Pathway 19

\$POSCAR 1 Au

1.000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.5000000000000000	0.5000000000000000	0.4350510000000000	T T T
0.5720280000000000	0.6175430000000000	0.4585070000000000	T T T
0.3621900000000000	0.5036070000000000	0.4585070000000000	T T T
0.5657810000000000	0.3788500000000000	0.4585070000000000	T T T
0.4279720000000000	0.6175430000000000	0.4585070000000000	T T T
0.4342190000000000	0.3788500000000000	0.4585070000000000	T T T
0.6378100000000000	0.5036070000000000	0.4585070000000000	T T T
0.5000000000000000	0.7076460000000000	0.5293610000000000	T T T
0.3201730000000000	0.3961770000000000	0.5293610000000000	T T T
0.6798270000000000	0.3961770000000000	0.5293610000000000	T T T
0.5000000000000000	0.5778390000000000	0.5752750000000000	T T T
0.4325900000000000	0.4610810000000000	0.5752750000000000	T T T
0.5674110000000000	0.4610810000000000	0.5752750000000000	T T T

Au

1.0000000000000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Au

13

Selective dynamics

Direct

0.5039359550837765	0.4976556060086577	0.4336088201182857	T T T
0.5724103309902655	0.6163647062722664	0.4636556730710849	T T T
0.3654807974717980	0.5013773800314488	0.4568706610311914	T T T
0.5661917681996239	0.3744080089499869	0.4561058612834766	T T T
0.4315588499454416	0.6158510295457247	0.4569129948547800	T T T
0.4353757367785339	0.3789984434529806	0.4636845780218802	T T T
0.6418344767639853	0.5053804444145433	0.4560189743169549	T T T
0.4965441740707849	0.7082017895658794	0.5307106939901570	T T T
0.3179348546482108	0.3990033279797115	0.5307198600333353	T T T
0.6790745205933999	0.3966270989306556	0.5257066056598939	T T T
0.4966351685855867	0.5798089442742153	0.5793020517071970	T T T
0.4292636977150166	0.4630761994690176	0.5792143687546045	T T T

0. 5637601678339359 0. 4632475197853206 0. 5674896064973730 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5049986660550955 0. 4971029348194489 0. 4327063176843852 T T T

0. 5729306276722286 0. 6150792137208867 0. 4682035870208749 T T T

0. 3666303086032174 0. 5007633169022366 0. 4552308854407867 T T T

0. 5671569700635324 0. 3736366749992736 0. 4589704301771320 T T T

0. 4327719121677787 0. 6152401551629364 0. 4551982089177393 T T T

0. 4367291026407014 0. 3793191365067288 0. 4681908358922905 T T T

0. 6429676291820516 0. 5049071845757183 0. 4588754040947012 T T T

0. 4948397231006019 0. 7088954347992685 0. 5299032406999701 T T T

0. 3164230835113340 0. 4001255193050301 0. 5298045363940153 T T T

0. 6863937825282859 0. 3923601369783253 0. 5144808859994425 T T T

0. 4927095376118191 0. 5818904453466804 0. 5814718381837750 T T T

0. 4253912321576315 0. 4653622987090059 0. 5814674134956015 T T T

0. 5600577247988698 0. 4653178482676623 0. 5654970660458996 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5053699380934479 0. 4969047406052372 0. 4322366783536464 T T T

0. 5733353782963785 0. 6134279047252580 0. 4711808902859400 T T T

0. 3670749023395427 0. 5004496801848662 0. 4543708928112750 T T T

0. 5690441358968873 0. 3742187447795340 0. 4623400596285624 T T T

0. 4332467741267538 0. 6149916516326919 0. 4543221657726420 T T T

0. 4384158951166929 0. 3798120216319365 0. 4711716908265418 T T T

0. 6433617056348605 0. 5030314597281853 0. 4622469696992564 T T T

0. 4944920434600674 0. 7095261238649996 0. 5287931461390761 T T T

0. 3157593082336660 0. 4000474873971077 0. 5287140343943270 T T T

0. 6944030794189006 0. 3877902741555843 0. 5028294260415753 T T T

0. 4889393782558835 0. 5843262541559395 0. 5830688228841554 T T T

0. 4213915728828909 0. 4674067287893159 0. 5831007334075250 T T T

0. 5551661366441375 0. 4680671767495110 0. 5656251139555737 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5058400996115737 0. 4966253477256418 0. 4317294321663657 T T T

0. 5737346090441406 0. 6120640061982356 0. 4740762879258327 T T T

0. 3676582967021854 0. 5000142942384839 0. 4534511466949956 T T T

0. 5704778275827196 0. 3745262922395370 0. 4647141457016638 T T T

0. 4338693679767178 0. 6145769531968172 0. 4534591930517296 T T T

0. 4398041654501669 0. 3801323146551305 0. 4740593114882609 T T T

0. 6438639296431924 0. 5016560502831415 0. 4647126470475325 T T T

0. 4944095645748006 0. 7099196793409480 0. 5277577283262704 T T T

0. 3154247897644802 0. 3998563034819860 0. 5277627911040428 T T T

0. 6990823922486308 0. 3850382510772256 0. 4940270901895183 T T T

0. 4858584250491998 0. 5861852240311547 0. 5843424422195382 T T T

0. 4182670156967608 0. 4692757039897761 0. 5842730251453279 T T T

0. 5517096915668560 0. 4701297544534250 0. 5656353463946908 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5065432039631724 0. 4963144530747150 0. 4307205678513649 T T T

0. 5742650367045206 0. 6105705839979952 0. 4779251687498557 T T T

0. 3686759434437695 0. 4994021064641914 0. 4524424945346596 T T T

0. 5719253161465019 0. 3747010168998808 0. 4666231221310109 T T T

0. 4348801252813626 0. 6140232678760780 0. 4523835559602396 T T T

0. 4413834425906279 0. 3805504655422535 0. 4779144395778320 T T T

0. 6444653146596350 0. 5003537847252478 0. 4666701399054440 T T T

0. 4943726241926438 0. 7101705985348969 0. 5268034901345621 T T T

0. 3151792620458698 0. 3997201076982050 0. 5268398739826757 T T T

0. 7026466610403636 0. 3829629419448693 0. 4852368533532447 T T T

0. 4823775101527423 0. 5879299388249508 0. 5856278991894736 T T T

0. 4149555291701449 0. 4712831785856846 0. 5857183753948424 T T T

0. 5483300749186752 0. 4720176001411523 0. 5650945413898866 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5072914911498959 0. 4958771261322469 0. 4294445287461716 T T T

0. 5746200307348959 0. 6089069488471930 0. 4823161789237679 T T T

0. 3699097613271784 0. 4986096979241839 0. 4513876551906935 T T T

0. 5733686483482546 0. 3748106920713297 0. 4683445163521399 T T T

0. 4360332040843441 0. 6133092791667157 0. 4513846982490041 T T T

0. 4431072562644991 0. 3809611012080161 0. 4823060238718194 T T T

0. 6450567997156156 0. 4991708123130440 0. 4683745736539539 T T T

0. 4944414093994326 0. 7103163826146737 0. 5258807656799817 T T T

0. 3151581015295689 0. 3994710013411343 0. 5258718496185615 T T T

0. 7053150998838209 0. 3816096828854588 0. 4763063126248666 T T T

0. 4788446162747599 0. 5896931224655082 0. 5869972344204291 T T T

0. 4117094223346006 0. 4733969824891630 0. 5870525607549190 T T T

0. 5451440164207763 0. 4738670280090608 0. 5643335306475977 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5083054886804482 0. 4952401202040848 0. 4279329717465623 T T T

0. 5751027502547873 0. 6072576242951759 0. 4871092704310506 T T T

0. 3715204261074495 0. 4976880806067330 0. 4503187119766349 T T T

0. 5745078881883410 0. 3748031440013249 0. 4699266115079545 T T T

0. 4377350783511534 0. 6124248338791571 0. 4503553240795096 T T T

0. 4446969597906964 0. 3813743411856458 0. 4871052041354291 T T T

0. 6456320779505845 0. 4980725924084681 0. 4699059253201563 T T T

0. 4947239629965718 0. 7103876624124584 0. 5249883324015074 T T T

0. 3151840926657151 0. 3992988822733653 0. 5249172509408104 T T T

0. 7067517656609349 0. 3806459138616118 0. 4673880709852851 T T T

0. 4753351458204320 0. 5914718044568062 0. 5882890978413032 T T T

0. 4084010021497890 0. 4756591310882497 0. 5882581682694124 T T T

0. 5421029842705980 0. 4756754922145435 0. 5635053718082328 T T T
Au
1. 0000000000000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5096094175494124 0. 4944694315391829 0. 4264175153376200 T T T
0. 5757265939476890 0. 6058270674722693 0. 4921258581142354 T T T
0. 3734745231273662 0. 4965919714694554 0. 4494551979832520 T T T
0. 5753933424814607 0. 3748131221967247 0. 4711903831015422 T T T
0. 4398698616614232 0. 6113810212097102 0. 4494262957617341 T T T
0. 4461330367013164 0. 3816120378481865 0. 4920440190731021 T T T
0. 6461137978860595 0. 4972185843287114 0. 4712137659559085 T T T
0. 4952064973006006 0. 7103946363945063 0. 5242408952104897 T T T
0. 3152998089507359 0. 3990597892322261 0. 5240931674523907 T T T
0. 7071005930443541 0. 3803422030517037 0. 4582336221683342 T T T
0. 4717598273393429 0. 5931858250748714 0. 5893485139292516 T T T
0. 4051088106209031 0. 4777910988916626 0. 5893831312103655 T T T
0. 5392032225011455 0. 4773125444027465 0. 5628278012577961 T T T

\$POSCAR 1 Au

1. 000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

13

Selective dynamics

Direct

0. 5111200000000000 0. 4935800000000000 0. 4254930000000000 T T T
0. 5764650000000000 0. 6046810000000000 0. 4970450000000000 T T T
0. 3756260000000000 0. 4951310000000000 0. 4486120000000000 T T T
0. 5762260000000000 0. 3748930000000000 0. 4726280000000000 T T T
0. 4420290000000000 0. 6101450000000000 0. 4486120000000000 T T T
0. 4475760000000000 0. 3814390000000000 0. 4970450000000000 T T T
0. 6464590000000000 0. 4965390000000000 0. 4726280000000000 T T T
0. 4960580000000000 0. 7104970000000000 0. 5231340000000000 T T T
0. 3157330000000000 0. 3981650000000000 0. 5231340000000000 T T T
0. 7065439999999999 0. 3807520000000000 0. 4492240000000000 T T T
0. 4680640000000000 0. 5951149999999999 0. 5898150000000000 T T T
0. 4016600000000000 0. 4801000000000000 0. 5898150000000000 T T T
0. 5364390000000000 0. 4789620000000000 0. 5628150000000000 T T T

Pathway 20

\$POSCAR 1 Au

1.000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.5000000000000000	0.5000000000000000	0.4350510000000000	T T T
0.5720280000000000	0.6175430000000000	0.4585070000000000	T T T
0.3621900000000000	0.5036070000000000	0.4585070000000000	T T T
0.5657810000000000	0.3788500000000000	0.4585070000000000	T T T
0.4279720000000000	0.6175430000000000	0.4585070000000000	T T T
0.4342190000000000	0.3788500000000000	0.4585070000000000	T T T
0.6378100000000000	0.5036070000000000	0.4585070000000000	T T T
0.5000000000000000	0.7076460000000000	0.5293610000000000	T T T
0.3201730000000000	0.3961770000000000	0.5293610000000000	T T T
0.6798270000000000	0.3961770000000000	0.5293610000000000	T T T
0.5000000000000000	0.5778390000000000	0.5752750000000000	T T T
0.4325900000000000	0.4610810000000000	0.5752750000000000	T T T
0.5674110000000000	0.4610810000000000	0.5752750000000000	T T T

Au

1.0000000000000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Au

13

Selective dynamics

Direct

0.4954879517890174	0.5023326320471465	0.4326371199526441	T T T
0.5709084707852583	0.6197348002291717	0.4496350878300046	T T T
0.3590260065190874	0.5051323256741791	0.4603610788208987	T T T
0.5645126263153573	0.3835553989678875	0.4620433306166942	T T T
0.4242748778984599	0.6186825408522619	0.4596990637841772	T T T
0.4328046845532735	0.3786793878170180	0.4550230313143300	T T T
0.6328871399348727	0.5046161499086971	0.4656709395200083	T T T
0.5038542976060341	0.7061619648975649	0.5273027465581434	T T T
0.3223989300811841	0.3938684235305518	0.5298047473454721	T T T
0.6805832103269722	0.3961741811290607	0.5322669836696615	T T T
0.5067157456588672	0.5745693189668247	0.5683431151326199	T T T
0.4363365682725646	0.4596411954605968	0.5716101001263496	T T T

0. 5702100615955399 0. 4568518231920542 0. 5856027980019649 T T T

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Selective dynamics

Direct

0. 4919201729772761 0. 5027278114827441 0. 4290594281540943 T T T

0. 5686763240551941 0. 6181759872797354 0. 4391025896998725 T T T

0. 3559190793590046 0. 5057791849828499 0. 4637427539334313 T T T

0. 5661263679240143 0. 3893499896857362 0. 4594986011579442 T T T

0. 4224489179716539 0. 6187769742932705 0. 4628075065495124 T T T

0. 4341887613457838 0. 3790684628724962 0. 4560185559044208 T T T

0. 6321873715450504 0. 5096065895215331 0. 4770873239873862 T T T

0. 5100507473366666 0. 7038014912879731 0. 5238730871481433 T T T

0. 3224841287565633 0. 3919222837885307 0. 5292930916987736 T T T

0. 6803064268622783 0. 3971610144368896 0. 5346902121283504 T T T

0. 5127201367424536 0. 5716191679708020 0. 5630358730717934 T T T

0. 4353208996425973 0. 4608517128923547 0. 5716113318559701 T T T

0. 5676511167511250 0. 4511592320444819 0. 5901795472497260 T T T

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Selective dynamics

Direct

0. 4842216014588976 0. 5027616965703517 0. 4237545890284579 T T T

0. 5675725500039233 0. 6120522039293064 0. 4343825566369973 T T T

0. 3516216151703909 0. 5071048790001919 0. 4672652192347262 T T T

0. 5678459769500136 0. 3996122697212571 0. 4560640527755093 T T T

0. 4209574405713972 0. 6189350056745582 0. 4653966827115613 T T T

0. 4365892149276373 0. 3777877183467193 0. 4575431373679985 T T T

0. 6380478391921747 0. 5148225260388265 0. 4879792802520279 T T T

0. 5149660345845140 0. 7011497762184473 0. 5202082340397617 T T T

0. 3228915491716666 0. 3900279690305519 0. 5280800773961106 T T T

0. 6796942842110033 0. 3963960966821152 0. 5360801438376377 T T T

0. 5150887067086726 0. 5696413358497326 0. 5606997884131061 T T T

0. 4345240821638376 0. 4613829349098673 0. 5709719566384083 T T T

0. 5659795418064231 0. 4483254618692491 0. 5915741555089117 T T T

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Selective dynamics

Direct

0. 4751058418318085 0. 5017999765366575 0. 4184134090579708 T T T

0. 5664538372086972 0. 6037693771704080 0. 4326566577258494 T T T

0. 3470823229785175 0. 5093537611527751 0. 4704067770621598 T T T

0. 5691021291126340 0. 4109922311403277 0. 4536098886182238 T T T

0. 4205679717777633 0. 6189567977566139 0. 4672112985171281 T T T

0. 4403387581109531 0. 3756725628173277 0. 4592986228091350 T T T

0. 6447079864109329 0. 5189238253701013 0. 4968090159494404 T T T

0. 5193708416875968 0. 6986107933093059 0. 5164670950394166 T T T

0. 3239332647838182 0. 3886885391306136 0. 5259541419626753 T T T

0. 6786100990846152 0. 3955238785412036 0. 5366501211395575 T T T

0. 5162147023013821 0. 5687608886931103 0. 5606782032656104 T T T

0. 4337863002498065 0. 4620868409900443 0. 5698648286887160 T T T

0. 5647263752095024 0. 4468603888876460 0. 5919798016602886 T T T

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Selective dynamics

Direct

0. 4662225885792624 0. 5000730837695748 0. 4141189350455833 T T T

0. 5643528224219826 0. 5940341409141540 0. 4320952753918513 T T T

0. 3426759241516061 0. 5121462029665753 0. 4730211667866945 T T T

0. 5698417415131801 0. 4227519838396271 0. 4517384932055600 T T T

0. 4211742307752184 0. 6185345349995220 0. 4692440561077681 T T T

0. 4452411212000369 0. 3735541570868334 0. 4609488414945566 T T T

0. 6498807064868941 0. 5224356272277472 0. 5036954121383871 T T T

0. 5244593222413657 0. 6956917088554131 0. 5124832444766995 T T T

0. 3257809482251275 0. 3877270997890852 0. 5230615126158484 T T T

0. 6768741464081289 0. 3952146675170335 0. 5361339719638673 T T T

0. 5169272659598112 0. 5688095755469762 0. 5628736271374220 T T T

0. 4330462166768808 0. 4631070097979012 0. 5684005162650200 T T T

0. 5635233904104017 0. 4459200577894488 0. 5921847974706808 T T T

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Selective dynamics

Direct

0. 4580724984818447 0. 4981951088422273 0. 4122624690556259 T T T

0. 5627066767380854 0. 5841101831935878 0. 4313818434143053 T T T

0. 3383190245588171 0. 5154249268547968 0. 4758218669635131 T T T

0. 5704175589104927 0. 4332516477617568 0. 4499097299560458 T T T

0. 4223708771688547 0. 6179786684419729 0. 4714386159150434 T T T

0. 4506368967410628 0. 3720436759593500 0. 4629090928373744 T T T

0. 6525892275803137 0. 5264476788465536 0. 5113930722289779 T T T

0. 5305099428865596 0. 6919503730442725 0. 5077130347094677 T T T

0. 3278603422965258 0. 3871709270631976 0. 5191662492820949 T T T

0. 6751066009493373 0. 3961582500538503 0. 5341493868997600 T T T

0. 5180397249333204 0. 5687904013376203 0. 5650974885446515 T T T

0. 4318213398190895 0. 4646002422961315 0. 5670570609144334 T T T

0. 5615497090741068 0. 4438777565816475 0. 5916999295556901 T T T

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Selective dynamics

Direct

0. 4520608954942290 0. 4914643028686342 0. 4179937861102640 T T T

0. 5584808357763990 0. 5776907182909458 0. 4291486735974945 T T T

0. 3319527703664010 0. 5212142445726096 0. 4755667109557108 T T T

0. 5751904241173242 0. 4381954718410097 0. 4406440387554159 T T T

0. 4253251904238537 0. 6162300183882031 0. 4762208060056220 T T T

0. 4635200425312516 0. 3685603984826973 0. 4798923876501819 T T T

0. 6484770903394953 0. 5321237065768936 0. 5194619671642101 T T T

0. 5384514623527528 0. 6876630563754292 0. 5053724665571269 T T T

0. 3320975257170131 0. 3886381395080762 0. 5093731441205308 T T T

0. 6748564659280299 0. 4009070060043189 0. 5291398060232412 T T T

0. 5209246498170681 0. 5684894181304364 0. 5695303784113287 T T T

0. 4252304255541112 0. 4731226294306906 0. 5667447488519078 T T T

0. 5534326303287683 0. 4357007070235899 0. 5809109032904640 T T T
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Selective dynamics

Direct

0. 4466443525734737 0. 4844588197952681 0. 4230474639250625 T T T
0. 5508195812768863 0. 5715319916855940 0. 4200298869177564 T T T
0. 3303335330350719 0. 5281423794669723 0. 4784338366363742 T T T
0. 5746444896498932 0. 4376478771533043 0. 4396723112570088 T T T
0. 4303384963385773 0. 6175761762180869 0. 4777905193800414 T T T
0. 4681046586298158 0. 3626072203957723 0. 4862232293183331 T T T
0. 6400770710905257 0. 5436467497785112 0. 5192770512353392 T T T
0. 5569998929306204 0. 6749178210383566 0. 5068177904272190 T T T
0. 3356461592394186 0. 3924798812217671 0. 4970506037121252 T T T
0. 6767223036792112 0. 4138202393809996 0. 5281747641206789 T T T
0. 5151816509030500 0. 5669851105795047 0. 5766778565417904 T T T
0. 4223629205528027 0. 4714204722697851 0. 5678270059352937 T T T
0. 5521252953399255 0. 4347650714947514 0. 5789774910716122 T T T

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Selective dynamics

Direct

0. 4423610000000000 0. 4719530000000000 0. 4193950000000000 T T T
0. 5381190000000000 0. 5651470000000000 0. 4166980000000000 T T T
0. 3317620000000000 0. 5344390000000000 0. 4756450000000000 T T T
0. 5722270000000000 0. 4345940000000000 0. 4407640000000000 T T T
0. 4331980000000000 0. 6208330000000000 0. 4877650000000000 T T T
0. 4716900000000000 0. 3565930000000000 0. 4994720000000000 T T T
0. 6340660000000000 0. 5480750000000000 0. 5176010000000000 T T T
0. 5671130000000000 0. 6666670000000000 0. 5053980000000000 T T T
0. 3418610000000000 0. 3966950000000000 0. 4803540000000000 T T T
0. 6782920000000000 0. 4224620000000000 0. 5267930000000000 T T T
0. 5142420000000000 0. 5692320000000000 0. 5874090000000000 T T T
0. 4222850000000000 0. 4753880000000000 0. 5629340000000000 T T T
0. 5527840000000001 0. 4379210000000000 0. 5797710000000000 T T T

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Selective dynamics

Direct

```
0.5000000000000000 0.5000000000000000 0.4350510000000000 T T T
0.5720280000000000 0.6175430000000000 0.4585070000000000 T T T
0.3621900000000000 0.5036070000000000 0.4585070000000000 T T T
0.5657810000000000 0.3788500000000000 0.4585070000000000 T T T
0.4279720000000000 0.6175430000000000 0.4585070000000000 T T T
0.4342190000000000 0.3788500000000000 0.4585070000000000 T T T
0.6378100000000000 0.5036070000000000 0.4585070000000000 T T T
0.5000000000000000 0.7076460000000000 0.5293610000000000 T T T
0.3201730000000000 0.3961770000000000 0.5293610000000000 T T T
0.6798270000000000 0.3961770000000000 0.5293610000000000 T T T
0.5000000000000000 0.5778390000000000 0.5752750000000000 T T T
0.4325900000000000 0.4610810000000000 0.5752750000000000 T T T
0.5674110000000000 0.4610810000000000 0.5752750000000000 T T T
```

Au

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Au

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Selective dynamics

Direct

```
0.5011400898601480 0.5042367163782336 0.4323585218545264 T T T
0.5749820020257609 0.6209788613472033 0.4564733155213740 T T T
0.3642163737435209 0.5042068374840981 0.4631496967732399 T T T
0.5669255017705922 0.3827743014942963 0.4567039186043390 T T T
0.4254522516781319 0.6197789420644172 0.4530081282339643 T T T
0.4346693674189769 0.3828521796161578 0.4587438629815124 T T T
0.6373984003156645 0.5058923841307081 0.4638627775272076 T T T
0.4972024804594165 0.7050889854144092 0.5282842431849369 T T T
0.3207418480734007 0.3941307815958872 0.5309910348994447 T T T
0.6793313003436630 0.3941750623276111 0.5303252812360182 T T T
0.4990499909079149 0.5725786748684919 0.5668513528126421 T T T
0.4320308350933141 0.4566662966280614 0.5807365074372668 T T T
```

0. 5668595566943881 0. 4566399750353174 0. 5785108565108575 T T T

Au

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Selective dynamics

Direct

0. 5040318572092011 0. 5042039731449761 0. 4296369634021660 T T T

0. 5749760458389441 0. 6220603584642291 0. 4587780352868517 T T T

0. 3676696975189415 0. 5065662340184758 0. 4693949955907477 T T T

0. 5672419042368005 0. 3826384725202073 0. 4549890438006738 T T T

0. 4278889691538977 0. 6199438972712873 0. 4427086267771615 T T T

0. 4350089129470317 0. 3855326045268466 0. 4611092853106604 T T T

0. 6390570930363563 0. 5078754504734233 0. 4656685544918934 T T T

0. 4890906881779522 0. 7021822914065758 0. 5284719441260901 T T T

0. 3197677079048294 0. 3976476746104529 0. 5337489156376272 T T T

0. 6798922690335959 0. 3939109892432626 0. 5279540447476694 T T T

0. 4963545234747306 0. 5694839728396871 0. 5637458995439408 T T T

0. 4324985303415737 0. 4533031769073760 0. 5869342657525329 T T T

0. 5665215544832077 0. 4546506579302416 0. 5768585555675748 T T T

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Selective dynamics

Direct

0. 5052984647555758 0. 5048072112081163 0. 4271705790898268 T T T

0. 5739265439514407 0. 6229403447792263 0. 4602935216267252 T T T

0. 3707953531696849 0. 5110305360778011 0. 4752220309711379 T T T

0. 5667109453632535 0. 3835049987130241 0. 4547294303471286 T T T

0. 4287855739455314 0. 6202745146762749 0. 4319100968253216 T T T

0. 4344513022095909 0. 3884120377969765 0. 4612066201308894 T T T

0. 6389649348965221 0. 5092089973254119 0. 4689524675052897 T T T

0. 4804893552887231 0. 6969922033056948 0. 5283678033407029 T T T

0. 3191615387739379 0. 4022495661303317 0. 5350156392410024 T T T

0. 6811018952219428 0. 3933529779505334 0. 5257474225202319 T T T

0. 4979562195024658 0. 5658343899641153 0. 5629708537164717 T T T

0. 4343205375933758 0. 4504694570992901 0. 5898372741761241 T T T

0. 5680370859349358 0. 4509225155801532 0. 5785753864195753 T T T

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Selective dynamics

Direct

0. 5063122507741376 0. 5055664616567356 0. 4247250677986801 T T T

0. 5723882031846838 0. 6234021020213547 0. 4615023284074830 T T T

0. 3745080451958306 0. 5160325477043380 0. 4807170621531761 T T T

0. 5661786289153595 0. 3844213361038423 0. 4547260883108682 T T T

0. 4284922047111307 0. 6200624231058339 0. 4218583104522292 T T T

0. 4339046524548858 0. 3914809456461864 0. 4607498628129540 T T T

0. 6385318881802925 0. 5102143786241475 0. 4722166514144138 T T T

0. 4720157691251464 0. 6907696665011275 0. 5272906847431402 T T T

0. 3189026949212338 0. 4071702278300430 0. 5356227159162121 T T T

0. 6820787688728690 0. 3928689987118346 0. 5240920092070229 T T T

0. 5009763153275462 0. 5626828369472591 0. 5639441448471848 T T T

0. 4360231841174210 0. 4481110214089330 0. 5918786991835268 T T T

0. 5696871449355816 0. 4472168044544755 0. 5806755008272688 T T T

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Selective dynamics

Direct

0. 5072713633385564 0. 5064789361288781 0. 4223035509324014 T T T

0. 5710519642611869 0. 6238743497161260 0. 4625368815830312 T T T

0. 3787167033156638 0. 5213455135141414 0. 4859452657346851 T T T

0. 5654779223925818 0. 3855104881854428 0. 4547757828710305 T T T

0. 4274260643619814 0. 6190337319716092 0. 4129210515092536 T T T

0. 4332456355011943 0. 3946537035319269 0. 4601259804109609 T T T

0. 6377755468714956 0. 5110057281546078 0. 4756069953507563 T T T

0. 4640012196727598 0. 6834949909051137 0. 5256418780877967 T T T

0. 3189430228800806 0. 4123479632276535 0. 5357376158791874 T T T

0. 6826745902860603 0. 3923177336849215 0. 5226637144554300 T T T

0. 5047638180874003 0. 5600428297366079 0. 5655132464975111 T T T

0. 4375219177555469 0. 4463759652735115 0. 5932681021409698 T T T

0. 5711299823414577 0. 4435178170354233 0. 5829590611459482 T T T

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Selective dynamics

Direct

0. 5083796324156874 0. 5072251065033866 0. 4201265349128559 T T T

0. 5699560176554542 0. 6240709161676021 0. 4639049101198218 T T T

0. 3832014374778483 0. 5271618105300665 0. 4912446461836930 T T T

0. 5647727692422951 0. 3861567809534127 0. 4547007135613169 T T T

0. 4262237429097903 0. 6170756436347322 0. 4050482867944570 T T T

0. 4326225214915513 0. 3980556006319955 0. 4594738827396410 T T T

0. 6373794575718537 0. 5113965424945867 0. 4777648972436793 T T T

0. 4558645049025665 0. 6751077229999365 0. 5241268905838246 T T T

0. 3191789874406471 0. 4176469663249044 0. 5353743733774333 T T T

0. 6829937194268441 0. 3918417372754440 0. 5213048644997004 T T T

0. 5084214188643241 0. 5582982425675561 0. 5680696908580644 T T T

0. 4387040743894263 0. 4452553131119463 0. 5943467535350904 T T T

0. 5723014679033622 0. 4407073684960708 0. 5845126831279182 T T T

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Selective dynamics

Direct

0. 4947406314912282 0. 5038321463823795 0. 3981867253091731 T T T

0. 5574968947558723 0. 6142645882335996 0. 4510561500796394 T T T

0. 3820344406100651 0. 5334642533141523 0. 4873719673961643 T T T

0. 5655604445441996 0. 4059484874638531 0. 4569380166502657 T T T

0. 4275173170996285 0. 6233366924937320 0. 3953708841473224 T T T

0. 4318970319005909 0. 4017394084390661 0. 4631604056600491 T T T

0. 6425900641357146 0. 5199940230474273 0. 4876141624415229 T T T

0. 4449750009754336 0. 6429805101531345 0. 5342623105973171 T T T

0. 3197517153667104 0. 4268750478983921 0. 5380467678920299 T T T

0. 6837840294247323 0. 3970518465880810 0. 5246137710054419 T T T

0. 5368163638620016 0. 5513116107748887 0. 5733418772740576 T T T

0. 4415882672015222 0. 4565739853836956 0. 5931790300251814 T T T

0. 5712475379581979 0. 4226271391534729 0. 5968570405106736 T T T
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Selective dynamics

Direct

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0. 5603987303292886 0. 6162299588997039 0. 4455895670411064 T T T
0. 3641198342373407 0. 5311830290750730 0. 4746182830662841 T T T
0. 5668930306958226 0. 4182457120746806 0. 4622194808322712 T T T
0. 4265050993454670 0. 6300377782878712 0. 4026941568617370 T T T
0. 4339583797460373 0. 4027715490090364 0. 4684919126851625 T T T
0. 6578368398842027 0. 5277664084982986 0. 4717415220525510 T T T
0. 4511063632568663 0. 6124232237612252 0. 5395764384566601 T T T
0. 3202541791876874 0. 4235402425143098 0. 5406854800404904 T T T
0. 6776891857637676 0. 4111643106385329 0. 5393663869469894 T T T
0. 5590647673739215 0. 5355978859918135 0. 5632022733712743 T T T
0. 4385482189905330 0. 4769323048090695 0. 5876020679938581 T T T
0. 5550885441370781 0. 4062539608722978 0. 6026630762719136 T T T

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Selective dynamics

Direct

0. 4728260000000000 0. 5044270000000000 0. 3910120000000000 T T T
0. 5599550000000000 0. 6042440000000000 0. 4310710000000000 T T T
0. 3620930000000000 0. 5294800000000000 0. 4734080000000000 T T T
0. 5724770000000000 0. 4423840000000000 0. 4549050000000000 T T T
0. 4223360000000000 0. 6318960000000000 0. 4057490000000000 T T T
0. 4435660000000000 0. 4032270000000000 0. 4786990000000000 T T T
0. 6673240000000000 0. 5408510000000000 0. 4795810000000000 T T T
0. 4663180000000000 0. 6020470000000000 0. 5329870000000000 T T T
0. 3251590000000000 0. 4229950000000000 0. 5449330000000000 T T T
0. 6654890000000000 0. 4269490000000000 0. 5578149999999999 T T T
0. 5670050000000000 0. 5244670000000000 0. 5742820000000000 T T T
0. 4382670000000000 0. 4827180000000000 0. 5943070000000000 T T T
0. 5371840000000000 0. 3843140000000000 0. 5812490000000000 T T T

Pathway 22

\$POSCAR 1 Au

1.000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.5000000000000000	0.5000000000000000	0.4350510000000000	T T T
0.5720280000000000	0.6175430000000000	0.4585070000000000	T T T
0.3621900000000000	0.5036070000000000	0.4585070000000000	T T T
0.5657810000000000	0.3788500000000000	0.4585070000000000	T T T
0.4279720000000000	0.6175430000000000	0.4585070000000000	T T T
0.4342190000000000	0.3788500000000000	0.4585070000000000	T T T
0.6378100000000000	0.5036070000000000	0.4585070000000000	T T T
0.5000000000000000	0.7076460000000000	0.5293610000000000	T T T
0.3201730000000000	0.3961770000000000	0.5293610000000000	T T T
0.6798270000000000	0.3961770000000000	0.5293610000000000	T T T
0.5000000000000000	0.5778390000000000	0.5752750000000000	T T T
0.4325900000000000	0.4610810000000000	0.5752750000000000	T T T
0.5674110000000000	0.4610810000000000	0.5752750000000000	T T T

Au

1.0000000000000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Au

13

Selective dynamics

Direct

0.4915755654229686	0.5062553154253743	0.4280848452783098	T T T
0.5712105825066974	0.6167504692586105	0.4558048348671924	T T T
0.3569934225101322	0.5088482517954297	0.4615667711355824	T T T
0.5620714786109356	0.3756119943460026	0.4771982671538033	T T T
0.4229845110524801	0.6224150192353111	0.4653436122714155	T T T
0.4356823633650160	0.3809126863515649	0.4433060596593355	T T T
0.6257375813927675	0.4959218823482912	0.4567779860395611	T T T
0.5064507461574156	0.7077685499918395	0.5301243828319353	T T T
0.3275113834355369	0.3902620815423800	0.5215255934760018	T T T
0.6821117069580134	0.3990563529990934	0.5351799770591982	T T T
0.5025063442093234	0.5761875837437139	0.5728407933942931	T T T
0.4412575292155425	0.4562994957357214	0.5642080388727813	T T T

0. 5739066980519407 0. 4637102301155203 0. 5880387508493428 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4835713450588717 0. 5195580497294946 0. 4167675146041241 T T T

0. 5750004330132708 0. 6130220914656712 0. 4586922763609298 T T T

0. 3550851325756493 0. 5108026089155999 0. 4640169343226707 T T T

0. 5665969613905335 0. 3591204995143685 0. 4909397947322056 T T T

0. 4176420887214971 0. 6271885739530951 0. 4712693664139523 T T T

0. 4481254009474525 0. 3886925674106455 0. 4416237612071762 T T T

0. 6087069509754809 0. 4838155294866420 0. 4514338797483506 T T T

0. 5095983461717118 0. 7078703563523512 0. 5286977733437500 T T T

0. 3348906615989942 0. 3863163423481598 0. 5147297539446288 T T T

0. 6842977000390219 0. 4045515728652823 0. 5364627440724465 T T T

0. 5019135324643088 0. 5769912624467697 0. 5728579909883129 T T T

0. 4413053951819917 0. 4576506675323045 0. 5642194799424620 T T T

0. 5732659463405617 0. 4644197724590025 0. 5882886247983683 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4795999080498207 0. 5352447806474933 0. 4114123484003285 T T T

0. 5840464620678615 0. 6066052486773434 0. 4614699201280640 T T T

0. 3560484081923824 0. 5093261094038417 0. 4659222615284025 T T T

0. 5684621538918149 0. 3475295291159182 0. 4990391951667513 T T T

0. 4085029809178332 0. 6309296803802280 0. 4769000018205047 T T T

0. 4611362063441175 0. 4026821495858118 0. 4431842136941553 T T T

0. 5932292139769773 0. 4728679265876896 0. 4482089947744560 T T T

0. 5130371192113516 0. 7052337881563382 0. 5222442657654994 T T T

0. 3448701040036984 0. 3802359109205914 0. 5079482568148440 T T T

0. 6822935346961978 0. 4084344230609919 0. 5346528504182975 T T T

0. 5008177037995930 0. 5774437535666330 0. 5702658182033015 T T T

0. 4374563876876059 0. 4596010165362343 0. 5706025110030993 T T T

0. 5704996833778995 0. 4638655495780915 0. 5881492284995070 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4807400407722741 0. 5399954540060548 0. 4128546678108923 T T T

0. 5879123123300393 0. 6031540694403725 0. 4690078015923465 T T T

0. 3600998148170353 0. 5085680209654971 0. 4728066608509092 T T T

0. 5516756354686042 0. 3543066376406393 0. 5148978290563609 T T T

0. 4042000773921812 0. 6337886895966703 0. 4763753775270007 T T T

0. 4609987359416159 0. 4054937114690965 0. 4302532330238910 T T T

0. 5915943059185332 0. 4695879282543251 0. 4463038918858627 T T T

0. 5124670648565469 0. 7044103882112408 0. 5192428794062598 T T T

0. 3510603317166526 0. 3766618551931735 0. 5044927469548428 T T T

0. 6766808976116785 0. 4004975939792528 0. 5318249969907646 T T T

0. 4922135157961491 0. 5767817892933911 0. 5684087590055421 T T T

0. 4499754736739513 0. 4483562547556984 0. 5655959959270379 T T T

0. 5803816372644700 0. 4783974507543638 0. 5879350035280246 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4875785926678119 0. 5549254549508346 0. 4226577752329023 T T T

0. 6044228437827097 0. 5939291613323993 0. 4915773317969259 T T T

0. 3638223284044226 0. 5058778845874257 0. 4814152368646237 T T T

0. 5426225085230513 0. 3566446172896309 0. 5189837531586718 T T T

0. 3907182257543502 0. 6361085978518587 0. 4766575683904935 T T T

0. 4622963071714399 0. 4196648409488586 0. 4278982898646866 T T T

0. 5910890502969004 0. 4673334844785125 0. 4373934786245806 T T T

0. 5131208143694871 0. 6929226586449927 0. 4951819371785515 T T T

0. 3618691254630106 0. 3691723718798590 0. 5031752091921599 T T T

0. 6705424305763713 0. 3976641802526130 0. 5252800818498493 T T T

0. 4814093005692837 0. 5760093263459851 0. 5652327643898862 T T T

0. 4497092184523173 0. 4444590827768358 0. 5746215117415485 T T T

0. 5807990718301671 0. 4852881565214656 0. 5799248795764192 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4859867750880065 0. 5547202321366298 0. 4227144162284878 T T T

0. 6208957113222127 0. 5800608207864422 0. 4985729358180329 T T T

0. 3639054923367580 0. 5097332521003353 0. 4855575009341734 T T T

0. 5557702664442883 0. 3622907339780140 0. 5192141289137197 T T T

0. 3882285899561536 0. 6407336345442270 0. 4768008390774725 T T T

0. 4591890498200125 0. 4175341603738660 0. 4318328268795154 T T T

0. 5857357385814267 0. 4662684789881809 0. 4307896867106449 T T T

0. 5231793779270645 0. 6725439147799896 0. 4881216536743129 T T T

0. 3462499700199834 0. 3780772370322524 0. 4995005669614121 T T T

0. 6791650154240050 0. 4295130681952849 0. 5221244765334565 T T T

0. 4719828675345096 0. 5697745937976436 0. 5653114033193178 T T T

0. 4469206672799145 0. 4339144752394508 0. 5744790960725317 T T T

0. 5727902898289581 0. 4848352096109870 0. 5849802804402707 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4910262305899201 0. 5531494760336169 0. 4231428567191967 T T T

0. 6144147434521998 0. 5767757547036467 0. 5025292403428865 T T T

0. 3635072448733214 0. 5119945273076261 0. 4866337842597777 T T T

0. 5383412200986811 0. 3504202162045263 0. 5178446323478696 T T T

0. 3927422477361204 0. 6401304054938274 0. 4770264669813098 T T T

0. 4551699007652021 0. 4194708792607867 0. 4298745921655130 T T T

0. 5860753969261091 0. 4537389330224958 0. 4378495161003614 T T T

0. 5277768879239034 0. 6747943858167444 0. 4861585231085351 T T T

0. 3422771569960472 0. 3804872189384774 0. 4974733773984685 T T T

0. 6946272287724686 0. 4709946127128945 0. 5197540571043537 T T T

0. 4785361093064405 0. 5665816224153484 0. 5630826775009792 T T T

0. 4422664523718298 0. 4335620873644897 0. 5750863605738856 T T T

```
0. 5732389652271280 0. 4678996657649254 0. 5835437004363254 T T T
Au
1. 0000000000000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000
```

Au

13

Selective dynamics

Direct

```
0. 5013114369468016 0. 5584990604635484 0. 4207900412633492 T T T
0. 6154437591492313 0. 5777802169042378 0. 5034654961403952 T T T
0. 3511907296902632 0. 5019074246879768 0. 4859480653387234 T T T
0. 5089899713727336 0. 3511402179368797 0. 5145639633508475 T T T
0. 3965405983858765 0. 6277496616692618 0. 4786850979321499 T T T
0. 4526324800907806 0. 4347908434181453 0. 4200016314738729 T T T
0. 5854890618572001 0. 4487417446639407 0. 4416406383149278 T T T
0. 5283489441525127 0. 6790933786586492 0. 4862655101718736 T T T
0. 3664511994928505 0. 3641557251478554 0. 5001060758951441 T T T
0. 6954478735677903 0. 4729251879245820 0. 5206002736642689 T T T
0. 4879315219098582 0. 5719652408442517 0. 5663645738722864 T T T
0. 4377064305308837 0. 4497072469474808 0. 5803808663865598 T T T
0. 5725157286598817 0. 4615437865398760 0. 5811875020022157 T T T
```

\$POSCAR 1 Au

```
1. 000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000
```

13

Selective dynamics

Direct

```
0. 5173850000000000 0. 5629350000000000 0. 4084940000000000 T T T
0. 6187850000000000 0. 5804370000000000 0. 5038370000000000 T T T
0. 3275780000000000 0. 4902400000000000 0. 4839230000000000 T T T
0. 5077640000000000 0. 3548060000000000 0. 5150250000000000 T T T
0. 4051220000000000 0. 5992240000000000 0. 4808820000000000 T T T
0. 4476380000000000 0. 4503620000000000 0. 4265130000000000 T T T
0. 5834880000000000 0. 4477800000000000 0. 4424990000000000 T T T
0. 5243120000000000 0. 6774670000000000 0. 4849740000000000 T T T
0. 3713720000000000 0. 3602870000000000 0. 5010120000000000 T T T
0. 6928430000000000 0. 4708570000000000 0. 5219150000000000 T T T
0. 5005120000000000 0. 5797050000000000 0. 5792659999999999 T T T
0. 4334510000000000 0. 4644630000000000 0. 5701030000000000 T T T
0. 5697489999999999 0. 4614360000000000 0. 5815560000000000 T T T
```

Pathway 23

\$POSCAR 1 Au

1.000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.5000000000000000	0.5000000000000000	0.4350510000000000	T T T
0.5720280000000000	0.6175430000000000	0.4585070000000000	T T T
0.3621900000000000	0.5036070000000000	0.4585070000000000	T T T
0.5657810000000000	0.3788500000000000	0.4585070000000000	T T T
0.4279720000000000	0.6175430000000000	0.4585070000000000	T T T
0.4342190000000000	0.3788500000000000	0.4585070000000000	T T T
0.6378100000000000	0.5036070000000000	0.4585070000000000	T T T
0.5000000000000000	0.7076460000000000	0.5293610000000000	T T T
0.3201730000000000	0.3961770000000000	0.5293610000000000	T T T
0.6798270000000000	0.3961770000000000	0.5293610000000000	T T T
0.5000000000000000	0.5778390000000000	0.5752750000000000	T T T
0.4325900000000000	0.4610810000000000	0.5752750000000000	T T T
0.5674110000000000	0.4610810000000000	0.5752750000000000	T T T

Au

1.0000000000000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Au

13

Selective dynamics

Direct

0.5002513835997555	0.4928478672031947	0.4305660990480356	T T T
0.5645615243176092	0.6131202388499357	0.4593891656100834	T T T
0.3617528981590719	0.5009413335111201	0.4445608372339941	T T T
0.5667696281649394	0.3737745431750711	0.4625153497865582	T T T
0.4268883829065136	0.6115380747285475	0.4725031865409828	T T T
0.4356971492724106	0.3734667390801468	0.4619047866509947	T T T
0.6374126981166020	0.5028839249892840	0.4548226342676324	T T T
0.5001005673299198	0.7080763063090999	0.5334526014956920	T T T
0.3192018418597279	0.4034368893683938	0.5259427221920548	T T T
0.6821830372336452	0.4006097294340883	0.5292096978144011	T T T
0.5060430138540205	0.5828668686607278	0.5878970532689342	T T T
0.4322129108113716	0.4720810936444149	0.5654901534633345	T T T

0. 5669259643744534 0. 4643573910459963 0. 5717467126273126 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5055414772442323 0. 4830864667742103 0. 4229032085262413 T T T

0. 5505603362535263 0. 6077544881645784 0. 4542857206983624 T T T

0. 3698795215395855 0. 5035278809729627 0. 4367083545314415 T T T

0. 5683017829580123 0. 3673246211221846 0. 4679644691971451 T T T

0. 4166642301021735 0. 6148417231189234 0. 4886101845121696 T T T

0. 4366096018299245 0. 3712651466355904 0. 4660533212539831 T T T

0. 6370806797042994 0. 5066086644465674 0. 4568947815405361 T T T

0. 5018524122645275 0. 7078136802111635 0. 5351959128091950 T T T

0. 3186760384659290 0. 4119091298990020 0. 5207845011336941 T T T

0. 6842945942031280 0. 4025120413766183 0. 5275483618886120 T T T

0. 5111993539109824 0. 5831239896080096 0. 5904843768805806 T T T

0. 4326671977641608 0. 4772575269531744 0. 5617269517727258 T T T

0. 5666737737595506 0. 4629756407169969 0. 5708408552553021 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5142339868377910 0. 4724719535079187 0. 4159168022789805 T T T

0. 5351516604567496 0. 6008498385533274 0. 4508905149395462 T T T

0. 3828154270828135 0. 5078546559985299 0. 4348118424881951 T T T

0. 5681814841825638 0. 3594117405147050 0. 4725450756737761 T T T

0. 4076346561704366 0. 6204141378575361 0. 4995057007568015 T T T

0. 4365408479040913 0. 3714173802672001 0. 4687488045838902 T T T

0. 6368144104495460 0. 5140058968977159 0. 4600033270109141 T T T

0. 5037971997998886 0. 7066053688781869 0. 5352166566216625 T T T

0. 3183449508788391 0. 4201423106358461 0. 5151824132334759 T T T

0. 6845691968764654 0. 4048758159355142 0. 5238857093451423 T T T

0. 5132496110761219 0. 5823685550604586 0. 5906083802033480 T T T

0. 4325257770064960 0. 4782864658707796 0. 5634992198591060 T T T

0. 5661417912782135 0. 4612968800222439 0. 5691865530051435 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5227446913816264 0. 4641386265332534 0. 4121496282520486 T T T

0. 5212322278917715 0. 5942779588851845 0. 4487177410509010 T T T

0. 3962393191284873 0. 5123921686334755 0. 4322572622421827 T T T

0. 5679927312166707 0. 3520210529318364 0. 4758000299807298 T T T

0. 4003993634365484 0. 6193031660539796 0. 5122380520098642 T T T

0. 4371004048341102 0. 3735207454510079 0. 4718301237950670 T T T

0. 6346353496949392 0. 5222996811778969 0. 4636453855921948 T T T

0. 5028828778615567 0. 7034790793430924 0. 5332086646707880 T T T

0. 3187924201677476 0. 4299678821811092 0. 5076828409223453 T T T

0. 6839832555612343 0. 4083494509072607 0. 5187520073240036 T T T

0. 5181136827464941 0. 5812368778770006 0. 5906926508430463 T T T

0. 4313128962609076 0. 4808796338002419 0. 5657938647258313 T T T

0. 5645717798178627 0. 4581346762246571 0. 5672327485910023 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5325529972029416 0. 4631497713131433 0. 4180296882129895 T T T

0. 5154778471045013 0. 5963241601793470 0. 4396856433561757 T T T

0. 4041997821216214 0. 5115045973240897 0. 4296567097910865 T T T

0. 5662351140892076 0. 3431311981964557 0. 4740682742228125 T T T

0. 3978983816785736 0. 6122559892465353 0. 5202885405344190 T T T

0. 4376418151207180 0. 3778471102792107 0. 4772747343485952 T T T

0. 6316714842381687 0. 5356983096397196 0. 4822520101943879 T T T

0. 4985459047353407 0. 7005741705690338 0. 5287820075901271 T T T

0. 3183263332875176 0. 4392421890047004 0. 5051064514505315 T T T

0. 6798642597544200 0. 4112869479455656 0. 5081929673939883 T T T

0. 5292749698134628 0. 5776594783577652 0. 5800971907787646 T T T

0. 4291703798488316 0. 4841557579858785 0. 5707856240312290 T T T

0. 5591417310046560 0. 4471713199585408 0. 5657811580949195 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5416697499734716 0. 4618781874191733 0. 4229538658094288 T T T

0. 5167219343453378 0. 5959317544044270 0. 4394368674346168 T T T

0. 4137927322393660 0. 5075262837405765 0. 4200318897241258 T T T

0. 5606797961308188 0. 3382235231752471 0. 4772173849930570 T T T

0. 3917744634936436 0. 5985245416514752 0. 5196025091024906 T T T

0. 4336733209143612 0. 3813238123234777 0. 4790314598850446 T T T

0. 6349708383640047 0. 5426851212763646 0. 4879282951807412 T T T

0. 4856801864745876 0. 6955397906637005 0. 5282237508608054 T T T

0. 3202736716816547 0. 4628750276193390 0. 5068615272549282 T T T

0. 6743024945384474 0. 4127291009895603 0. 4944599672846374 T T T

0. 5300743906758790 0. 5771877196830770 0. 5789112535540484 T T T

0. 4337853287475684 0. 4794407837810642 0. 5784378752000803 T T T

0. 5626020924208465 0. 4461353532725262 0. 5669043537160455 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5484139113168811 0. 4613573393762781 0. 4223831125677198 T T T

0. 5152371031124523 0. 5927595821274713 0. 4391051210776456 T T T

0. 4180906475088259 0. 4958925971930793 0. 4246512549368733 T T T

0. 5674460323808359 0. 3342927012774057 0. 4766374761057149 T T T

0. 3937597756455568 0. 5977306086572208 0. 5194743037669330 T T T

0. 4390356957096160 0. 3723980456975957 0. 4807139527984614 T T T

0. 6344067290106092 0. 5515534594771252 0. 4967792330124711 T T T

0. 4866601438368847 0. 6934320861373221 0. 5278812209440971 T T T

0. 3117441603395824 0. 4904865768142584 0. 5097337876526196 T T T

0. 6710819811420985 0. 4219308623167858 0. 4822319649437775 T T T

0. 5245370482259639 0. 5730050177762913 0. 5805559096612384 T T T

0. 4295895136944252 0. 4719470367871701 0. 5754287729131956 T T T

0. 5599982580762137 0. 4432150863620117 0. 5644248896193043 T T T
Au
1. 0000000000000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5460653157272372 0. 4589286091601830 0. 4196396149492753 T T T
0. 5110585478124622 0. 5879745441808018 0. 4356096132141372 T T T
0. 4139504720602576 0. 4892181946329366 0. 4304748529585395 T T T
0. 5813255924535058 0. 3324008229190913 0. 4711569530494852 T T T
0. 3980931438553332 0. 6023551018774633 0. 5204969495415918 T T T
0. 4507915269511339 0. 3658765321666272 0. 4826522723809312 T T T
0. 6291858811575517 0. 5617079370013781 0. 5007942261015701 T T T
0. 5015658705871346 0. 6882929554259590 0. 5277646089560571 T T T
0. 3047863917686789 0. 5073551625685947 0. 5115822405362573 T T T
0. 6689697558278586 0. 4352192301548861 0. 4824331077155093 T T T
0. 5197978758354939 0. 5653111972378454 0. 5841576173153499 T T T
0. 4213429363353474 0. 4682855680158929 0. 5721786547038710 T T T
0. 5530676896279737 0. 4370751446583438 0. 5610602885773904 T T T

\$POSCAR 1 Au

1. 000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
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13

Selective dynamics

Direct

0. 5429010000000000 0. 4549780000000000 0. 4179110000000000 T T T
0. 5050900000000000 0. 5830040000000000 0. 4243640000000000 T T T
0. 4100300000000000 0. 4845320000000000 0. 4316660000000000 T T T
0. 5889489999999999 0. 3346380000000000 0. 4715560000000000 T T T
0. 4053100000000000 0. 6059130000000000 0. 5202680000000000 T T T
0. 4549550000000000 0. 3620130000000000 0. 4827460000000000 T T T
0. 6178510000000000 0. 5728540000000000 0. 5039990000000000 T T T
0. 5222010000000000 0. 6767510000000000 0. 5240300000000000 T T T
0. 3050210000000000 0. 5181010000000000 0. 5131790000000001 T T T
0. 6650820000000000 0. 4493180000000000 0. 4837940000000000 T T T
0. 5143520000000000 0. 5586680000000001 0. 5948080000000000 T T T
0. 4175710000000000 0. 4647160000000000 0. 5704550000000000 T T T
0. 5506880000000000 0. 4345150000000000 0. 5612250000000000 T T T

Pathway 24

\$POSCAR 1 Au

1.000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.5721840000000000	0.5664030000000000	0.4077320000000000	T T T
0.5721840000000000	0.4335970000000000	0.4077320000000000	T T T
0.4278160000000000	0.5664030000000000	0.4077320000000000	T T T
0.4278160000000000	0.4335970000000000	0.4077320000000000	T T T
0.5000000000000000	0.6803250000000000	0.3889020000000000	T T T
0.5000000000000000	0.3196750000000000	0.3889020000000000	T T T
0.4298000000000000	0.5000000000000000	0.5280730000000000	T T T
0.5702000000000000	0.5000000000000000	0.5280730000000000	T T T
0.5000000000000000	0.6288890000000000	0.5141910000000000	T T T
0.5000000000000000	0.3711110000000000	0.5141910000000000	T T T
0.5000000000000000	0.5702320000000000	0.6314490000000000	T T T
0.5000000000000000	0.4297680000000000	0.6314490000000000	T T T
0.5000000000000000	0.5000000000000000	0.7438420000000000	T T T

Au

1.0000000000000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Au

13

Selective dynamics

Direct

0.5647333449746474	0.5623526588772604	0.4025434169597407	T T T
0.5793928720595602	0.4305955542151205	0.4078600625516865	T T T
0.4207115791171600	0.5707100582366761	0.4176514800722749	T T T
0.4353963459250114	0.4383415568456442	0.4089623160065204	T T T
0.4974109481387473	0.6788886834279853	0.3863714281242518	T T T
0.5010888184969179	0.3218491006316894	0.3867158391366635	T T T
0.4281605786250466	0.4979703934713732	0.5322905772896782	T T T
0.5690651234894469	0.4990826897718506	0.5266107669039752	T T T
0.5089215709388225	0.6294061594488669	0.5130368290140276	T T T
0.5037027056934720	0.3702073201038364	0.5142890941011379	T T T
0.5036986574190938	0.5706564128771033	0.6301971064811924	T T T
0.4989754231262776	0.4283341844650603	0.6316691300637574	T T T

0. 4887428990889098 0. 5016052276276280 0. 7418019532950937 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

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Au

13

Selective dynamics

Direct

0. 5555402178995866 0. 5573297548958369 0. 3968733988682938 T T T

0. 5854355875896788 0. 4285753324739126 0. 4078010399234876 T T T

0. 4157834486443749 0. 5745864485065975 0. 4279258267081516 T T T

0. 4430343139095943 0. 4444319058629936 0. 4097483336063661 T T T

0. 4948413197060506 0. 6775284775006898 0. 3847420689146736 T T T

0. 5012868498583850 0. 3248117526909214 0. 3858750082624980 T T T

0. 4259613987424266 0. 4944094328722824 0. 5359900598812783 T T T

0. 5679290634401567 0. 4974165151661513 0. 5254469832961072 T T T

0. 5188069978900141 0. 6292253486265952 0. 5106639864239956 T T T

0. 5067121918021752 0. 3691574381048621 0. 5153578968852787 T T T

0. 5062855437489753 0. 5708117405238621 0. 6280344569752653 T T T

0. 4987908979766650 0. 4270443457563483 0. 6327141165427894 T T T

0. 4795932751560171 0. 5046715070190902 0. 7388268237117455 T T T

Au

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Au

13

Selective dynamics

Direct

0. 5456992861906896 0. 5545797689223536 0. 3864780525078855 T T T

0. 5884915846997266 0. 4313128594579982 0. 4081396715013063 T T T

0. 4135813275914302 0. 5765780494020187 0. 4361388419301537 T T T

0. 4455806090031605 0. 4475915321454029 0. 4121269937413233 T T T

0. 4914282288600465 0. 6781101149848492 0. 3863394397574265 T T T

0. 5033878186464923 0. 3284159342496563 0. 3858069326554868 T T T

0. 4259690946469881 0. 4920916012010664 0. 5395071123024071 T T T

0. 5703758088860673 0. 4942484618644478 0. 5276128324446612 T T T

0. 5297423840618328 0. 6243058157684547 0. 5061515212035361 T T T

0. 5091823698992732 0. 3680895820696041 0. 5166096649829629 T T T

0. 5080997288751635 0. 5711934045731454 0. 6257754046814424 T T T

0. 4988349623778483 0. 4255767282128848 0. 6345627639327162 T T T

0. 4696279942164079 0. 5079061471481907 0. 7347507683586392 T T T

Au

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Au

13

Selective dynamics

Direct

0. 5377202856326618 0. 5548130019918379 0. 3734348396590675 T T T

0. 5881533837804409 0. 4379724647463996 0. 4107654658010204 T T T

0. 4134053107100772 0. 5777671164626194 0. 4408119644998025 T T T

0. 4456395800682598 0. 4492654445036825 0. 4138852292312677 T T T

0. 4897849740619047 0. 6792617218398784 0. 3885723849306444 T T T

0. 5064372421276161 0. 3322698090061685 0. 3853369517917344 T T T

0. 4265209181487120 0. 4911871439673848 0. 5418793617553123 T T T

0. 5748221421588313 0. 4891088137790435 0. 5362028181101665 T T T

0. 5374081222216844 0. 6150193421045669 0. 5003026712362111 T T T

0. 5092924593699439 0. 3673327788301873 0. 5170787411170791 T T T

0. 5079711720805535 0. 5728377757977782 0. 6237153760194776 T T T

0. 4976586227268291 0. 4231769295320484 0. 6364754333788232 T T T

0. 4651869906499572 0. 5099876574385249 0. 7315387624693481 T T T

Au

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Au

13

Selective dynamics

Direct

0. 5309811034738396 0. 5549237648280098 0. 3645492045713820 T T T

0. 5871811839029755 0. 4446645361090739 0. 4136413602720796 T T T

0. 4139246635701864 0. 5785850062010238 0. 4464723164289925 T T T

0. 4454480678304492 0. 4502490552825287 0. 4180659396047304 T T T

0. 4883290787293131 0. 6792310015064883 0. 3908678629234625 T T T

0. 5095639250888904 0. 3363687773596122 0. 3842815534608592 T T T

0. 4260555682324059 0. 4906448209614678 0. 5463175805064793 T T T

0. 5783675953707932 0. 4851656945842417 0. 5433975488733934 T T T

0. 5444536969084302 0. 6064391834817956 0. 4940463737880883 T T T

0. 5114782983717137 0. 3661118240981581 0. 5170318270029238 T T T

0. 5092940192858378 0. 5760039205294442 0. 6200498472839889 T T T

0. 4974288944489172 0. 4192929424973295 0. 6376018833310640 T T T

0. 4574951099345115 0. 5123194725609169 0. 7236767019525333 T T T

Au

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20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

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Au

13

Selective dynamics

Direct

0. 5264241217194070 0. 5538903803333496 0. 3590013116581384 T T T

0. 5864915750362965 0. 4503613045993183 0. 4178659317248277 T T T

0. 4150513980860976 0. 5794419465130460 0. 4519173609466636 T T T

0. 4449544073610174 0. 4512019349600956 0. 4232773737700588 T T T

0. 4887000745663098 0. 6780652671552679 0. 3925298023805144 T T T

0. 5123498110740455 0. 3412486255770389 0. 3823382842589702 T T T

0. 4251019490639442 0. 4913283020528795 0. 5522551883429354 T T T

0. 5798500481716820 0. 4824520745990211 0. 5498782033832862 T T T

0. 5503270812225386 0. 5989439911106553 0. 4884087515963056 T T T

0. 5132910446319255 0. 3648091040910496 0. 5161672611740696 T T T

0. 5109939941825740 0. 5809364577021423 0. 6158537843752593 T T T

0. 4971174405820373 0. 4136651375640488 0. 6381133041931421 T T T

0. 4493482581719505 0. 5136554737422216 0. 7123934421959000 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

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0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5165646737533054 0. 5491222095187194 0. 3531096070951216 T T T

0. 5861429324006253 0. 4585835605226491 0. 4247170598717944 T T T

0. 4221264448481536 0. 5822963674959644 0. 4672273763372358 T T T

0. 4429498142480927 0. 4534019388915218 0. 4300530886168041 T T T

0. 4917865850007549 0. 6742959472347890 0. 3944171487747776 T T T

0. 5167097033591498 0. 3510816050240222 0. 3785882525522581 T T T

0. 4218017049309761 0. 4858051974634334 0. 5606798176819511 T T T

0. 5758293907519832 0. 4820195847433083 0. 5594490510987565 T T T

0. 5628578997129612 0. 5906222691394893 0. 4792258156161274 T T T

0. 5157283442720629 0. 3640786624390314 0. 5140399667549612 T T T

0. 5038300044762395 0. 5918721446073169 0. 6020092665975688 T T T

0. 4980935363035057 0. 4023245581301032 0. 6400246174000719 T T T

0. 4455801740491311 0. 5144959547897809 0. 6964589316024909 T T T
Au
1. 000000000000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5139732244368622 0. 5357792246323108 0. 3540677471788181 T T T
0. 5905876916360125 0. 4606624483176518 0. 4377899370289536 T T T
0. 4251019663608459 0. 5835931688886823 0. 4716777694632137 T T T
0. 4355038972787439 0. 4529098077902468 0. 4333423768560328 T T T
0. 4960352401222561 0. 6648675239379932 0. 3880474962436086 T T T
0. 5195080247885702 0. 3688632185086856 0. 3686183528499056 T T T
0. 4202098896592706 0. 4839687408388277 0. 5636342537251154 T T T
0. 5660237286735742 0. 4867098763474824 0. 5692780680940464 T T T
0. 5664565852872128 0. 5900055339488574 0. 4792002566709115 T T T
0. 5145322503677161 0. 3646864837705156 0. 5084543380494028 T T T
0. 4937261612319090 0. 6032531794495705 0. 5960438920493661 T T T
0. 4951160859961625 0. 3917951880150316 0. 6377327180528193 T T T
0. 4632264673448050 0. 5129056055542129 0. 6921127937377510 T T T

\$POSCAR 1 Au

1. 000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
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0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

13

Selective dynamics

Direct

0. 5124810000000000 0. 5248119999999999 0. 3592050000000000 T T T
0. 5943410000000000 0. 4605780000000000 0. 4532870000000000 T T T
0. 4266980000000000 0. 5816080000000000 0. 4688480000000000 T T T
0. 4232080000000000 0. 4485830000000000 0. 4360030000000000 T T T
0. 5010880000000000 0. 6560240000000001 0. 3809480000000000 T T T
0. 5218820000000000 0. 3884130000000000 0. 3607850000000000 T T T
0. 4215270000000000 0. 4842240000000000 0. 5648010000000000 T T T
0. 5654210000000000 0. 4943100000000000 0. 5793340000000000 T T T
0. 5660480000000000 0. 5913750000000000 0. 4829220000000000 T T T
0. 5096550000000000 0. 3617270000000000 0. 5003670000000000 T T T
0. 4827550000000000 0. 6106410000000000 0. 5939600000000000 T T T
0. 4947280000000000 0. 3864510000000000 0. 6310040000000000 T T T
0. 4801700000000000 0. 5112540000000000 0. 6885360000000000 T T T

Pathway 25

Au

1.000000		
20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.5721840000000000	0.5664030000000000	0.4077320000000000	T T T
0.5721840000000000	0.4335970000000000	0.4077320000000000	T T T
0.4278160000000000	0.5664030000000000	0.4077320000000000	T T T
0.4278160000000000	0.4335970000000000	0.4077320000000000	T T T
0.5000000000000000	0.6803250000000000	0.3889020000000000	T T T
0.5000000000000000	0.3196750000000000	0.3889020000000000	T T T
0.4298000000000000	0.5000000000000000	0.5280730000000000	T T T
0.5702000000000000	0.5000000000000000	0.5280730000000000	T T T
0.5000000000000000	0.6288900000000000	0.5141910000000000	T T T
0.5000000000000000	0.3711110000000000	0.5141910000000000	T T T
0.5000000000000000	0.5702320000000000	0.6314490000000000	T T T
0.5000000000000000	0.4297680000000000	0.6314490000000000	T T T
0.5000000000000000	0.5000000000000000	0.7438420000000000	T T T

Au

1.0000000000000000		
20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Au

13

Selective dynamics

Direct

0.5786677218666725	0.5724905299306258	0.4212087799904936	T T T
0.5649100554227005	0.4399475453132524	0.4099666411151972	T T T
0.4358433839675442	0.5613491730829097	0.4005377690394951	T T T
0.4215908511248472	0.4296754834468715	0.4062515074019544	T T T
0.5012286009619800	0.6793119942128669	0.3866514496021125	T T T
0.5018446347674725	0.3222310385689298	0.3866473746369010	T T T
0.4316244457962739	0.4977738613639531	0.5253227448538240	T T T
0.5727213344143607	0.4974268845083358	0.5339067596850313	T T T
0.4853478238221101	0.6296074316273490	0.5127489566801415	T T T
0.4962437156839883	0.3696854706703832	0.5144824903810914	T T T
0.4939049364307948	0.5702693727028105	0.6295319931274506	T T T
0.5015208848527877	0.4277727675590697	0.6318703084396944	T T T

0. 5145516108884678 0. 5024588239283574 0. 7408732250466485 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5836423444802250 0. 5780102991734850 0. 4338148417521737 T T T

0. 5558628121290070 0. 4483752541340209 0. 4098779037085194 T T T

0. 4484528673626542 0. 5552636967105045 0. 3921944383370572 T T T

0. 4139412216313545 0. 4283249956925772 0. 4073246169581282 T T T

0. 5032562416751460 0. 6787347650954274 0. 3868083884385598 T T T

0. 5011476779598425 0. 3273039199489318 0. 3849681293330676 T T T

0. 4317879383487977 0. 4944334805981399 0. 5256629175376162 T T T

0. 5749642894101399 0. 4931037512973333 0. 5375993430486687 T T T

0. 4716841743632330 0. 6269030078696076 0. 5093054685695648 T T T

0. 4948611263457963 0. 3683068771548861 0. 5153579533591426 T T T

0. 4919379399256840 0. 5698087369932026 0. 6267849492957609 T T T

0. 5029954302502873 0. 4255457539358645 0. 6333685054831193 T T T

0. 5254659361178327 0. 5058859253281298 0. 7369325441786572 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5842460353635417 0. 5799845242338506 0. 4399559899865935 T T T

0. 5547794779171298 0. 4511413934408210 0. 4111917188717911 T T T

0. 4589427321433135 0. 5554411580031200 0. 3756308845144360 T T T

0. 4128452500753639 0. 4360668096035312 0. 4103432092208692 T T T

0. 5050680523967728 0. 6807792922617253 0. 3904049304831574 T T T

0. 4967884128072839 0. 3321877167986571 0. 3847630490777902 T T T

0. 4265592600146917 0. 4875597151056681 0. 5354682625129072 T T T

0. 5743278609947566 0. 4915379975953300 0. 5397611386914392 T T T

0. 4608583582312846 0. 6152298549390736 0. 5024277249738063 T T T

0. 4948203661236974 0. 3672573710839089 0. 5163463779311570 T T T

0. 4923236381224569 0. 5709099403610693 0. 6243701754824542 T T T

0. 5054810483661285 0. 4229809153902764 0. 6359196804627771 T T T

0. 5329595074435716 0. 5089237881418711 0. 7334168577908500 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5835745700675048 0. 5811187367478041 0. 4462868357955969 T T T

0. 5554691890378436 0. 4528679067036308 0. 4130290292829741 T T T

0. 4678971161879346 0. 5564577955143761 0. 3624958293306051 T T T

0. 4142979990379061 0. 4461843133241032 0. 4153513396991215 T T T

0. 5057224485058569 0. 6811272382203697 0. 3943540487387409 T T T

0. 4914275656084754 0. 3377904054150989 0. 3838797858321001 T T T

0. 4216778741265159 0. 4812826666690526 0. 5463489475896210 T T T

0. 5750289002684426 0. 4892676295843259 0. 5427487537267339 T T T

0. 4522011277822955 0. 6018422495212974 0. 4940462645610282 T T T

0. 4949765986689982 0. 3667127317904217 0. 5164818550948596 T T T

0. 4925450074491664 0. 5736698002390455 0. 6193444797478662 T T T

0. 5077170914000035 0. 4190113603498844 0. 6380595259209656 T T T

0. 5374645118590635 0. 5126676454145240 0. 7275733046798294 T T T

Au

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Au

13

Selective dynamics

Direct

0. 5814081643281028 0. 5822846269324771 0. 4548416286938419 T T T

0. 5570287862736052 0. 4543318819891837 0. 4159383817394513 T T T

0. 4772261279143777 0. 5559662522902329 0. 3534977008710456 T T T

0. 4161604659348086 0. 4566387748053344 0. 4210120350772470 T T T

0. 5041728636592069 0. 6796329207615344 0. 3985426150197711 T T T

0. 4853888013933627 0. 3448157950700548 0. 3823647869962912 T T T

0. 4191325315301171 0. 4766213091817022 0. 5551660796726736 T T T

0. 5767057360830066 0. 4862955683993135 0. 5472896373538845 T T T

0. 4440812973806700 0. 5900146910446367 0. 4857000131671043 T T T

0. 4948832494974482 0. 3663565483879410 0. 5158529492354802 T T T

0. 4929514824724137 0. 5775501053521381 0. 6116890805918089 T T T

0. 5090352516407464 0. 4133579124975242 0. 6397370010680916 T T T

0. 5418252418921341 0. 5161340929894038 0. 7183680905133514 T T T

Au

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Au

13

Selective dynamics

Direct

0. 5734805958719136 0. 5840663862293951 0. 4702797489410528 T T T

0. 5596457523630178 0. 4555120056506681 0. 4266537787866724 T T T

0. 4845511811625656 0. 5497982451040997 0. 3533155840296303 T T T

0. 4155885270753785 0. 4586337983053923 0. 4267395044015316 T T T

0. 5014987452712489 0. 6751800041269647 0. 3980363746638531 T T T

0. 4845534451949760 0. 3531377386484138 0. 3767192628270664 T T T

0. 4268053080440524 0. 4806736019825166 0. 5620371778108719 T T T

0. 5776257145243875 0. 4828793001747655 0. 5595357595769457 T T T

0. 4315161767396134 0. 5884989409268115 0. 4796669411845826 T T T

0. 4906196796917399 0. 3649941258245661 0. 5123429373624404 T T T

0. 5003068625447185 0. 5936864442697498 0. 5984419072937897 T T T

0. 5046125769639431 0. 3985402120355417 0. 6404014432018528 T T T

0. 5491954345524448 0. 5143996774231283 0. 6958295799197600 T T T

Au

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Au

13

Selective dynamics

Direct

0. 5746141313556379 0. 5793433320265109 0. 4680772906804407 T T T

0. 5616563048841172 0. 4512406614422417 0. 4207025464220138 T T T

0. 4873759772605126 0. 5543592246609848 0. 3594422435517046 T T T

0. 4183558438639281 0. 4569537173252485 0. 4335324656767554 T T T

0. 4991854432759979 0. 6794401719868688 0. 4148992268833211 T T T

0. 4814474002003664 0. 3471150303063553 0. 3790694531053234 T T T

0. 4352518373399619 0. 4842734264275350 0. 5697715154622003 T T T

0. 5772962780297064 0. 4780752108761845 0. 5554380368745626 T T T

0. 4260627660022180 0. 5851028705813803 0. 4819518731529868 T T T

0. 4938623157573971 0. 3645509642570275 0. 5111559552529741 T T T

0. 5110455966255358 0. 6139787045498863 0. 5862938501068484 T T T

0. 5080168778406247 0. 3875572597278776 0. 6413989305561287 T T T

0. 5258292275639960 0. 5180099110954615 0. 6782666122747685 T T T

Au

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Au

13

Selective dynamics

Direct

0. 5791778434287309 0. 5729805845857925 0. 4678884630577826 T T T

0. 5594373595434661 0. 4500324716610180 0. 4147296878690767 T T T

0. 4862706917791968 0. 5629012475253035 0. 3650192280385482 T T T

0. 4194409876449754 0. 4552054629490954 0. 4308461278318703 T T T

0. 5001185946790514 0. 6819466180731837 0. 4423013400797586 T T T

0. 4807162555514708 0. 3422687552671064 0. 3817277196676301 T T T

0. 4309999178555941 0. 4732865651830025 0. 5685926423917707 T T T

0. 5788424064594579 0. 4697569121870515 0. 5514480740941892 T T T

0. 4227307588790978 0. 5782558965742766 0. 4877383000740210 T T T

0. 4966152882633423 0. 3608124404897382 0. 5124690534322696 T T T

0. 5148610595787559 0. 6336356061398547 0. 5739320470370188 T T T

0. 5123180383420518 0. 3888968578514422 0. 6436740257018059 T T T

0. 5184707979948158 0. 5300212099464545 0. 6596332907243081 T T T

Au

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20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

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13

Selective dynamics

Direct

0. 5732400000000000 0. 5704040000000000 0. 4831110000000000 T T T

0. 5591870000000000 0. 4527240000000000 0. 4147630000000000 T T T

0. 4865430000000000 0. 5634900000000000 0. 3690220000000000 T T T

0. 4198210000000000 0. 4570910000000000 0. 4311980000000000 T T T

0. 4985870000000000 0. 6802230000000000 0. 4401380000000000 T T T

0. 4810850000000000 0. 3453080000000000 0. 3807080000000000 T T T

0. 4199530000000000 0. 4603240000000000 0. 5682240000000000 T T T

0. 5911040000000000 0. 4549610000000000 0. 5480400000000000 T T T

0. 4293310000000000 0. 5749130000000000 0. 5000820000000000 T T T

0. 4970220000000000 0. 3570870000000000 0. 5127170000000000 T T T

0. 5137550000000000 0. 6556500000000000 0. 5752810000000000 T T T

0. 5135830000000000 0. 3928100000000000 0. 6436570000000000 T T T

0. 5167890000000000 0. 5350160000000000 0. 6330590000000000 T T T

Pathway 26

Au

1.000000		
20.0000000000000000	0.0000000000000000	0.0000000000000000
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13

Selective dynamics

Direct

0.5721840000000000	0.5664030000000000	0.4077320000000000	T T T
0.5721840000000000	0.4335970000000000	0.4077320000000000	T T T
0.4278160000000000	0.5664030000000000	0.4077320000000000	T T T
0.4278160000000000	0.4335970000000000	0.4077320000000000	T T T
0.5000000000000000	0.6803250000000000	0.3889020000000000	T T T
0.5000000000000000	0.3196750000000000	0.3889020000000000	T T T
0.4298000000000000	0.5000000000000000	0.5280730000000000	T T T
0.5702000000000000	0.5000000000000000	0.5280730000000000	T T T
0.5000000000000000	0.6288900000000000	0.5141910000000000	T T T
0.5000000000000000	0.3711110000000000	0.5141910000000000	T T T
0.5000000000000000	0.5702320000000000	0.6314490000000000	T T T
0.5000000000000000	0.4297680000000000	0.6314490000000000	T T T
0.5000000000000000	0.5000000000000000	0.7438420000000000	T T T

Au

1.0000000000000000		
20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
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Au

13

Selective dynamics

Direct

0.5878929641750011	0.5698634798500430	0.4152245354362808	T T T
0.5582842843199733	0.4409290638443780	0.4039626078249025	T T T
0.4406721106236304	0.5604402974587980	0.4064241724272497	T T T
0.4147726494291667	0.4298803450615786	0.4155223018821618	T T T
0.5081184392855248	0.6746847620712987	0.3831494456901403	T T T
0.4942259765692711	0.3240186002555937	0.3842280376317155	T T T
0.4292144937050009	0.5016257196288489	0.5307808088694747	T T T
0.5704865549775134	0.4982001658849159	0.5304294324330089	T T T
0.5029840623946159	0.6287638400388518	0.5130114016952172	T T T
0.5019505680936583	0.3712745689105499	0.5130355206485642	T T T
0.4985254661895530	0.5719485685284168	0.6310762928591167	T T T
0.5005018943562091	0.4282723745324255	0.6311821806584166	T T T

0. 4923714413749428 0. 5000986666813355 0. 7419728091967169 T T T

Au

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Au

13

Selective dynamics

Direct

0. 6036315858387453 0. 5715274775912005 0. 4254719546229323 T T T

0. 5445133242229335 0. 4555339787183242 0. 4019085053331088 T T T

0. 4341934533869664 0. 5578564230458027 0. 4075345734753957 T T T

0. 4071384962874536 0. 4269650902709872 0. 4187274769468058 T T T

0. 5130521456193405 0. 6604059716843630 0. 3749741747778031 T T T

0. 4967799316670136 0. 3316622986087051 0. 3807488291869235 T T T

0. 4297957583685942 0. 4997491416438036 0. 5324870492177379 T T T

0. 5726234159978200 0. 4967952677700258 0. 5342664335608007 T T T

0. 5032407423975698 0. 6251777008777498 0. 5091274631032195 T T T

0. 5041423380217411 0. 3727473720091987 0. 5117551375376435 T T T

0. 4981794831165111 0. 5731199914346301 0. 6301153701257001 T T T

0. 5007983164084433 0. 4269560310474427 0. 6318833702573051 T T T

0. 4919119842201132 0. 5015037430743792 0. 7409991740779976 T T T

Au

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Au

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Selective dynamics

Direct

0. 6165859604304288 0. 5699005803986255 0. 4319379738849505 T T T

0. 5354815874711052 0. 4696381495056834 0. 4017281771721314 T T T

0. 4192322234553952 0. 5601499909549738 0. 4118714005334666 T T T

0. 4049121295066852 0. 4263193331137146 0. 4189811754749887 T T T

0. 5164291404453231 0. 6413409339944937 0. 3688653315021539 T T T

0. 5018144604957693 0. 3403119864322021 0. 3776917867583211 T T T

0. 4294889100907763 0. 4983199897775719 0. 5339505811208380 T T T

0. 5741417892173277 0. 4965926074336817 0. 5373548199229414 T T T

0. 5048398222040347 0. 6204841440040313 0. 5057527213059314 T T T

0. 5063606292877560 0. 3749688261019314 0. 5099533871859508 T T T

0. 4973595010630126 0. 5741124010849930 0. 6295429967079443 T T T

0. 5011220648181621 0. 4259559545959160 0. 6321069654141447 T T T

0. 4922327538760732 0. 5019055887831030 0. 7402621968353161 T T T

Au

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Au

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Selective dynamics

Direct

0. 6260665909470206 0. 5689988657068221 0. 4394752434145546 T T T

0. 5306981429391787 0. 4816662261624362 0. 4011481536075558 T T T

0. 4049933625196677 0. 5633602689425132 0. 4166153685757180 T T T

0. 4048997613741327 0. 4281685001039212 0. 4157690657645644 T T T

0. 5178247744128991 0. 6178359674047508 0. 3643711820852172 T T T

0. 5078337767806961 0. 3488711208246059 0. 3756695611694087 T T T

0. 4283992935685784 0. 4968168503450932 0. 5341485476280492 T T T

0. 5748325363890647 0. 4968535846375095 0. 5403193756896773 T T T

0. 5033384095130105 0. 6163853683733074 0. 5030010200704826 T T T

0. 5068092687817736 0. 3777342924593685 0. 5082570692269091 T T T

0. 4949342317367261 0. 5749885237336353 0. 6290046605233077 T T T

0. 5012715881920173 0. 4255079658726684 0. 6322821059962948 T T T

0. 4980992050678087 0. 5028129365446413 0. 7399381751369805 T T T

Au

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Au

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Selective dynamics

Direct

0. 6284320831927351 0. 5633468088128983 0. 4322227235790013 T T T

0. 5287603894875299 0. 4809423444215522 0. 3957362777389354 T T T

0. 4093032701645609 0. 5653398250257403 0. 4244136765707542 T T T

0. 4049419431377451 0. 4290155349285241 0. 4283216347135461 T T T

0. 5183223770151815 0. 6182304334166885 0. 3639023566270385 T T T

0. 5015166398403271 0. 3496192718892534 0. 3734724158304549 T T T

0. 4278673384687997 0. 5004391205659611 0. 5419431157584701 T T T

0. 5752735134520544 0. 4962804771520301 0. 5368356002101106 T T T

0. 5135124756456363 0. 6181906107225906 0. 5034194641545502 T T T

0. 5135772196034644 0. 3764803971862482 0. 5063098667759891 T T T

0. 5011187253482947 0. 5772786143710386 0. 6292404789512054 T T T

0. 5031529864803872 0. 4238470516805936 0. 6302011950758906 T T T

0. 4742220786943449 0. 5009900300924117 0. 7339806737485303 T T T

Au

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Au

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Selective dynamics

Direct

0. 6285808138526401 0. 5627357419199503 0. 4290552871892776 T T T

0. 5292209354345648 0. 4788381109476531 0. 3947863841653101 T T T

0. 4133569687185849 0. 5650360323892594 0. 4340243610095623 T T T

0. 4072246352690655 0. 4288764025156898 0. 4401134640747147 T T T

0. 5169889943213696 0. 6153061738807347 0. 3627479273191054 T T T

0. 4950964695220801 0. 3498495583666677 0. 3712606908908735 T T T

0. 4236980689586036 0. 5016856958673488 0. 5529106570044960 T T T

0. 5742486561371376 0. 4989213122934635 0. 5359863195744857 T T T

0. 5199432258688140 0. 6229107300928993 0. 5031847266785546 T T T

0. 5238093735098222 0. 3755112128204894 0. 5018283893724130 T T T

0. 5042403956636289 0. 5820960919335457 0. 6283140979239019 T T T

0. 5076627995042354 0. 4196014556158380 0. 6262307591428226 T T T

0. 4559297016727868 0. 4986320005731234 0. 7195564164378125 T T T

Au

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20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

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Au

13

Selective dynamics

Direct

0. 6421555234716402 0. 5388924880345274 0. 4397099362410276 T T T

0. 5243166743199956 0. 5003921346612576 0. 3830140857135156 T T T

0. 4093598978260660 0. 5666608517159786 0. 4490789812333918 T T T

0. 4250447103841435 0. 4318830009645321 0. 4550888400459238 T T T

0. 4894777256136967 0. 6291221345367236 0. 3580056395491739 T T T

0. 5119370013339616 0. 3667612500855790 0. 3721420736781750 T T T

0. 4123719833447002 0. 5032356371966366 0. 5681710425138949 T T T

0. 5643843236115581 0. 4863457497319875 0. 5364081541467665 T T T

0. 5348806531930661 0. 6129860278377061 0. 4856974971667692 T T T

0. 5294669506583687 0. 3578999864447984 0. 5082411965451313 T T T

0. 5114101080679533 0. 5890060933112805 0. 6150323622264672 T T T

0. 4993764655707377 0. 4088590508555651 0. 6272489594332475 T T T

0. 4458190390089840 0. 5079561228258386 0. 7021607033041046 T T T

Au

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20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

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Au

13

Selective dynamics

Direct

0. 6195298083685499 0. 4899602555345443 0. 4377184044129411 T T T

0. 5103958832810123 0. 5137036331104444 0. 3615339931884801 T T T

0. 4101310209143173 0. 5672240459636712 0. 4519436887262032 T T T

0. 4354662459669008 0. 4336075958552896 0. 4550109607355535 T T T

0. 4813499499072622 0. 6435978731527018 0. 3634579609086622 T T T

0. 5346713394632540 0. 3818694172606535 0. 3743245289809692 T T T

0. 4134631994511565 0. 5008331066695306 0. 5688807243453563 T T T

0. 5625482456346759 0. 4911003950744444 0. 5594899676281536 T T T

0. 5431846298935428 0. 6009659043628078 0. 4789137578948464 T T T

0. 5395957424170958 0. 3634815189723498 0. 5104372588904525 T T T

0. 5030221540577966 0. 6028108282914426 0. 6089036929128717 T T T

0. 4935862670663184 0. 3997753758984388 0. 6310223100874403 T T T

0. 4530565772031114 0. 5110705816661671 0. 6983622194755903 T T T

Au

1. 000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

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13

Selective dynamics

Direct

0. 5975700000000000 0. 4664650000000000 0. 4553690000000000 T T T

0. 5106690000000000 0. 5179360000000000 0. 3580170000000000 T T T

0. 4199170000000000 0. 5730040000000000 0. 4644950000000000 T T T

0. 4281990000000000 0. 4385650000000000 0. 4391180000000000 T T T

0. 4877530000000000 0. 6486490000000000 0. 3724400000000000 T T T

0. 5319870000000000 0. 3831870000000000 0. 3671740000000000 T T T

0. 4230230000000000 0. 4810340000000000 0. 5657340000000000 T T T

0. 5654360000000000 0. 5044930000000000 0. 5793980000000000 T T T

0. 5578330000000000 0. 5957230000000000 0. 4777280000000000 T T T

0. 5217390000000000 0. 3633420000000000 0. 5080500000000000 T T T

0. 4728470000000000 0. 6137600000000000 0. 5876850000000000 T T T

0. 5043200000000000 0. 3938950000000000 0. 6371360000000000 T T T

0. 4787090000000000 0. 5199480000000000 0. 6876550000000000 T T T

Pathway 27

Au

```
1.000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
```

13

Selective dynamics

Direct

```
0.4900460000000000 0.6390840000000000 0.5000000000000000 T T T
0.6311810000000000 0.6345790000000000 0.5000000000000000 T T T
0.5658930000000000 0.7480240000000000 0.5000000000000000 T T T
0.5610210000000000 0.5192460000000000 0.5000000000000000 T T T
0.4270120000000000 0.5180870000000000 0.5000000000000000 T T T
0.4943580000000000 0.4024630000000000 0.5000000000000000 T T T
0.3573640000000000 0.3976690000000000 0.5000000000000000 T T T
0.4296270000000000 0.2838050000000000 0.5000000000000000 T T T
0.2914460000000000 0.5136039999999999 0.5000000000000000 T T T
0.5656130000000000 0.2875150000000000 0.5000000000000000 T T T
0.3552510000000000 0.6325090000000000 0.5000000000000000 T T T
0.6324930000000000 0.4027530000000000 0.5000000000000000 T T T
0.6986940000000000 0.5206620000000000 0.5000000000000000 T T T
```

Au

```
1.0000000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
```

Au

13

Selective dynamics

Direct

```
0.4906769803462218 0.6386519220279149 0.5024574428713406 T T T
0.6318252732830726 0.6326477438936653 0.5011923040222337 T T T
0.5679193435928841 0.7433871195082298 0.5287945410071438 T T T
0.5603074698683000 0.5191486183370927 0.4861136088928701 T T T
0.4265476415460915 0.5184630024493824 0.4929502934142113 T T T
0.4938330522018272 0.4027819261783580 0.4960519032865632 T T T
0.3568946013578849 0.3986922809449822 0.5034525809372878 T T T
0.4295129600211665 0.2854182401155433 0.5139235408196234 T T T
0.2912226156908782 0.5148535216843898 0.5000481659560689 T T T
0.5655660445932738 0.2889807727834419 0.5089765169446506 T T T
0.3559269018344496 0.6333991978186178 0.4964936269851651 T T T
0.6322243005556358 0.4031835200428993 0.4931626017935163 T T T
```

0. 6975437198522471 0. 5203930427386542 0. 4763837784723459 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4903879092173856 0. 6368170780134119 0. 5032990365277357 T T T

0. 6315198525441934 0. 6277932111250880 0. 5049774437833900 T T T

0. 5689512316262009 0. 7313640690941662 0. 5537902761396082 T T T

0. 5581195511573124 0. 5199200630609885 0. 4686246243908628 T T T

0. 4250800034179270 0. 5184631954613261 0. 4819868606217325 T T T

0. 4938847806219328 0. 4036421054897093 0. 4901243553046543 T T T

0. 3571702036961743 0. 3992052393300702 0. 5034851088000428 T T T

0. 4319556979509356 0. 2889990920497110 0. 5249165354835578 T T T

0. 2910185108232461 0. 5151833399527880 0. 5009308792630518 T T T

0. 5681543695269810 0. 2956012518423307 0. 5238112067311926 T T T

0. 3557910070954127 0. 6337217148432024 0. 4926236887142170 T T T

0. 6324536508517351 0. 4074933662804251 0. 4926164842371979 T T T

0. 6955130735480994 0. 5217961034660168 0. 4588133440676397 T T T

Au

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Au

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Selective dynamics

Direct

0. 4906557059513434 0. 6333501276742109 0. 5034509328160623 T T T

0. 6297622464919638 0. 6142449108685749 0. 5136959707410932 T T T

0. 5716901780241946 0. 7164332951628057 0. 5685451610434068 T T T

0. 5547425121450367 0. 5207828473936299 0. 4481242252303377 T T T

0. 4229263735019883 0. 5189363838842654 0. 4709212032782872 T T T

0. 4940264844704098 0. 4060186464676300 0. 4863918652091124 T T T

0. 3575238224277704 0. 3998371700071761 0. 5023384759018089 T T T

0. 4350604738953456 0. 2928932902798311 0. 5293792589837516 T T T

0. 2914831361146892 0. 5158063855269540 0. 5021783957585760 T T T

0. 5707162436953210 0. 3071727691949090 0. 5388075766321386 T T T

0. 3561252931566385 0. 6346094893677788 0. 4912249159346052 T T T

0. 6312342856652975 0. 4176289813961620 0. 4994439142913463 T T T

0. 6940528675564576 0. 5222849714914223 0. 4454976931453628 T T T

Au

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Au

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Selective dynamics

Direct

0. 4908346575051723 0. 6302746320572953 0. 5040398215962489 T T T

0. 6246128898114189 0. 5906802842325514 0. 5264210132893473 T T T

0. 5791174001374344 0. 7041458759495181 0. 5703862465239445 T T T

0. 5504844752145300 0. 5222365013693331 0. 4329290307663493 T T T

0. 4205624834848750 0. 5193629645480159 0. 4652160888137301 T T T

0. 4947801378267951 0. 4093130166301943 0. 4850789003911811 T T T

0. 3581200863914915 0. 3998071794296991 0. 5016432961418151 T T T

0. 4392619780584377 0. 2956978581335639 0. 5298171003442362 T T T

0. 2916000239524258 0. 5156207442526238 0. 5038543241036145 T T T

0. 5745584502300635 0. 3188450366779653 0. 5457473869929538 T T T

0. 3561776409254867 0. 6350872618426270 0. 4917186135966044 T T T

0. 6286170304168969 0. 4344929691147710 0. 5098104902947926 T T T

0. 6912738510333619 0. 5244354392136041 0. 4333385658831460 T T T

Au

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Au

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Selective dynamics

Direct

0. 4894888971186747 0. 6312135025373065 0. 5049936184316053 T T T

0. 6107624992772880 0. 5681627676520865 0. 5461913935839547 T T T

0. 5942137651316611 0. 6973478239815134 0. 5523832889404251 T T T

0. 5484608079746018 0. 5258737990179496 0. 4292347703727860 T T T

0. 4193569960689184 0. 5203456257254999 0. 4645322238386194 T T T

0. 4964307025999693 0. 4118688655103787 0. 4835099794988373 T T T

0. 3597593122707852 0. 4003597242254476 0. 5017285454486221 T T T

0. 4423536277166368 0. 2967817810714651 0. 5266867200305487 T T T

0. 2915043199887534 0. 5149882602322902 0. 5072096378789475 T T T

0. 5762216050395053 0. 3225091612418272 0. 5462165765164035 T T T

0. 3547899033216812 0. 6351697910243643 0. 4940645057687049 T T T

0. 6310814137322749 0. 4367711140260642 0. 5065944377216911 T T T

0. 6855771259789114 0. 5386064686977844 0. 4366542946974408 T T T

Au

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Selective dynamics

Direct

0. 4879284479961464 0. 6336542117854619 0. 5053711773955329 T T T

0. 5948638190498994 0. 5556207859828801 0. 5596615615919646 T T T

0. 6095784965734314 0. 6827174695583694 0. 5293162466780208 T T T

0. 5479276824883406 0. 5291263220045476 0. 4295501627387224 T T T

0. 4190624009642753 0. 5211594354217777 0. 4657464373301661 T T T

0. 4979486263748502 0. 4144100914682283 0. 4850346074616960 T T T

0. 3613395863304293 0. 4009123853710257 0. 5027377695467750 T T T

0. 4447879628564616 0. 2973882237674210 0. 5250547645075073 T T T

0. 2911183785032039 0. 5145166953547713 0. 5081936201076150 T T T

0. 5781273887464751 0. 3233835887592457 0. 5436833089338505 T T T

0. 3534300846655125 0. 6353740579081807 0. 4939625094895578 T T T

0. 6337836201134130 0. 4377058623263377 0. 5028462055196719 T T T

0. 6801024560232538 0. 5540309278015340 0. 4488415547981851 T T T

Au

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Au

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Selective dynamics

Direct

0. 4936865767796345 0. 6478033510084971 0. 4825943479264037 T T T

0. 5613999218465330 0. 5437265611086303 0. 5581510687524887 T T T

0. 6176575624948909 0. 6660564754142247 0. 5348911307603675 T T T

0. 5377252439820340 0. 5297923580383495 0. 4213191278238234 T T T

0. 4293221751581847 0. 5282246924361472 0. 5173795048826024 T T T

0. 5074356177598884 0. 4213375766345716 0. 5401490301906666 T T T

0. 3676758933435682 0. 4066781000098315 0. 5262355294052282 T T T

0. 4499150686320703 0. 3012258496203114 0. 5216435572743093 T T T

0. 2950612921418979 0. 5163536911802956 0. 4969273561334447 T T T

0. 5853847967274043 0. 3133086689120891 0. 5111441749083021 T T T

0. 3629668946974586 0. 6281924444875839 0. 4580808348654389 T T T

0. 6261691663457847 0. 4345876853950908 0. 4696945386930395 T T T

0. 6655998115706493 0. 5627125450427646 0. 4617877575587817 T T T
Au
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Selective dynamics

Direct

0. 5104866955950417 0. 6408181433182339 0. 4594357804596358 T T T
0. 5528652078829734 0. 5542197719477117 0. 5674200864295086 T T T
0. 6132360242196362 0. 6763351890535079 0. 5387935896668159 T T T
0. 5233493188542208 0. 5122209356851707 0. 4192691003070472 T T T
0. 4225651148466348 0. 5295222178062547 0. 5762772641492663 T T T
0. 5090294241303056 0. 4292053411111313 0. 5427163500749012 T T T
0. 3730166183136193 0. 4240180735109062 0. 5000945962364777 T T T
0. 4452030732845138 0. 3140379910521661 0. 5030099224039279 T T T
0. 2950464599038350 0. 5296934284301736 0. 5172345844603395 T T T
0. 5804268142506407 0. 3191578305622935 0. 5052456599207991 T T T
0. 4013920172777572 0. 5659357047900517 0. 4417370119813790 T T T
0. 6277205690566989 0. 4367704741986406 0. 4626587639268667 T T T
0. 6456626610303320 0. 5680657919346926 0. 4661088655980325 T T T

\$POSCAR 1 Au

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Selective dynamics

Direct

0. 5113820000000000 0. 6349200000000000 0. 4510790000000000 T T T
0. 5452720000000000 0. 5669689999999999 0. 5720480000000000 T T T
0. 6221110000000000 0. 6691930000000000 0. 5210170000000000 T T T
0. 5005080000000000 0. 4964180000000000 0. 4351510000000000 T T T
0. 4220160000000000 0. 5123770000000000 0. 5740980000000000 T T T
0. 5309460000000000 0. 4331090000000000 0. 5793290000000000 T T T
0. 3757970000000000 0. 4386180000000000 0. 4608600000000000 T T T
0. 4820950000000000 0. 3612660000000000 0. 4659650000000000 T T T
0. 2933060000000000 0. 5235620000000000 0. 5264870000000000 T T T
0. 5838940000000000 0. 3121030000000000 0. 5404420000000000 T T T
0. 3911040000000000 0. 5816470000000000 0. 4530800000000000 T T T
0. 6137950000000000 0. 4195970000000000 0. 4637740000000000 T T T
0. 6277740000000001 0. 5502220000000000 0. 4566690000000000 T T T

Pathway 28

\$POSCAR 1 Au

1.000000

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Selective dynamics

Direct

0.4900460000000000	0.6390840000000000	0.5000000000000000	T T T
0.6311810000000000	0.6345790000000000	0.5000000000000000	T T T
0.5658930000000000	0.7480240000000000	0.5000000000000000	T T T
0.5610210000000000	0.5192460000000000	0.5000000000000000	T T T
0.4270120000000000	0.5180870000000000	0.5000000000000000	T T T
0.4943580000000000	0.4024630000000000	0.5000000000000000	T T T
0.3573640000000000	0.3976690000000000	0.5000000000000000	T T T
0.4296270000000000	0.2838050000000000	0.5000000000000000	T T T
0.2914460000000000	0.5136039999999999	0.5000000000000000	T T T
0.5656130000000000	0.2875150000000000	0.5000000000000000	T T T
0.3552510000000000	0.6325090000000000	0.5000000000000000	T T T
0.6324930000000000	0.4027530000000000	0.5000000000000000	T T T
0.6986940000000000	0.5206620000000000	0.5000000000000000	T T T

Au

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Selective dynamics

Direct

0.4895631749019867	0.6388059939350281	0.5041176196206701	T T T
0.6311702456701704	0.6333284988090542	0.5078956825288435	T T T
0.5650825016414992	0.7399003027361200	0.5451293507745263	T T T
0.5606313086488574	0.5198294635848050	0.4898314844759536	T T T
0.4267976120968073	0.5183012161026692	0.4918306048823326	T T T
0.4944988257109024	0.4031059462008992	0.4967822936553817	T T T
0.3572765758211641	0.3986062107921302	0.5013615924486491	T T T
0.4302248938205683	0.2853808949219014	0.5107917853784930	T T T
0.2915023374664236	0.5145995703392831	0.4928840102367086	T T T
0.5663471278003629	0.2889904228431762	0.5037477004229992	T T T
0.3562470653803419	0.6329293076283333	0.4828610180631868	T T T
0.6328977354622465	0.4039970288904616	0.4928757367373019	T T T

0. 6977600743013014 0. 5222256219387671 0. 4798911207749662 T T T

Au

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Au

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Selective dynamics

Direct

0. 4881825902995015 0. 6410139935148811 0. 4960366376519527 T T T

0. 6318234445050210 0. 6345909310692619 0. 5038449506204543 T T T

0. 5603994267636480 0. 7106328596016165 0. 5826822589774800 T T T

0. 5605665911511820 0. 5222006409489915 0. 4871502216210091 T T T

0. 4266970963166899 0. 5197048480767065 0. 4893415784710839 T T T

0. 4952848057333384 0. 4059822285466446 0. 5013805411363612 T T T

0. 3576682665389970 0. 4018211826702265 0. 5081776519184630 T T T

0. 4313583519624422 0. 2889325221658865 0. 5179640795425314 T T T

0. 2920940159500220 0. 5176371556708310 0. 4911277458472448 T T T

0. 5675489043220503 0. 2924744974955056 0. 5065632602050248 T T T

0. 3581265814662433 0. 6324150387229409 0. 4606526660482056 T T T

0. 6334843759096935 0. 4073374082113492 0. 4893466863727937 T T T

0. 6967650471778750 0. 5252571914018791 0. 4657317215874014 T T T

Au

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Selective dynamics

Direct

0. 4891218151543970 0. 6453203569114975 0. 4791285444206443 T T T

0. 6318577110168266 0. 6417868266991511 0. 4942353580953984 T T T

0. 5503904303398568 0. 6660046098191360 0. 5958634266237528 T T T

0. 5623198927668067 0. 5265928420574674 0. 4971958377076722 T T T

0. 4278753902315007 0. 5241848204621155 0. 4971751388817872 T T T

0. 4969233804335119 0. 4102370973576111 0. 5095759875423088 T T T

0. 3593299173116430 0. 4061017917614466 0. 5139866485875950 T T T

0. 4320177379096500 0. 2926129384587154 0. 5179111613945838 T T T

0. 2932942363974690 0. 5214331034049992 0. 4937972341404787 T T T

0. 5676180198743266 0. 2954312805982792 0. 5040710586457124 T T T

0. 3600415416036206 0. 6309763278380556 0. 4475899116004067 T T T

0. 6335135019066929 0. 4106972312749966 0. 4874073284995378 T T T

0. 6956959245807772 0. 5286212728835842 0. 4620623638601312 T T T

Au

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Au

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Selective dynamics

Direct

0. 4944096977019293 0. 6469620542871576 0. 4594739129294466 T T T

0. 6286596609020262 0. 6471501395807807 0. 4956893771699028 T T T

0. 5270859505212211 0. 6274437606093952 0. 5903056712588055 T T T

0. 5669055058885506 0. 5272198871185477 0. 5066890322714768 T T T

0. 4320128146383944 0. 5324873621983913 0. 5129313001442368 T T T

0. 4992079290689133 0. 4130046234913574 0. 5167482589826859 T T T

0. 3627358630068420 0. 4121631349849455 0. 5182419748782876 T T T

0. 4316786857244287 0. 2967891843057754 0. 5161037830173602 T T T

0. 2968553345298433 0. 5272708713000265 0. 5001570620354514 T T T

0. 5675069794894961 0. 2971225775165011 0. 5005112238071771 T T T

0. 3650189743358795 0. 6282733356225724 0. 4399693872366765 T T T

0. 6340694776506042 0. 4119756178058289 0. 4823986123087775 T T T

0. 6938526313604303 0. 5321379559972529 0. 4607804039597282 T T T

Au

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Au

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Selective dynamics

Direct

0. 5103663906978995 0. 6538677143237810 0. 4444084302476160 T T T

0. 6304972015434902 0. 6511145458107723 0. 5090507101790410 T T T

0. 5123772154930682 0. 6290369476725237 0. 5823252242725788 T T T

0. 5589371625775789 0. 5310069763424636 0. 5013228003948039 T T T

0. 4290362924842119 0. 5281304713289277 0. 5407049742520921 T T T

0. 4998076901342794 0. 4124887995834188 0. 5231176327385617 T T T

0. 3613940321135591 0. 4099318361558978 0. 5223198468959686 T T T

0. 4331683646231531 0. 2970103573384632 0. 5231704058790878 T T T

0. 2986301209651537 0. 5260208108240182 0. 4978766807220441 T T T

0. 5660973381122766 0. 2983611807934888 0. 4885938775478155 T T T

0. 3876208734383399 0. 6090645005963014 0. 4386316133906187 T T T

0. 6276503556936381 0. 4163185335110838 0. 4726106688401383 T T T

0. 6844165492815608 0. 5376479128771930 0. 4558671346395172 T T T

Au

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Au

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Selective dynamics

Direct

0. 5218443705638930 0. 6637534568023271 0. 4384515173654223 T T T

0. 6332077165537022 0. 6600692893799888 0. 5155601651396737 T T T

0. 5166623887437591 0. 6193394196019029 0. 5779613570225708 T T T

0. 5390971397080340 0. 5328075043550279 0. 4754739012363113 T T T

0. 4254505040341964 0. 5222961832113638 0. 5632853870504856 T T T

0. 4977026793262087 0. 4132585249568402 0. 5247160699506042 T T T

0. 3588022897559446 0. 4087932552403073 0. 5232745060983488 T T T

0. 4328147077289591 0. 2972395174607033 0. 5276340556217572 T T T

0. 3040718264769915 0. 5258078626761252 0. 4904689926577589 T T T

0. 5647173776716857 0. 3002834096788824 0. 4876212373762679 T T T

0. 4110543907595623 0. 5923816965304444 0. 4437870400571205 T T T

0. 6219134865820855 0. 4205560022733758 0. 4703683158744869 T T T

0. 6726607092478359 0. 5434144649856967 0. 4613974545490677 T T T

Au

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Au

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Selective dynamics

Direct

0. 5237970447164166 0. 6552947138965157 0. 4502061062292473 T T T

0. 6316783222107963 0. 6723216747866859 0. 5296268890930896 T T T

0. 5460427570839046 0. 5689836170143960 0. 5663790136014412 T T T

0. 5261775104760111 0. 5203459480470890 0. 4349638296381916 T T T

0. 4200359115725549 0. 5300290428277863 0. 5608067369341432 T T T

0. 5035332423322513 0. 4258229619063859 0. 5386526686248084 T T T

0. 3601530521152015 0. 4135673318901737 0. 5216710821130396 T T T

0. 4363131700184206 0. 3067391964948701 0. 5333369096983704 T T T

0. 3006895394830870 0. 5288380820773441 0. 4905903443674107 T T T

0. 5663775299560704 0. 3086808411190788 0. 4980271792246950 T T T

0. 4086444551854883 0. 5904289742812495 0. 4357426696583578 T T T

0. 6209240762026289 0. 4257790828618037 0. 4647758083690293 T T T

0. 6556329762115196 0. 5531691203610398 0. 4752207624480759 T T T
 Au
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Au

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Selective dynamics

Direct

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 0. 6246124867574695 0. 6703737033592997 0. 5299308894075477 T T T
 0. 5494969156929609 0. 5601976042869165 0. 5697077296466880 T T T
 0. 5158710670675728 0. 4998268639692399 0. 4267239756143935 T T T
 0. 4190773010240759 0. 5346000417822752 0. 5769455474530740 T T T
 0. 5077262486254598 0. 4322130396886016 0. 5550490336495955 T T T
 0. 3823288749864653 0. 4389944406069915 0. 4820626074468151 T T T
 0. 4411225797147352 0. 3226608358135031 0. 5020617323869837 T T T
 0. 2964980617696589 0. 5380006563693271 0. 5116963313056336 T T T
 0. 5730463385985647 0. 3145764935179270 0. 5261489426308756 T T T
 0. 4043039741563704 0. 5758653078307967 0. 4394543342240074 T T T
 0. 6215347371730400 0. 4233333259471881 0. 4654453905371357 T T T
 0. 6420418975517093 0. 5535956831189291 0. 4659143733032775 T T T

\$POSCAR 1 Au

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Selective dynamics

Direct

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 0. 6299070000000000 0. 6636320000000000 0. 5181080000000000 T T T
 0. 5468430000000000 0. 5672640000000000 0. 5707560000000000 T T T
 0. 5018740000000000 0. 4940120000000000 0. 4353540000000000 T T T
 0. 4209900000000000 0. 5189230000000000 0. 5715860000000000 T T T
 0. 5256520000000000 0. 4346320000000000 0. 5824270000000000 T T T
 0. 3738430000000000 0. 4434110000000000 0. 4598970000000000 T T T
 0. 4759760000000000 0. 3611570000000000 0. 4704760000000000 T T T
 0. 2941750000000000 0. 5346730000000000 0. 5203220000000000 T T T
 0. 5733770000000000 0. 3098160000000000 0. 5492410000000000 T T T
 0. 3964860000000000 0. 5851290000000000 0. 4474270000000000 T T T
 0. 6104510000000000 0. 4128110000000000 0. 4695890000000000 T T T
 0. 6311290000000001 0. 5422380000000000 0. 4582000000000000 T T T

Pathway 29

\$POSCAR 1 Au

1.000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.4900460000000000	0.6390840000000000	0.5000000000000000	T T T
0.6311810000000000	0.6345790000000000	0.5000000000000000	T T T
0.5658930000000000	0.7480240000000000	0.5000000000000000	T T T
0.5610210000000000	0.5192460000000000	0.5000000000000000	T T T
0.4270120000000000	0.5180870000000000	0.5000000000000000	T T T
0.4943580000000000	0.4024630000000000	0.5000000000000000	T T T
0.3573640000000000	0.3976690000000000	0.5000000000000000	T T T
0.4296270000000000	0.2838050000000000	0.5000000000000000	T T T
0.2914460000000000	0.5136039999999999	0.5000000000000000	T T T
0.5656130000000000	0.2875150000000000	0.5000000000000000	T T T
0.3552510000000000	0.6325090000000000	0.5000000000000000	T T T
0.6324930000000000	0.4027530000000000	0.5000000000000000	T T T
0.6986940000000000	0.5206620000000000	0.5000000000000000	T T T

Au

1.0000000000000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Au

13

Selective dynamics

Direct

0.4913479448815718	0.6370495815447049	0.5146519875078865	T T T
0.6279856756276769	0.6339257820770147	0.4894315511582084	T T T
0.5550962128275275	0.7400879987214454	0.4624609116716570	T T T
0.5626196742837423	0.5186382900459404	0.5221544489779019	T T T
0.4277961163831661	0.5176415716581583	0.5208050592267878	T T T
0.4956021308723456	0.4021837092250725	0.5159930578076832	T T T
0.3587048043886751	0.3994927888871992	0.5008566441038517	T T T
0.4300509886638808	0.2858114656654944	0.4931912166595037	T T T
0.2941447606824505	0.5157297663189506	0.4942689420896860	T T T
0.5658570225314283	0.2898506669818814	0.4889736882597311	T T T
0.3588989521334614	0.6329557595306564	0.4974347569544357	T T T
0.6333424017611933	0.4041363669605410	0.4983520709924765	T T T

0. 6985523149628136 0. 5224957624965815 0. 5014256645902089 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4957968751513793 0. 6344079076251495 0. 5437807657242378 T T T

0. 6229395465142611 0. 6351449151878270 0. 4894797198748968 T T T

0. 5290082572060747 0. 7196284018153963 0. 4470403479432191 T T T

0. 5652726477468840 0. 5172476018718980 0. 5319979924253869 T T T

0. 4296812163122035 0. 5174233066489837 0. 5313511049460257 T T T

0. 4966556958030397 0. 4020586872424204 0. 5222301319739224 T T T

0. 3597729767722683 0. 4042872594423484 0. 4984496645598380 T T T

0. 4284979643598584 0. 2888993258508094 0. 4922013324817092 T T T

0. 3007368008939421 0. 5242202403851024 0. 4882507735223172 T T T

0. 5642754047028512 0. 2919519646097112 0. 4841975058540361 T T T

0. 3767762956781922 0. 6341050235582281 0. 4813834413941441 T T T

0. 6334074723127654 0. 4055667362585371 0. 4938610695432182 T T T

0. 6971778465461680 0. 5250581304305455 0. 4957761497571517 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4960037058594751 0. 6337469336185599 0. 5625450866001693 T T T

0. 6222708982477653 0. 6419539849313145 0. 5072316177649306 T T T

0. 5121862743354397 0. 6868029393473039 0. 4360039714859507 T T T

0. 5650482289227132 0. 5201479476419328 0. 5326050276436487 T T T

0. 4294908078394025 0. 5180127552701932 0. 5401940889485004 T T T

0. 4985942457190878 0. 4042026888380251 0. 5231204477016901 T T T

0. 3599445610553373 0. 4092618478912786 0. 4996236514369912 T T T

0. 4287575968709206 0. 2945501651879336 0. 4939610483279573 T T T

0. 3040673614931991 0. 5328872634130295 0. 4870863501666288 T T T

0. 5646768582319530 0. 2922959808705992 0. 4812920796896135 T T T

0. 3955877990309774 0. 6280665169907678 0. 4638434862239723 T T T

0. 6312196729194525 0. 4091012677484446 0. 4869495804406566 T T T

0. 6921509894742131 0. 5289692033697998 0. 4855435635694526 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 4976420537355379 0. 6324538438030156 0. 5752503574567899 T T T

0. 6292629475150707 0. 6483652382376173 0. 5281999091573838 T T T

0. 5248733726796323 0. 6569286763648167 0. 4405005997058078 T T T

0. 5575066239322923 0. 5292958153560969 0. 5114517771289029 T T T

0. 4252133120455653 0. 5214006932822640 0. 5449208835301722 T T T

0. 4972627215512083 0. 4094809476882120 0. 5201860364724724 T T T

0. 3580762363692321 0. 4100395416886264 0. 5058132274336394 T T T

0. 4291089106484491 0. 2965511785657542 0. 5047845722733911 T T T

0. 3015967153721791 0. 5307986139647519 0. 4837015840761875 T T T

0. 5645703757152629 0. 2971557633695285 0. 4806280191908658 T T T

0. 4006580137232564 0. 6154307532929646 0. 4489130774893897 T T T

0. 6276556306336106 0. 4155851136529969 0. 4793811617119772 T T T

0. 6865720860786726 0. 5365133124703471 0. 4762687943732580 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5113281111206714 0. 6172054813866061 0. 5802120673639557 T T T

0. 6338266633011215 0. 6605732925889548 0. 5326175837098860 T T T

0. 5309533499869031 0. 6638589277527731 0. 4441130108745289 T T T

0. 5402595923736271 0. 5315560949551221 0. 4786250104988309 T T T

0. 4215042798908985 0. 5196916474275104 0. 5595838868870212 T T T

0. 4949779225569167 0. 4111491523426577 0. 5216767051687923 T T T

0. 3565101092845379 0. 4103085687881791 0. 5077701293085490 T T T

0. 4279672900624298 0. 2969567110592282 0. 5109903314124552 T T T

0. 3055406472287384 0. 5298304239309169 0. 4779239250698586 T T T

0. 5628500116053268 0. 2994967745045570 0. 4819928709252784 T T T

0. 4167865680076137 0. 5972732656286138 0. 4443416686185792 T T T

0. 6231080509828921 0. 4195870168547187 0. 4772022955546971 T T T

0. 6743864035982797 0. 5425121340447012 0. 4829505146077956 T T T
Au
1. 000000000000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5375371681485273 0. 5860572054154540 0. 5761708648696565 T T T
0. 6368450058108469 0. 6747397972834738 0. 5413275740336679 T T T
0. 5323978832402922 0. 6595801822476012 0. 4544813377828379 T T T
0. 5290116099706851 0. 5233443619863212 0. 4489447832317736 T T T
0. 4224137140127640 0. 5239737670341248 0. 5554690353083652 T T T
0. 4965536469546343 0. 4141639934323118 0. 5275155955621698 T T T
0. 3571001736947358 0. 4119339390099376 0. 5082507026040380 T T T
0. 4283503156385121 0. 2994747563184378 0. 5144829786546503 T T T
0. 3052361812395963 0. 5311079197690275 0. 4788909213541648 T T T
0. 5632370206110973 0. 3027615856254116 0. 4866584954150823 T T T
0. 4150924741990775 0. 5987105253686440 0. 4373609755611189 T T T
0. 6216002829604260 0. 4237501288068854 0. 4735946374025145 T T T
0. 6546235235186807 0. 5504013292423996 0. 4968520982201134 T T T

Au

1. 000000000000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5402021444133921 0. 5639169552858135 0. 5746083692362917 T T T
0. 6315269865815049 0. 6655113964372366 0. 5480588871068451 T T T
0. 5279309540660611 0. 6518397847433021 0. 4629949699819025 T T T
0. 5288680128398575 0. 5191797486162697 0. 4316007961872796 T T T
0. 4094496317544047 0. 5393316833283881 0. 5605964236529812 T T T
0. 4994375638799372 0. 4366269159130035 0. 5471023889468756 T T T
0. 3630618098663250 0. 4211355224001890 0. 5078643566213215 T T T
0. 4483347740581463 0. 3200753482411920 0. 5076784644150186 T T T
0. 2980718507982980 0. 5355727295551457 0. 4804144198493616 T T T
0. 5753542672108565 0. 2926968648341561 0. 4825076846786245 T T T
0. 4130738574979299 0. 5912406580528097 0. 4327165977301873 T T T
0. 6134194329661221 0. 4187083109955837 0. 4703831896745868 T T T

0. 6512677140670466 0. 5441635709451610 0. 4934734519187989 T T T
Au

1. 0000000000000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5328815144930317 0. 5807418229790875 0. 5875569739723707 T T T
0. 6326376742354629 0. 6628113027518230 0. 5435308251692291 T T T
0. 5290258550586425 0. 6397162795942654 0. 4591077398575765 T T T
0. 5234594929560162 0. 5073234987752715 0. 4241881942800554 T T T
0. 4041936499836954 0. 5483431074741808 0. 5693038458269597 T T T
0. 5033181025195093 0. 4530421200889949 0. 5565219868556909 T T T
0. 3771360918131613 0. 4322390967842249 0. 4980830102190882 T T T
0. 4691297103625366 0. 3376094656251168 0. 4962771231230724 T T T
0. 2946925582522756 0. 5382390289898595 0. 4868978913875566 T T T
0. 5828799330205177 0. 2771094417176585 0. 4705871980346956 T T T
0. 4115341217530035 0. 5816059907364434 0. 4332366971501727 T T T
0. 6046395592875270 0. 4075111360277882 0. 4727627865734647 T T T
0. 6344707362644848 0. 5337071908252078 0. 5019457275501357 T T T

\$POSCAR 1 Au

1. 000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

13

Selective dynamics

Direct

0. 5274000000000000 0. 5985390000000000 0. 5875939999999999 T T T
0. 6297420000000000 0. 6651640000000000 0. 5273409999999999 T T T
0. 5320930000000000 0. 6185090000000000 0. 4446910000000000 T T T
0. 5121380000000000 0. 4836350000000000 0. 4271920000000000 T T T
0. 4031220000000000 0. 5528980000000000 0. 5771350000000000 T T T
0. 5075740000000000 0. 4642130000000000 0. 5661670000000000 T T T
0. 3843700000000000 0. 4425240000000000 0. 4881710000000000 T T T
0. 4804250000000000 0. 3537670000000000 0. 4789220000000000 T T T
0. 2922520000000000 0. 5412220000000000 0. 4989390000000000 T T T
0. 5856050000000000 0. 2735070000000000 0. 4711600000000000 T T T
0. 4078140000000000 0. 5728680000000000 0. 4342320000000000 T T T
0. 6118700000000000 0. 4020400000000000 0. 4899840000000000 T T T
0. 6255940000000000 0. 5311129999999999 0. 5084720000000000 T T T

Pathway 30

\$POSCAR 1 Au

1.000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.5669720000000000	0.5618430000000000	0.5000000000000000	T T T
0.7022180000000000	0.5622530000000000	0.5000000000000000	T T T
0.6335700000000000	0.6794410000000000	0.5000000000000000	T T T
0.6374700000000000	0.4439330000000000	0.5000000000000000	T T T
0.5000000000000000	0.4455030000000000	0.5000000000000000	T T T
0.5706300000000000	0.3296890000000000	0.5000000000000000	T T T
0.4293700000000000	0.3296890000000000	0.5000000000000000	T T T
0.5000000000000000	0.2176350000000000	0.5000000000000000	T T T
0.3625300000000000	0.4439330000000000	0.5000000000000000	T T T
0.4330280000000000	0.5618430000000000	0.5000000000000000	T T T
0.2977820000000000	0.5622530000000000	0.5000000000000000	T T T
0.3664300000000000	0.6794410000000000	0.5000000000000000	T T T
0.5000000000000000	0.6825460000000000	0.5000000000000000	T T T

Au

1.0000000000000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Au

13

Selective dynamics

Direct

0.5667722294643071	0.5616077982696430	0.5085486877238310	T T T
0.7011009320792136	0.5617617189108353	0.4914335373253472	T T T
0.6342309623381938	0.6786924520462499	0.5074664912647799	T T T
0.6342104456519735	0.4457264585848550	0.4789801000443071	T T T
0.4994951735496097	0.4454624578673261	0.5057473750682344	T T T
0.5695973117196276	0.3308348204882212	0.4870952876352877	T T T
0.4296178880057775	0.3291061223948283	0.5046364454883826	T T T
0.5024825789001238	0.2181733824205129	0.5037998921214190	T T T
0.3624495189144381	0.4434081276612761	0.5046522267790986	T T T
0.4329108435938524	0.5618582434021958	0.5109805471668849	T T T
0.2985607896404585	0.5620371901424749	0.4977819743667518	T T T
0.3680001551751604	0.6787693456616934	0.4915831211470493	T T T

0. 5005717092876412 0. 6825628055091389 0. 5072948521890112 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5661261716724199 0. 5604669010067943 0. 5200771621816515 T T T

0. 6988908269800049 0. 5581767822424506 0. 4915826484734319 T T T

0. 6362967221410080 0. 6758831089938393 0. 5122012705463765 T T T

0. 6246077460720333 0. 4520435479290523 0. 4584920956996715 T T T

0. 4983679480043463 0. 4452003721657564 0. 5137972391444444 T T T

0. 5686102281434586 0. 3349541017789204 0. 4782102566068744 T T T

0. 4302031669325458 0. 3283724003674336 0. 5068698506352858 T T T

0. 5094716789165600 0. 2212539086578477 0. 5073916155912895 T T T

0. 3617249344833436 0. 4423363634461621 0. 5067640988855076 T T T

0. 4319566811939607 0. 5615565167259825 0. 5194679804337893 T T T

0. 2998197185861920 0. 5613764897437629 0. 4921858918143808 T T T

0. 3715864543035212 0. 6768187800784564 0. 4837216783559793 T T T

0. 5023383083406884 0. 6815615553233527 0. 5092387974013910 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5652510229372678 0. 5589891974662601 0. 5322188767298306 T T T

0. 6951020768908552 0. 5508259580248891 0. 4920727948221990 T T T

0. 6395824610826633 0. 6709768962126366 0. 5142130082676678 T T T

0. 6097665873845687 0. 4610377113022655 0. 4437557224120106 T T T

0. 4971092594257697 0. 4447673405849127 0. 5243440578002261 T T T

0. 5696069718872283 0. 3410299065351984 0. 4756338543362628 T T T

0. 4313670759148950 0. 3283158421292050 0. 5059329610705191 T T T

0. 5178933361877565 0. 2260743046731989 0. 5095357202954699 T T T

0. 3613097663360545 0. 4416444025958776 0. 5053106419250414 T T T

0. 4308224388501345 0. 5612971754374552 0. 5249165093579867 T T T

0. 3009342016205090 0. 5609920581790940 0. 4878455819946348 T T T

0. 3758357700733351 0. 6745493583695525 0. 4773087297597678 T T T

0. 5054196186363075 0. 6795006740347810 0. 5069121284557169 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5642778986950735 0. 5576647440251681 0. 5424946527242875 T T T

0. 6900561388286690 0. 5405690606909779 0. 4924061821291153 T T T

0. 6431949915070574 0. 6644025503847064 0. 5139480015770825 T T T

0. 5926968483770229 0. 4708951166692377 0. 4347984767846188 T T T

0. 4957051434960366 0. 4443478798996562 0. 5348841942407172 T T T

0. 5725319162512902 0. 3489680233139731 0. 4756896563438669 T T T

0. 4334728769443590 0. 3291982607085615 0. 5040285336055303 T T T

0. 5264239548051173 0. 2322749808052925 0. 5094655687024624 T T T

0. 3612685835535865 0. 4412623841369933 0. 5039824480051952 T T T

0. 4300161333127705 0. 5608888598614383 0. 5277473779176821 T T T

0. 3017295686372011 0. 5606811355518544 0. 4845674370245195 T T T

0. 3795560036789210 0. 6724534117274310 0. 4731584290779100 T T T

0. 5090705288154503 0. 6763944184195464 0. 5028296287695987 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5632095774545928 0. 5563099351420739 0. 5508038209498547 T T T

0. 6835180130986516 0. 5283121001556100 0. 4923641059631876 T T T

0. 6465950461286742 0. 6564500624616905 0. 5129693102271360 T T T

0. 5758703213107753 0. 4804515615300629 0. 4303087161102073 T T T

0. 4938742140872352 0. 4438051397244712 0. 5437411863945831 T T T

0. 5775058283704477 0. 3587525736854128 0. 4775808462728205 T T T

0. 4359706791876694 0. 3305803696991403 0. 5017306531624095 T T T

0. 5348477521313929 0. 2401184729519712 0. 5088009303469049 T T T

0. 3613355858267037 0. 4410023029981233 0. 5022192614193242 T T T

0. 4297147814682077 0. 5601071910808857 0. 5279488740168574 T T T

0. 3021348716209439 0. 5605612381684125 0. 4820222626701396 T T T

0. 3826878294663006 0. 6708792921205232 0. 4705375606993751 T T T

0. 5127360865610983 0. 6726705868562394 0. 4989730584798449 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5621614713489962 0. 5552783205922309 0. 5573953455270116 T T T

0. 6752605533503029 0. 5146709310850087 0. 4923218067316693 T T T

0. 6495017937604363 0. 6480415173805585 0. 5115765065572420 T T T

0. 5607206634869599 0. 4889955352012726 0. 4289418942408889 T T T

0. 4922743884948770 0. 4430487594051795 0. 5500697555137518 T T T

0. 5853975876857347 0. 3702206791185372 0. 4808897790428327 T T T

0. 4379922086368074 0. 3320198485921318 0. 5002147228390984 T T T

0. 5423577538772808 0. 2494872065799476 0. 5074884670619089 T T T

0. 3611738201316499 0. 4408742251040373 0. 5013632402691460 T T T

0. 4298768524543256 0. 5589887435930926 0. 5264988445879825 T T T

0. 3021360038264226 0. 5605132326584457 0. 4803342948008871 T T T

0. 3852347400910747 0. 6693927038615634 0. 4677938096607516 T T T

0. 5159127494536754 0. 6684691236309899 0. 4951121197652323 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5633608212956195 0. 5550391123795763 0. 5727202467928241 T T T

0. 6506083180026468 0. 5031643275207441 0. 4778973607884766 T T T

0. 6537521657150838 0. 6367007257157177 0. 5092987948243691 T T T

0. 5189744941931625 0. 4931435069615778 0. 4426054709523644 T T T

0. 4898617385049120 0. 4427312966063002 0. 5722527964391456 T T T

0. 5896006496640730 0. 3834434692826589 0. 4829435740953613 T T T

0. 4514387630207821 0. 3397262830444769 0. 4921869955329882 T T T

0. 5536688738285882 0. 2578754631181749 0. 5051422644891920 T T T

0. 3777060663323237 0. 4476575886516000 0. 4776237239662537 T T T

0. 4305025407756798 0. 5603220390824140 0. 5381723754445110 T T T

0. 3054213678314601 0. 5605404920069444 0. 4798623466311420 T T T

0. 3920779131823433 0. 6650835427101174 0. 4644821128753716 T T T

0. 5230268767207994 0. 6545729747848299 0. 4848125262353838 T T T
Au
1. 0000000000000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5635547238611432 0. 5536734239133344 0. 5877247280778568 T T T
0. 6315451035579404 0. 5183367283654846 0. 4659196530134099 T T T
0. 6551443864663633 0. 6372426580973904 0. 5261095036206640 T T T
0. 5022082614566908 0. 4872883691516496 0. 4337290452537904 T T T
0. 5006039653923670 0. 4363362508039511 0. 5753280019118127 T T T
0. 5947638040815298 0. 3918650403772833 0. 4767994845124542 T T T
0. 4553910486240419 0. 3544436933528142 0. 4744990805510493 T T T
0. 5495079739154091 0. 2779647999609094 0. 5273655227235995 T T T
0. 3720989081352891 0. 4545220599867135 0. 4596635077425930 T T T
0. 4326952350750340 0. 5498884440016695 0. 5482980811336561 T T T
0. 3057461228889857 0. 5645602405018422 0. 4969356343714283 T T T
0. 4036433718917354 0. 6484095303340324 0. 4573847449041217 T T T
0. 5330976912966048 0. 6254695678667539 0. 4702436088266331 T T T

\$POSCAR 1 Au

1. 000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

13

Selective dynamics

Direct

0. 5541390000000000 0. 5539620000000000 0. 5766970000000000 T T T
0. 6381890000000000 0. 5215520000000000 0. 4658610000000000 T T T
0. 6546390000000000 0. 6376170000000000 0. 5335750000000000 T T T
0. 5038700000000000 0. 4976010000000000 0. 4352100000000000 T T T
0. 5103660000000000 0. 4264620000000000 0. 5788030000000000 T T T
0. 5954739999999999 0. 3971330000000000 0. 4679170000000000 T T T
0. 4543250000000000 0. 3693060000000000 0. 4605160000000000 T T T
0. 5378690000000000 0. 2974940000000000 0. 5391950000000000 T T T
0. 3681320000000000 0. 4683100000000000 0. 4517010000000000 T T T
0. 4220390000000000 0. 5279180000000000 0. 5697700000000000 T T T
0. 3022440000000000 0. 5681430000000000 0. 5150970000000000 T T T
0. 4149040000000000 0. 6045440000000000 0. 4494500000000000 T T T
0. 5438110000000000 0. 6299580000000000 0. 4562090000000000 T T T

Pathway 31

\$POSCAR 1 Au

1.000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.5669720000000000	0.5618430000000000	0.5000000000000000	T T T
0.7022180000000000	0.5622530000000000	0.5000000000000000	T T T
0.6335700000000000	0.6794410000000000	0.5000000000000000	T T T
0.6374700000000000	0.4439330000000000	0.5000000000000000	T T T
0.5000000000000000	0.4455030000000000	0.5000000000000000	T T T
0.5706300000000000	0.3296890000000000	0.5000000000000000	T T T
0.4293700000000000	0.3296890000000000	0.5000000000000000	T T T
0.5000000000000000	0.2176350000000000	0.5000000000000000	T T T
0.3625300000000000	0.4439330000000000	0.5000000000000000	T T T
0.4330280000000000	0.5618430000000000	0.5000000000000000	T T T
0.2977820000000000	0.5622530000000000	0.5000000000000000	T T T
0.3664300000000000	0.6794410000000000	0.5000000000000000	T T T
0.5000000000000000	0.6825460000000000	0.5000000000000000	T T T

Au

1.0000000000000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Au

13

Selective dynamics

Direct

0.5664327692907081	0.5615404698911524	0.5128527776791928	T T T
0.7015197795885597	0.5614594532756890	0.5196116168705192	T T T
0.6345572837036145	0.6762875683811046	0.4918371310995402	T T T
0.6361521973484399	0.4436454692321176	0.5248168121403528	T T T
0.4988921773568024	0.4456293197268571	0.5179235935356090	T T T
0.5702303697767381	0.3311594002719351	0.5024063252869506	T T T
0.4293750862652683	0.3310763250887747	0.4959826815837566	T T T
0.5015550881738835	0.2250696306069682	0.4629764803663942	T T T
0.3617610909481871	0.4439894496950899	0.5096896666836959	T T T
0.4327239061308362	0.5617260590476454	0.5050646703550045	T T T
0.2978304596980063	0.5619360778807021	0.4960406134287579	T T T
0.3678506298190979	0.6764927776443143	0.4755285716124807	T T T

0. 5011191618998447 0. 6799890015751028 0. 4852695581990462 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5662489834081444 0. 5596490978871718 0. 5195040374321261 T T T

0. 7013924149369035 0. 5589602803121578 0. 5268153475587306 T T T

0. 6361623833481916 0. 6679727851215325 0. 4792019538678248 T T T

0. 6347364410966150 0. 4431679026984693 0. 5458250912043351 T T T

0. 4972263101552881 0. 4460479446357100 0. 5384654547930657 T T T

0. 5697873511785689 0. 3387415243086299 0. 4972144579462920 T T T

0. 4293531463679472 0. 3352483113152502 0. 4975430994686057 T T T

0. 5022850483162062 0. 2472516855471110 0. 4302596394447638 T T T

0. 3602235175975434 0. 4437710767979571 0. 5289784481673915 T T T

0. 4322244005178074 0. 5601959156773902 0. 5105026399694212 T T T

0. 2980143419240115 0. 5596450867924928 0. 4980622461196636 T T T

0. 3695721492722913 0. 6681713175418309 0. 4582512880978012 T T T

0. 5027735118804665 0. 6711780639788490 0. 4693767996226765 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5667576004872452 0. 5510526828689506 0. 5146801213969999 T T T

0. 7010434194286995 0. 5533656031504185 0. 5308444569524752 T T T

0. 6378130437541880 0. 6579740263289423 0. 4728211380586496 T T T

0. 6328113896476281 0. 4417224488906173 0. 5657526348731051 T T T

0. 4943273682126999 0. 4467481446760751 0. 5621347577690377 T T T

0. 5669059281809486 0. 3643379006407355 0. 4805903791597734 T T T

0. 4309224187548189 0. 3399276164998590 0. 5023675808466974 T T T

0. 5039350285508380 0. 2729132948989590 0. 4126793334710162 T T T

0. 3585696970153490 0. 4426918080503033 0. 5450219462304385 T T T

0. 4322511626053211 0. 5534868525907584 0. 5063271044711951 T T T

0. 2987982860027915 0. 5559449237331743 0. 5000320443102354 T T T

0. 3713110515388990 0. 6606501700726909 0. 4494467800620187 T T T

0. 5045536058205036 0. 6591855214727800 0. 4573022254611895 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

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0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5704251321450896 0. 5357998584201473 0. 4943251093644564 T T T

0. 6978345526128906 0. 5506688221618512 0. 5400554387995226 T T T

0. 6386201435960446 0. 6531561612652843 0. 4758026430317886 T T T

0. 6299889475018420 0. 4383408866888225 0. 5721725637223676 T T T

0. 4929574301732534 0. 4468858615898496 0. 5781499519407385 T T T

0. 5539218455672152 0. 4018655954066432 0. 4619823766371679 T T T

0. 4330570436913690 0. 3441141152090522 0. 5076442233322088 T T T

0. 5092889643676889 0. 2873680295647958 0. 4158897794801216 T T T

0. 3582450882731363 0. 4436764319316053 0. 5552770549017728 T T T

0. 4345128111890981 0. 5397766656106335 0. 4921810481544568 T T T

0. 2998684188665958 0. 5518731999146793 0. 4996206854187044 T T T

0. 3743082642192262 0. 6558764588841426 0. 4530881038721538 T T T

0. 5069713577964921 0. 6505989071498971 0. 4538115244457082 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

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0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5856314777431960 0. 5363849351112122 0. 4748091278989054 T T T

0. 6940623314857847 0. 5576400257730584 0. 5500387057167488 T T T

0. 6416672113968445 0. 6615698913836364 0. 4818633520616825 T T T

0. 6267352689474294 0. 4409259658075402 0. 5665785687506727 T T T

0. 4928123820243060 0. 4427346381062585 0. 5887874442412265 T T T

0. 5442990508797633 0. 4097325867143092 0. 4561712160620413 T T T

0. 4268397174990980 0. 3552746829135958 0. 5062046234352432 T T T

0. 5030664933839661 0. 2881013301547743 0. 4226697150214614 T T T

0. 3607738421682530 0. 4597909238382190 0. 5572055298457810 T T T

0. 4516337829835972 0. 5184611952951342 0. 4739396949282151 T T T

0. 2819834250445527 0. 5506195489025666 0. 5018290742718183 T T T

0. 3800408068119018 0. 6316174945416145 0. 4657911681434432 T T T

0. 5104542096312794 0. 6471477745655049 0. 4541122830690446 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 6009436485923018 0. 5285786825987483 0. 4561248089868499 T T T

0. 6687105097354108 0. 5702702204905532 0. 5654517387884511 T T T

0. 6413526223399468 0. 6598363621432137 0. 4704148284767927 T T T

0. 6222803826912059 0. 4452743965913598 0. 5721543745106114 T T T

0. 4883454834866964 0. 4494743506698862 0. 5871276788679030 T T T

0. 5624448915053082 0. 4000103073428829 0. 4553729974182951 T T T

0. 4281015915551212 0. 3712064771993653 0. 4936766896478900 T T T

0. 5025470614301812 0. 2857007675137086 0. 4258532787946382 T T T

0. 3613181073430785 0. 4770614510312883 0. 5451537278738915 T T T

0. 4666425146499069 0. 5034610615537440 0. 4571279475534311 T T T

0. 2663255129690065 0. 5677315647551481 0. 5308552535106444 T T T

0. 3818547546201548 0. 6073038856201600 0. 4818913690311012 T T T

0. 5091329190815923 0. 6340914169297091 0. 4587958343196806 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 6083605281683806 0. 5245150691545337 0. 4426756551477313 T T T

0. 6038296821836618 0. 5688182862098048 0. 5742491662221570 T T T

0. 6467201936029302 0. 6531982196751381 0. 4774516801268398 T T T

0. 6294429014667705 0. 4382327259839537 0. 5571983561252760 T T T

0. 5007643997451505 0. 4700977701096255 0. 5854151471919872 T T T

0. 5646954753510044 0. 3982967905771701 0. 4414924336603199 T T T

0. 4378133037712130 0. 3759478643421403 0. 5043399963284645 T T T

0. 4998471032748587 0. 2834615712897844 0. 4329503218541879 T T T

0. 3685624178436385 0. 4819023260260077 0. 5488788396718305 T T T

0. 4697306443722075 0. 5017300064995385 0. 4506052016651065 T T T

0. 2697486971820174 0. 5690576960407244 0. 5339708950074509 T T T

0. 3854759229751868 0. 6053277203968331 0. 4816712853381519 T T T

0. 5150087300629015 0. 6294148999628503 0. 4691015485264096 T T T
Au
1. 000000000000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 6047469204677995 0. 5315715494132722 0. 4284789123377653 T T T
0. 6022193086664818 0. 5513646431535087 0. 5671953113962771 T T T
0. 6496204304117594 0. 6490214365059502 0. 4849840069092742 T T T
0. 6026579002160254 0. 4178014667066130 0. 5432674442961725 T T T
0. 4915114625940328 0. 4776145976709246 0. 5923490799265592 T T T
0. 5602924596051967 0. 4075953287245065 0. 4141390846257388 T T T
0. 4448894515535795 0. 3783079904686175 0. 5075658951430171 T T T
0. 5375828635244311 0. 2905891589855016 0. 4725058149109048 T T T
0. 3634622279086985 0. 4792953583659921 0. 5400640719035044 T T T
0. 4693357205052625 0. 5040966898885938 0. 4503292625387942 T T T
0. 2700412284893536 0. 5734768836375288 0. 5366489281230516 T T T
0. 3868893791961667 0. 6079605446232308 0. 4861452001508195 T T T
0. 5167506468611636 0. 6313052995163669 0. 4763275139077661 T T T

\$POSCAR 1 Au

1. 000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

13

Selective dynamics

Direct

0. 5969740000000000 0. 5381730000000000 0. 4147220000000000 T T T
0. 6152380000000000 0. 5387010000000000 0. 5579290000000000 T T T
0. 6551230000000000 0. 6427720000000000 0. 4796890000000000 T T T
0. 5790310000000000 0. 4110260000000000 0. 5630180000000000 T T T
0. 4821060000000000 0. 5079850000000000 0. 5730220000000000 T T T
0. 5607660000000000 0. 4104980000000000 0. 4198110000000000 T T T
0. 4513260000000000 0. 3799990000000000 0. 5066510000000000 T T T
0. 5567980000000000 0. 2960600000000000 0. 4935080000000000 T T T
0. 3554810000000000 0. 4686680000000000 0. 5185480000000000 T T T
0. 4643430000000000 0. 5074710000000000 0. 4337510000000000 T T T
0. 2674320000000000 0. 5671270000000000 0. 52941400000000001 T T T
0. 3937770000000000 0. 6037050000000000 0. 5131650000000000 T T T
0. 5216050000000000 0. 6278150000000000 0. 4967730000000000 T T T

Pathway 32

\$POSCAR 1 Au

1.000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.5669720000000000	0.5618430000000000	0.5000000000000000	T T T
0.7022180000000000	0.5622530000000000	0.5000000000000000	T T T
0.6335700000000000	0.6794410000000000	0.5000000000000000	T T T
0.6374700000000000	0.4439330000000000	0.5000000000000000	T T T
0.5000000000000000	0.4455030000000000	0.5000000000000000	T T T
0.5706300000000000	0.3296890000000000	0.5000000000000000	T T T
0.4293700000000000	0.3296890000000000	0.5000000000000000	T T T
0.5000000000000000	0.2176350000000000	0.5000000000000000	T T T
0.3625300000000000	0.4439330000000000	0.5000000000000000	T T T
0.4330280000000000	0.5618430000000000	0.5000000000000000	T T T
0.2977820000000000	0.5622530000000000	0.5000000000000000	T T T
0.3664300000000000	0.6794410000000000	0.5000000000000000	T T T
0.5000000000000000	0.6825460000000000	0.5000000000000000	T T T

Au

1.0000000000000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Au

13

Selective dynamics

Direct

0.5661985790095254	0.5619066882004934	0.4885179792867660	T T T
0.7014574695566008	0.5592602931076777	0.4947322271745571	T T T
0.6344180557008556	0.6744358941991850	0.5193534600626457	T T T
0.6355538763103467	0.4445007896606012	0.4705104436671588	T T T
0.4983786922125062	0.4463900686805812	0.4795411694818093	T T T
0.5700829077786603	0.3312232705286343	0.4884485597143585	T T T
0.4300322408101457	0.3312376296096001	0.5026541099263016	T T T
0.5035624230131768	0.2233389952202895	0.5259905268523135	T T T
0.3618756971987058	0.4444105743523141	0.4934238010748517	T T T
0.4323235120731084	0.5626610774251595	0.4933118108434798	T T T
0.2976880279215981	0.5625369849851185	0.5048977936023660	T T T
0.3674961635908631	0.6778740120687228	0.5219335767716052	T T T

0. 5009318284474238 0. 6802246692085032 0. 5166845415417834 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5636644411543770 0. 5618901081986640 0. 4771135576686041 T T T

0. 6956623761430443 0. 5459074592810886 0. 5022122875799009 T T T

0. 6350437007934908 0. 6609958773627406 0. 5362489038814220 T T T

0. 6309924305402365 0. 4466015911679673 0. 4391720252053776 T T T

0. 4944119673804596 0. 4481511063186088 0. 4614002720722952 T T T

0. 5719515888880234 0. 3383431085524523 0. 4852093125681247 T T T

0. 4340556017147726 0. 3360782024167579 0. 5101540801507830 T T T

0. 5158089410201850 0. 2383313747231005 0. 5490741774598901 T T T

0. 3610568664085981 0. 4452993075268772 0. 4928582153065204 T T T

0. 4296093031432781 0. 5646062150391389 0. 4832223399320237 T T T

0. 2965131006460559 0. 5631116250531901 0. 5066717444718043 T T T

0. 3690336764445639 0. 6756865072718282 0. 5313859294002792 T T T

0. 5021954449314688 0. 6749983955045171 0. 5252771543029807 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5605715315564231 0. 5632386837549486 0. 4666048443436986 T T T

0. 6801068774497432 0. 5218090682586580 0. 5148739525728875 T T T

0. 6350294858282892 0. 6426821446385236 0. 5491874713054589 T T T

0. 6250655935313776 0. 4501054987278899 0. 4151118404048350 T T T

0. 4901284660428769 0. 4503191988824890 0. 4479636751973511 T T T

0. 5784925940638034 0. 3534357367727927 0. 4913787256320989 T T T

0. 4408957921353541 0. 3425241711456403 0. 5156966117390392 T T T

0. 5303141661190738 0. 2530819486145475 0. 5593103591783209 T T T

0. 3618981898848556 0. 4470135889436000 0. 4950629122831461 T T T

0. 4263886771149748 0. 5677602336896629 0. 4729896506506464 T T T

0. 2955200003964000 0. 5640544242147096 0. 5064619013855931 T T T

0. 3713978805834738 0. 6743762734435536 0. 5351974074289267 T T T

0. 5041901828294482 0. 6695999039850411 0. 5301606478779892 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5595272237913347 0. 5675315619614165 0. 4550421888997403 T T T

0. 6541843488561617 0. 4949494503348448 0. 5259649142736051 T T T

0. 6358166654172540 0. 6251835789122772 0. 5536894310532455 T T T

0. 6168468562485356 0. 4544190228049598 0. 4004818101609977 T T T

0. 4872770899482655 0. 4524203077355727 0. 4415298430431491 T T T

0. 5889916354047690 0. 374160009910511 0. 5059912167311071 T T T

0. 448851926869694 0. 3484208103454572 0. 5189774886024120 T T T

0. 5425008945134066 0. 2625253537552596 0. 5574607241437864 T T T

0. 3641004068371847 0. 4487409684767565 0. 4986342270055922 T T T

0. 4244496372892987 0. 5706796570870236 0. 4656113617725634 T T T

0. 2953064749787948 0. 5641935383387705 0. 5055170610858409 T T T

0. 3748658182927025 0. 6724677608851078 0. 5379817734783120 T T T

0. 5072471926606749 0. 6643088622221268 0. 5331179597496782 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5615210721693326 0. 5785433160061312 0. 4412495497685768 T T T

0. 6421941901760971 0. 4961775292164333 0. 5242116139818891 T T T

0. 6408249688511685 0. 6265798077730368 0. 5468809909027627 T T T

0. 6113591335843802 0. 4559256530736001 0. 3977085094958662 T T T

0. 4965011536074575 0. 4613165590219223 0. 4690554549100348 T T T

0. 5930801808767383 0. 3702881839331519 0. 5061429716218274 T T T

0. 4480634848038937 0. 3540097767507888 0. 5313898883329393 T T T

0. 5385231166521668 0. 2589256237063221 0. 5498769526767825 T T T

0. 3674299587685262 0. 4572153339694824 0. 5083225395674468 T T T

0. 4254313804491185 0. 5751518516320349 0. 4501194197564242 T T T

0. 2923476911509467 0. 5647827220744508 0. 4834851285305676 T T T

0. 3752248126666105 0. 6516580923900653 0. 5480555130048232 T T T

0. 5074982900590421 0. 6494264180836194 0. 5435014674501070 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5625553747988993 0. 5842302107979338 0. 4329462735058350 T T T

0. 6428237957265991 0. 4975607959459752 0. 5203014894062659 T T T

0. 6442380414958947 0. 6273477036322946 0. 5426750788562351 T T T

0. 5966910661690130 0. 4558318131918501 0. 3978392363679759 T T T

0. 5030658383484040 0. 4796322412612068 0. 5014362264513705 T T T

0. 5922278092771325 0. 3715497733409226 0. 5057287848563977 T T T

0. 4486468278112390 0. 3613451730616113 0. 5336690271802005 T T T

0. 5352708004389481 0. 2611770766819880 0. 5466797445439185 T T T

0. 3693396427096721 0. 4654784625214758 0. 5121375772919156 T T T

0. 4268965591589997 0. 5768314750982378 0. 4364974924287200 T T T

0. 2915692278766066 0. 5645869722596881 0. 4674588168332220 T T T

0. 3773821583239013 0. 6265003223109453 0. 5513732635111790 T T T

0. 5092922915043325 0. 6279288471752620 0. 5512569887668035 T T T

Au

1. 0000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5608276365205516 0. 5930163505183091 0. 4379971490339212 T T T

0. 6395407381967780 0. 5004088283839344 0. 5171676071965354 T T T

0. 6528205104694219 0. 6309892065887777 0. 5365187247931246 T T T

0. 5687538682707387 0. 4636239890594381 0. 4011680920723669 T T T

0. 4988678580233024 0. 4909000993529577 0. 5243712721190714 T T T

0. 5868764307771988 0. 3767889519826178 0. 5049748468132786 T T T

0. 4493999102813988 0. 3640187606753416 0. 5365094799386342 T T T

0. 5362031110043159 0. 2628255004308040 0. 5446167296826329 T T T

0. 3662281100814437 0. 4629362324825397 0. 5101386122385226 T T T

0. 4312411018577747 0. 5637633198346489 0. 4201315752925827 T T T

0. 2972186197030713 0. 5646093576142104 0. 4558807642272418 T T T

0. 3922110163723040 0. 6019533702782744 0. 5451946612724327 T T T

0. 5198105220559840 0. 6241669000267488 0. 5653304853197380 T T T
Au
1. 0000000000000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5597582696725940 0. 6017998186551508 0. 4319466923374651 T T T
0. 6296451972787573 0. 5094223641628662 0. 5209728497230136 T T T
0. 6560952233183565 0. 6416153036919582 0. 5207561717259581 T T T
0. 5425442444922770 0. 4680493583847274 0. 4155549726668645 T T T
0. 4940848650769618 0. 4853004957691341 0. 5520058577632987 T T T
0. 5868408077233307 0. 3836159943928422 0. 5156374551878808 T T T
0. 4470791199671857 0. 3587841783687850 0. 5294769718398296 T T T
0. 5377091059258522 0. 2625540312913113 0. 5352647034110779 T T T
0. 3676573372102349 0. 4599343197064353 0. 5012020674679923 T T T
0. 4359800455355558 0. 5523399462099111 0. 4116540607363550 T T T
0. 3061454968256107 0. 5697291691855876 0. 4521424074904599 T T T
0. 4043028373991627 0. 5915679962768128 0. 5441309165802802 T T T
0. 5321568799462596 0. 6152878846487182 0. 5692548730695838 T T T

\$POSCAR 1 Au

1. 000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

13

Selective dynamics

Direct

0. 5584000000000000 0. 5964830000000000 0. 4264210000000000 T T T
0. 6280250000000001 0. 5109350000000000 0. 5174290000000000 T T T
0. 6557110000000000 0. 6432670000000000 0. 5093960000000000 T T T
0. 5149760000000000 0. 4662820000000000 0. 4340080000000000 T T T
0. 4950590000000000 0. 4788500000000000 0. 5724180000000000 T T T
0. 5918730000000000 0. 3850610000000000 0. 5236570000000000 T T T
0. 4551140000000000 0. 3580310000000000 0. 5064330000000000 T T T
0. 5435810000000000 0. 2617130000000000 0. 5279090000000000 T T T
0. 3770480000000000 0. 4613300000000000 0. 4858200000000000 T T T
0. 4290970000000000 0. 5709260000000000 0. 4101360000000000 T T T
0. 3045760000000000 0. 5738660000000000 0. 4651720000000000 T T T
0. 4086180000000000 0. 5838500000000000 0. 5524580000000000 T T T
0. 5379210000000000 0. 6094060000000000 0. 5687430000000000 T T T

Pathway 33

\$POSCAR 1 Au

1.000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.5669720000000000	0.5618430000000000	0.5000000000000000	T T T
0.7022180000000000	0.5622530000000000	0.5000000000000000	T T T
0.6335700000000000	0.6794410000000000	0.5000000000000000	T T T
0.6374700000000000	0.4439330000000000	0.5000000000000000	T T T
0.5000000000000000	0.4455030000000000	0.5000000000000000	T T T
0.5706300000000000	0.3296890000000000	0.5000000000000000	T T T
0.4293700000000000	0.3296890000000000	0.5000000000000000	T T T
0.5000000000000000	0.2176350000000000	0.5000000000000000	T T T
0.3625300000000000	0.4439330000000000	0.5000000000000000	T T T
0.4330280000000000	0.5618430000000000	0.5000000000000000	T T T
0.2977820000000000	0.5622530000000000	0.5000000000000000	T T T
0.3664300000000000	0.6794410000000000	0.5000000000000000	T T T
0.5000000000000000	0.6825460000000000	0.5000000000000000	T T T

Au

1.0000000000000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Au

13

Selective dynamics

Direct

0.5669252042769735	0.5624892526306914	0.5084245165422155	T T T
0.7021610693268305	0.5622781106251700	0.5041617432287114	T T T
0.6337241086756017	0.6792456644567278	0.4957580720037214	T T T
0.6365742092473767	0.4448747905125596	0.4957267734118659	T T T
0.5001685917177348	0.4459512259002320	0.5123355756435881	T T T
0.5696079152615462	0.3309099415069737	0.4930451525350936	T T T
0.4295805514629076	0.3299362738107846	0.5089377574307075	T T T
0.4994906220526528	0.2186168946959088	0.4922197623418555	T T T
0.3628514686318959	0.4440921590028067	0.5142465865914705	T T T
0.4331331276943748	0.5622045574108534	0.5079501875872118	T T T
0.2981573888841157	0.5615141259523708	0.4998501194580587	T T T
0.3674534952349989	0.6759520220555348	0.4766101156241509	T T T

0. 5001722475329150 0. 6819352827359900 0. 4907336376013802 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

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0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5664129592090991 0. 5634543448502515 0. 5223431864935179 T T T

0. 7018527026654748 0. 5605316219396194 0. 5121437334365809 T T T

0. 6350925739098731 0. 6768407526331056 0. 4951516511138445 T T T

0. 6321347168389320 0. 4497260811400306 0. 4830301366372095 T T T

0. 4999118792386140 0. 4466474944725042 0. 5227328281938064 T T T

0. 5667588881086495 0. 3357683602018017 0. 4816287289927131 T T T

0. 4297244352488112 0. 3304804037384925 0. 5131933767486591 T T T

0. 5010595142485607 0. 2215778809927184 0. 4872334867651458 T T T

0. 3626094425186088 0. 4441821736655689 0. 5225931058014468 T T T

0. 4327131846532716 0. 5631047181888466 0. 5179450485390052 T T T

0. 2987728997750677 0. 5605001098233466 0. 4987215843238086 T T T

0. 3710611632951761 0. 6685200237235193 0. 4599640669395600 T T T

0. 5018956402897203 0. 6786662716916879 0. 4833190660146817 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5654819690465588 0. 5644576090949971 0. 5373534149299456 T T T

0. 7004545200595563 0. 5555323833940892 0. 5180654075421210 T T T

0. 6376140358950467 0. 6719222324937125 0. 4952453830698768 T T T

0. 6225126924766993 0. 4595582627920717 0. 4680745358901044 T T T

0. 4994168115887188 0. 4474671959282299 0. 5314897917026692 T T T

0. 5640335213842591 0. 3431569848913690 0. 4724208587812805 T T T

0. 4304751031395448 0. 3313380545441844 0. 5153377844876524 T T T

0. 5062559223302507 0. 2260939859309000 0. 4860997096860436 T T T

0. 3619945203150519 0. 4441085765484999 0. 5265785850184663 T T T

0. 4318492764067973 0. 5639502191151535 0. 5258505334443220 T T T

0. 2990842540843603 0. 5596900895168631 0. 4978850611706003 T T T

0. 3754144538599916 0. 6608764903934784 0. 4502414882706603 T T T

0. 5054129194130276 0. 6718481517515524 0. 4753574460062360 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5644626136021523 0. 5653084461344708 0. 5499869631892739 T T T

0. 6977146587178443 0. 5472550216962597 0. 5218665985115839 T T T

0. 6406902636128411 0. 6651841700469129 0. 4952841674952957 T T T

0. 6090463135772245 0. 4726799614361572 0. 4558658786577542 T T T

0. 4988810237675775 0. 4483001659766332 0. 5398130271123417 T T T

0. 5628163570985149 0. 3519745677798381 0. 4671467026562494 T T T

0. 4317856735634021 0. 3327215390488162 0. 5163661277093692 T T T

0. 5132167850708126 0. 2322475930732910 0. 4851602208392531 T T T

0. 3612289360190359 0. 4441641029285001 0. 5286601837066466 T T T

0. 4310400256894037 0. 5643906588723875 0. 5310290752973839 T T T

0. 2991678941384762 0. 5592688044912751 0. 4969643400159494 T T T

0. 3797521001607623 0. 6546045263824113 0. 4447088262309446 T T T

0. 5101973549818376 0. 6619006784936419 0. 4671478885779209 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5635299179131291 0. 5659089527477378 0. 5602955709644253 T T T

0. 6935447746012852 0. 5368787033247160 0. 5233659553527427 T T T

0. 6434354880586226 0. 6576372624878311 0. 4951945168937752 T T T

0. 5940471642404933 0. 4876829168051267 0. 4480784067699062 T T T

0. 4983384877305034 0. 4489175715786461 0. 5475316958628245 T T T

0. 5637976537816196 0. 3620310659096341 0. 4648599832725792 T T T

0. 4334150054713345 0. 3344890207457518 0. 5162491260899138 T T T

0. 5205995565390618 0. 2397995562642977 0. 4837770112414563 T T T

0. 3604840959405811 0. 4441940317558544 0. 5294379050351964 T T T

0. 4304338916534520 0. 5642998565504374 0. 5344107506040228 T T T

0. 2991866022478937 0. 5590791920064230 0. 4957881234283441 T T T

0. 3839412434822474 0. 6493405123927446 0. 4411555402848165 T T T

0. 5152461183396726 0. 6497415937565124 0. 4598554141999920 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5627282117039196 0. 5663088755125364 0. 5687386306553844 T T T

0. 6871392514317424 0. 5249571494258333 0. 5224786391393353 T T T

0. 6458219099640577 0. 6500271650598624 0. 4955689900020812 T T T

0. 5793740517970598 0. 5031346131105177 0. 4442102838340615 T T T

0. 4978758175376831 0. 4492245239422548 0. 5545372302956986 T T T

0. 5663935156808027 0. 3732442484698118 0. 4644237481525180 T T T

0. 4351153517799113 0. 3364221839751463 0. 5155560684337911 T T T

0. 5273848551758743 0. 2483017559891416 0. 4816093762167845 T T T

0. 3599680398653129 0. 4443031454884151 0. 5299688079498543 T T T

0. 4301665719862869 0. 5639525797458951 0. 5370426847622548 T T T

0. 2993407579898636 0. 5590768895817783 0. 4945067838989533 T T T

0. 3882715435456559 0. 6442123962531211 0. 4384316471406011 T T T

0. 5204201215417239 0. 6368347097120295 0. 4529271095186871 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5632169469925962 0. 5664131307584248 0. 5737682119630256 T T T

0. 6609197239507120 0. 4962140784764760 0. 4986088888879065 T T T

0. 6552691563807999 0. 6344637174683808 0. 4996767109453895 T T T

0. 5399638271651951 0. 5127341862200282 0. 4421983749687477 T T T

0. 4954057368278078 0. 4499632893441404 0. 5717768450369353 T T T

0. 5798497668038071 0. 3878467234406234 0. 4779803267186444 T T T

0. 4446349967252053 0. 3397565363386507 0. 5130567247212182 T T T

0. 5449969381284971 0. 2599076776518558 0. 4841748889719260 T T T

0. 3621478877847817 0. 4426632889905344 0. 5233438612458562 T T T

0. 4316448299636718 0. 5614457964177278 0. 5322752273649586 T T T

0. 3015320499402794 0. 5576007824338939 0. 4869759128632699 T T T

0. 3947797209516373 0. 6432210739302575 0. 4348815337290655 T T T

0. 5256384183849493 0. 6477699494558798 0. 4612824925830356 T T T
Au
1. 000000000000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5547365682176261 0. 5812674997321398 0. 5786660947475716 T T T
0. 6387169055860779 0. 5051264897439807 0. 4937757453621280 T T T
0. 6625414521115600 0. 6367188582589925 0. 5155679324327654 T T T
0. 5147595356292888 0. 5060674167123269 0. 4343314799970048 T T T
0. 5015680513067315 0. 4566936031330124 0. 5680784692014008 T T T
0. 5788011845801214 0. 3885986214918346 0. 4728859798045926 T T T
0. 4491453576561910 0. 3426610285520227 0. 5147975880851430 T T T
0. 5440335011177475 0. 2602133675447379 0. 4763889068986261 T T T
0. 3709458748250825 0. 4492705835361388 0. 5146992406962685 T T T
0. 4224320868831296 0. 5693325260558305 0. 5603013632849717 T T T
0. 3029917508503241 0. 5619575201006550 0. 4907374797269932 T T T
0. 4170631724361889 0. 6025940062735974 0. 4271742669148695 T T T
0. 5422645587998708 0. 6394986948089807 0. 4525954528476887 T T T

\$POSCAR 1 Au

1. 000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

13

Selective dynamics

Direct

0. 5478950000000000 0. 5962950000000000 0. 5810360000000000 T T T
0. 6292590000000000 0. 5102540000000000 0. 5008760000000000 T T T
0. 6562249999999999 0. 6424550000000000 0. 5126480000000000 T T T
0. 5052570000000000 0. 4787660000000000 0. 4276290000000000 T T T
0. 5052980000000000 0. 4663060000000000 0. 5674740000000000 T T T
0. 5936910000000000 0. 3845570000000000 0. 4896870000000000 T T T
0. 4557300000000000 0. 3582520000000000 0. 4873830000000000 T T T
0. 5458390000000000 0. 2614510000000000 0. 4787330000000000 T T T
0. 3760770000000000 0. 4619800000000000 0. 4966480000000000 T T T
0. 4174560000000000 0. 5714240000000000 0. 5788570000000000 T T T
0. 3020050000000000 0. 5749160000000000 0. 5067320000000000 T T T
0. 4174140000000000 0. 5842360000000000 0. 4350590000000000 T T T
0. 5478540000000000 0. 6091070000000000 0. 4372380000000000 T T T

Pathway 34

\$POSCAR 1 Au

1.000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.5669720000000000	0.5618430000000000	0.5000000000000000	T T T
0.7022180000000000	0.5622530000000000	0.5000000000000000	T T T
0.6335700000000000	0.6794410000000000	0.5000000000000000	T T T
0.6374700000000000	0.4439330000000000	0.5000000000000000	T T T
0.5000000000000000	0.4455030000000000	0.5000000000000000	T T T
0.5706300000000000	0.3296890000000000	0.5000000000000000	T T T
0.4293700000000000	0.3296890000000000	0.5000000000000000	T T T
0.5000000000000000	0.2176350000000000	0.5000000000000000	T T T
0.3625300000000000	0.4439330000000000	0.5000000000000000	T T T
0.4330280000000000	0.5618430000000000	0.5000000000000000	T T T
0.2977820000000000	0.5622530000000000	0.5000000000000000	T T T
0.3664300000000000	0.6794410000000000	0.5000000000000000	T T T
0.5000000000000000	0.6825460000000000	0.5000000000000000	T T T

Au

1.0000000000000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Au

13

Selective dynamics

Direct

0.5669058802444848	0.5615003928931841	0.4836932153175298	T T T
0.7017132502812041	0.5619600773016575	0.4939296211270422	T T T
0.6337425646380834	0.6791662200097182	0.4874411061842353	T T T
0.6368215435974472	0.4437626891826699	0.4927308049913667	T T T
0.4993924170461815	0.4453744880145480	0.4850666826794505	T T T
0.5690919512248200	0.3310143163844554	0.5072719157633159	T T T
0.4282760787666138	0.3308815327564947	0.5016078041145953	T T T
0.4980208444803834	0.2207811173431496	0.5253293158295892	T T T
0.3619388189992121	0.4448127175565835	0.4918789747513321	T T T
0.4331958469164272	0.5621959282521529	0.4894951040316771	T T T
0.2985187501552839	0.5632341840524966	0.5029154077922395	T T T
0.3706136961682467	0.6746064709106041	0.5310918972264520	T T T

0. 5017683574817452 0. 6807102238595235 0. 5075476030301362 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

0. 0000000000000000 20. 0000000000000000 0. 0000000000000000

0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5665709315553820 0. 5605452270179523 0. 4652008274131577 T T T

0. 6964272337987434 0. 5664563178807068 0. 5055149569040740 T T T

0. 6309088086067278 0. 6797750261651012 0. 4738086631284872 T T T

0. 6356830331837311 0. 4470263943356780 0. 4973283153598188 T T T

0. 4988379476681130 0. 4452390984555418 0. 4732996508576182 T T T

0. 5670061323924095 0. 3356418024243457 0. 5155158208011400 T T T

0. 4268682384714744 0. 3336386573007386 0. 5012635221725733 T T T

0. 4968558665532335 0. 2256226170848689 0. 5342412387069363 T T T

0. 3613733744510876 0. 4468635126984975 0. 4855392153488420 T T T

0. 4330832130367066 0. 5637603771187066 0. 4730713031849382 T T T

0. 2997873987100629 0. 5657380406431075 0. 4979132898808876 T T T

0. 3797532090251257 0. 6584351679796431 0. 5556077590612332 T T T

0. 5068446125472910 0. 6712581108608471 0. 5216948871686704 T T T

Au

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Au

13

Selective dynamics

Direct

0. 5661211607067301 0. 5584459055155748 0. 4471000992668492 T T T

0. 6845539644576492 0. 5752283031290892 0. 5174451219383842 T T T

0. 6241356100352191 0. 6802172699855670 0. 4603720650905016 T T T

0. 6332103207059241 0. 4529554401368742 0. 5034935815398105 T T T

0. 4979359312181479 0. 4455024486995466 0. 4690679551962182 T T T

0. 5661416990438148 0. 3405527353828640 0. 5212444176230006 T T T

0. 4248485326578409 0. 3372947732081253 0. 5032303134419701 T T T

0. 4969091468678183 0. 2300789809473701 0. 5352168179404786 T T T

0. 3608425008576628 0. 4505755028196776 0. 4852828275751242 T T T

0. 4332179984520387 0. 5660825563599460 0. 4596739838996144 T T T

0. 3013578194265085 0. 5704616808077962 0. 4938101465612309 T T T

0. 3918003582049300 0. 6409484756383738 0. 5661275735234680 T T T

0. 5189249573657890 0. 6516562772248035 0. 5379345463550717 T T T

Au

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Au

13

Selective dynamics

Direct

0. 5652831148913653 0. 5564693731879028 0. 4334292959299305 T T T

0. 6712808868483311 0. 5852705385632183 0. 5271640288608994 T T T

0. 6126755015996407 0. 6807634171038948 0. 4517733764780065 T T T

0. 6298582369598522 0. 4600745224837438 0. 5093052836864645 T T T

0. 4965937734629169 0. 4475464181598138 0. 4713830824302347 T T T

0. 5664687096857755 0. 3449022765959149 0. 5241013593468709 T T T

0. 4227371175189065 0. 3406566594755192 0. 5047344481407808 T T T

0. 4970472311125938 0. 2346129679638317 0. 5347207259399205 T T T

0. 3598770400722306 0. 4546108526674416 0. 4865646437774384 T T T

0. 4328159424638662 0. 5676649397295623 0. 4476631433910119 T T T

0. 3033370167817937 0. 5757486174580303 0. 4918315290706303 T T T

0. 4061056767328435 0. 6263761781585181 0. 5660694643104806 T T T

0. 5359197518699245 0. 6253035882932060 0. 5512590685840332 T T T

Au

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Au

13

Selective dynamics

Direct

0. 5641563121117430 0. 5551489959446462 0. 4228990878305174 T T T

0. 6795855400350066 0. 5899292317152370 0. 5202522623482366 T T T

0. 5999131829497040 0. 6793428210291059 0. 4575432791258061 T T T

0. 6262461539040161 0. 4687085277769242 0. 5175047333893827 T T T

0. 4932980762225914 0. 4583412338627946 0. 4896799749182178 T T T

0. 5659483266537977 0. 3505767408667790 0. 5271797627999913 T T T

0. 4221872381827532 0. 3448357959953195 0. 5046686681300105 T T T

0. 4976434038527658 0. 2390555022803824 0. 5321035011421121 T T T

0. 3575589607607026 0. 4585120403890805 0. 4878942377038803 T T T

0. 4311439945426153 0. 5696677220270162 0. 4353238309583410 T T T

0. 3045406969962209 0. 5815351252611056 0. 4864518291764660 T T T

0. 4137803617171870 0. 6088582283341338 0. 5636731789328132 T T T

0. 5439977520709531 0. 5954883843545661 0. 5548251034897717 T T T

Au

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Au

13

Selective dynamics

Direct

0. 5696388222238451 0. 5397507413895450 0. 4199640961419463 T T T

0. 6762299703983723 0. 5959381578707423 0. 5113102705238444 T T T

0. 5696514328126673 0. 6680101659607727 0. 4517015165955568 T T T

0. 6299398940544780 0. 4698366162939305 0. 5228787696195760 T T T

0. 4908376320427614 0. 4676689129198206 0. 5130661907485069 T T T

0. 5648066502217454 0. 3540684915533057 0. 5276778810275515 T T T

0. 4239260719611643 0. 3503401954852524 0. 4992198364733688 T T T

0. 4965362828458927 0. 2424086140886571 0. 5282320365955654 T T T

0. 3600106155784384 0. 4650956471388362 0. 4837078159469521 T T T

0. 4423598569512496 0. 5818258792225023 0. 4338954647107743 T T T

0. 3113134090357870 0. 5892022899036820 0. 4805514504286372 T T T

0. 4163935250147525 0. 5897463357423425 0. 5667067752566267 T T T

0. 5483558368588780 0. 5861083022655166 0. 5610873458758867 T T T

Au

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Au

13

Selective dynamics

Direct

0. 5564553975384653 0. 5151565602824031 0. 4173574100967711 T T T

0. 6727617129025103 0. 6042293937273711 0. 5205420044852536 T T T

0. 5611514103002929 0. 6458945178229827 0. 4469556301488313 T T T

0. 6332262595159217 0. 4747137366555486 0. 5227718292256627 T T T

0. 4935655022779060 0. 4703039755599633 0. 5378186579482940 T T T

0. 5675968501420638 0. 3601428927027087 0. 5124369611559243 T T T

0. 4252422959558365 0. 3561639810568619 0. 5039149007734584 T T T

0. 4989110923721263 0. 2472720143765335 0. 5167255043591901 T T T

0. 3660367325233670 0. 4733698905183135 0. 4864486662608519 T T T

0. 4412194776214845 0. 5841405243831128 0. 4243354035931216 T T T

0. 3143444556351632 0. 5963366707274422 0. 4730924659727468 T T T

0. 4186253559064432 0. 5835160664890762 0. 5628328904964223 T T T

0. 5508634573084055 0. 5887601254137060 0. 5747671253886654 T T T
Au
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20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
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Au

13

Selective dynamics

Direct

0. 5404679924099663 0. 4876475433163180 0. 4190425929178472 T T T
0. 6739424644664045 0. 6136542922696815 0. 5303992786182902 T T T
0. 5667183340548095 0. 6187013209531623 0. 4452072344346350 T T T
0. 6318609369925658 0. 4856360522564895 0. 5224884104095036 T T T
0. 4923038995935472 0. 4716726200147467 0. 5537921812641752 T T T
0. 5686777043518958 0. 3715330500314772 0. 4967706712620863 T T T
0. 4266335564980972 0. 3599883702157225 0. 5077877445549362 T T T
0. 5052068865375323 0. 2545810915816850 0. 5020062699528435 T T T
0. 3673668616177642 0. 4768151091027804 0. 4911177243397502 T T T
0. 4409874071606754 0. 5798167483752963 0. 4194818625513658 T T T
0. 3157036662673834 0. 5994790013886119 0. 4703602658694785 T T T
0. 4194577557523061 0. 5886043628738791 0. 5597336677130380 T T T
0. 5506725342970362 0. 5918707809360367 0. 5818115438838952 T T T

\$POSCAR 1 Au

1. 000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
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13

Selective dynamics

Direct

0. 5108350000000000 0. 4718120000000000 0. 4306880000000000 T T T
0. 6730440000000000 0. 6198860000000000 0. 5232930000000000 T T T
0. 5709520000000000 0. 5952880000000000 0. 4366020000000000 T T T
0. 6282489999999999 0. 4922060000000000 0. 5174700000000000 T T T
0. 4919030000000000 0. 4721100000000000 0. 5698050000000000 T T T
0. 5759160000000000 0. 3721890000000000 0. 5106050000000000 T T T
0. 4369020000000000 0. 3652360000000000 0. 4917020000000000 T T T
0. 5118890000000000 0. 2564570000000000 0. 5021400000000000 T T T
0. 3731350000000000 0. 4794470000000000 0. 4827790000000000 T T T
0. 4395180000000000 0. 5887150000000000 0. 4187290000000000 T T T
0. 3161220000000000 0. 6020360000000000 0. 4747570000000000 T T T
0. 4200500000000000 0. 5890220000000000 0. 5617780000000000 T T T
0. 5514850000000000 0. 5955950000000000 0. 5796510000000000 T T T

Pathway 35

\$POSCAR 1 Au

1.000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.5669720000000000	0.5618430000000000	0.5000000000000000	T T T
0.7022180000000000	0.5622530000000000	0.5000000000000000	T T T
0.6335700000000000	0.6794410000000000	0.5000000000000000	T T T
0.6374700000000000	0.4439330000000000	0.5000000000000000	T T T
0.5000000000000000	0.4455030000000000	0.5000000000000000	T T T
0.5706300000000000	0.3296890000000000	0.5000000000000000	T T T
0.4293700000000000	0.3296890000000000	0.5000000000000000	T T T
0.5000000000000000	0.2176350000000000	0.5000000000000000	T T T
0.3625300000000000	0.4439330000000000	0.5000000000000000	T T T
0.4330280000000000	0.5618430000000000	0.5000000000000000	T T T
0.2977820000000000	0.5622530000000000	0.5000000000000000	T T T
0.3664300000000000	0.6794410000000000	0.5000000000000000	T T T
0.5000000000000000	0.6825460000000000	0.5000000000000000	T T T

Au

1.0000000000000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
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Au

13

Selective dynamics

Direct

0.5651208616276759	0.5625087289173872	0.4812488657558211	T T T
0.6965755786752758	0.5647137205368078	0.4980878672460740	T T T
0.6334250540924617	0.6782555500636577	0.5332300298767069	T T T
0.6362097440908315	0.4445769111020439	0.4790852648791162	T T T
0.4994105850313171	0.4442051124638899	0.4902038315794240	T T T
0.5710086036748419	0.3292670304612219	0.4880486397889836	T T T
0.4305510869734995	0.3308443202923264	0.5128958930938464	T T T
0.4998086741213608	0.2186837756315833	0.5075137226240318	T T T
0.3621727729144766	0.4448005275918074	0.5116620692799289	T T T
0.4325789708606062	0.5598834729750964	0.4937537104494570	T T T
0.2979685312289478	0.5641931401376236	0.5066245849258900	T T T
0.3714724944620648	0.6783746120909262	0.4904912567618898	T T T

0. 5036970422467169 0. 6796930480355204 0. 5071537513137439 T T T

Au

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20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

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Au

13

Selective dynamics

Direct

0. 5564948683960138 0. 5554047762292995 0. 4508943192583973 T T T

0. 6761395954197073 0. 5742540620252745 0. 5034773251507406 T T T

0. 6394736502911682 0. 6925976807669846 0. 5516951751579517 T T T

0. 6352922002158552 0. 4469472010438998 0. 4735118304587482 T T T

0. 4988060146278336 0. 4395084589266104 0. 4923807283838539 T T T

0. 5738072930592754 0. 3286063683672495 0. 4870926846418784 T T T

0. 4291816261209584 0. 3302563564843444 0. 5179705737088715 T T T

0. 4996969551011615 0. 2199183694035535 0. 5082168114934751 T T T

0. 3601584440914853 0. 4449935983567477 0. 5162113507689311 T T T

0. 4326841357332445 0. 5558315051311294 0. 4989124745939994 T T T

0. 2984378349474610 0. 5669998549871689 0. 5069768891601887 T T T

0. 3835758595529474 0. 6754529964716900 0. 4829843139362306 T T T

0. 5162515224429832 0. 6692287219555074 0. 5096750108240081 T T T

Au

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20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

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Au

13

Selective dynamics

Direct

0. 5424923767676756 0. 5516038833258461 0. 4324529867032891 T T T

0. 6521928280675113 0. 5808898466506457 0. 5050030636199411 T T T

0. 6435137561679448 0. 6967341582040840 0. 5659425489671082 T T T

0. 6310828811739096 0. 4518293990761226 0. 4645752496270221 T T T

0. 4999446762252979 0. 4381337799763201 0. 4986251203104090 T T T

0. 5765662749316419 0. 3296446659519183 0. 4844584975111337 T T T

0. 4282179440444199 0. 3306630873804010 0. 5225307975395601 T T T

0. 5010693040366259 0. 2225050801367382 0. 5067019362749366 T T T

0. 3600992026545986 0. 4460300021355102 0. 5195396116787874 T T T

0. 4366007613563198 0. 5545927810412498 0. 5190146182916161 T T T

0. 3023925592542543 0. 5688566185171148 0. 5005701598939484 T T T

0. 3984777459407047 0. 6675957022670272 0. 4677350692425815 T T T

0. 5273496893791862 0. 6609209449181324 0. 5128498277348300 T T T

Au

1. 0000000000000000

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Au

13

Selective dynamics

Direct

0. 5303654727164081 0. 5575582813804750 0. 4326831637009456 T T T

0. 6469552809029288 0. 5823777487169434 0. 5006736375887938 T T T

0. 6444208947933471 0. 6919875870175471 0. 5744797582284246 T T T

0. 6240084988557215 0. 4576806398527129 0. 4549132845745865 T T T

0. 4984614902443811 0. 4413778032797694 0. 5026094507763943 T T T

0. 5748168506879279 0. 3338630857622999 0. 4793859559874955 T T T

0. 4283323667926708 0. 3320816114949664 0. 5264786958424348 T T T

0. 5024158360993295 0. 2256760038431616 0. 5045394979376305 T T T

0. 3607850155015168 0. 4473029962123341 0. 5229721400352320 T T T

0. 4368846856929960 0. 5561434275052801 0. 5427531159029685 T T T

0. 3075209729731456 0. 5692470884696241 0. 4941658079125173 T T T

0. 4166257503037217 0. 6423183628540209 0. 4443816764602630 T T T

0. 5284068844359968 0. 6623853118346690 0. 5199633021081551 T T T

Au

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Au

13

Selective dynamics

Direct

0. 5320283192985763 0. 5619432532089798 0. 4171238310187738 T T T

0. 6395157178949207 0. 5698772585029139 0. 5032197381237672 T T T

0. 6368793131097109 0. 6669803522377830 0. 5920463265519867 T T T

0. 6224458275633967 0. 4571311263640854 0. 4331954565250126 T T T

0. 5018781266837946 0. 4540587654459685 0. 4995397557028505 T T T

0. 5733116697425288 0. 3407382707543039 0. 4777643151391645 T T T

0. 4366569366995541 0. 3419486797278482 0. 5319880734039552 T T T

0. 5079429840871561 0. 2324782440883645 0. 5152318848734690 T T T

0. 3628016565290350 0. 4516180586026941 0. 5242633133157411 T T T

0. 4341556264459179 0. 5608780901775985 0. 5508706909038388 T T T

0. 3067680306139858 0. 5723764436490421 0. 4954581908306306 T T T

0. 4180486066776787 0. 6344543019641447 0. 4399008921424108 T T T

0. 5275671846540207 0. 6555170672080962 0. 5193970094512238 T T T

Au

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20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

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Au

13

Selective dynamics

Direct

0. 5394618826015833 0. 5552177268431969 0. 4006658608259512 T T T

0. 6316808517689263 0. 5410614035399345 0. 5110043385356395 T T T

0. 6392452039937409 0. 6462246681232805 0. 5885500915893663 T T T

0. 6380070919423558 0. 4574363273423677 0. 4097184449642352 T T T

0. 4994370405769085 0. 4828348152613894 0. 5130344439240407 T T T

0. 5734810283115780 0. 3688276700222595 0. 4817544804175234 T T T

0. 4415897341193685 0. 3579168300857575 0. 5249213850202303 T T T

0. 5237963296510525 0. 2535024299574518 0. 5172250860056584 T T T

0. 3618317023022219 0. 4611002625082929 0. 5152081518498484 T T T

0. 4103041892792707 0. 5741028506423069 0. 5769621330746139 T T T

0. 2978242454274312 0. 5787131220449129 0. 4965452717297620 T T T

0. 4195205682317683 0. 5960965205590729 0. 4394510480422963 T T T

0. 5238201317940414 0. 6269652822619861 0. 5249587413186986 T T T

Au

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Au

13

Selective dynamics

Direct

0. 5363397573224997 0. 5884447197724191 0. 4122550425127868 T T T

0. 6327942283543038 0. 5146048181751368 0. 5137231403262573 T T T

0. 6650524801491874 0. 6189757485121054 0. 5858947775871927 T T T

0. 6010565300081191 0. 4685769328428534 0. 3923115425979167 T T T

0. 4922675865691106 0. 4875666169479096 0. 4943110688230830 T T T

0. 5868790237395255 0. 3833695741917845 0. 4950608407126136 T T T

0. 4488031388225093 0. 3624784268820112 0. 5261243891408993 T T T

0. 5420045144696941 0. 2677140792796398 0. 5355162322391853 T T T

0. 3595147232157798 0. 4581444321771374 0. 5108725220974691 T T T

0. 4067588885236332 0. 5824608390063277 0. 5612512184004509 T T T

0. 2876047158782444 0. 5709499005591160 0. 4910171636745205 T T T

0. 4047424718386690 0. 5873156841238558 0. 4265149979608269 T T T

0. 5361819411088983 0. 6093981067772749 0. 5551465337385588 T T T
Au
1. 0000000000000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5541767842811447 0. 6076536979169087 0. 4423187404283131 T T T
0. 6337594307374037 0. 5069544217348867 0. 5101742924423849 T T T
0. 6602192452422132 0. 6311889317617325 0. 5452613162278752 T T T
0. 5535592735626170 0. 4803857074297706 0. 3974973698718559 T T T
0. 4956973989730592 0. 4856325141314310 0. 5280918524019819 T T T
0. 5840485110240957 0. 3829453988704778 0. 4910737947976937 T T T
0. 4483801844354442 0. 3576757412629630 0. 5251550450924538 T T T
0. 5424130783222343 0. 2637195493596485 0. 5278430212862198 T T T
0. 3626171497390072 0. 4561589715400999 0. 5044906907110778 T T T
0. 4042853135771297 0. 5844721799289612 0. 5577457659742013 T T T
0. 2999182976769466 0. 5698202737769876 0. 4708448280775542 T T T
0. 4288230031021140 0. 5643703215026497 0. 4213490715425803 T T T
0. 5321023293267514 0. 6090221644510367 0. 5781536795625607 T T T

\$POSCAR 1 Au

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0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

13

Selective dynamics

Direct

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0. 6289250000000000 0. 5103020000000000 0. 5092700000000000 T T T
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0. 5103080000000000 0. 4722910000000000 0. 4304150000000000 T T T
0. 5002170000000000 0. 4725640000000000 0. 5704510000000000 T T T
0. 5934420000000000 0. 3841060000000000 0. 5069580000000000 T T T
0. 4558370000000000 0. 3576880000000000 0. 4970940000000000 T T T
0. 5457070000000001 0. 2605100000000000 0. 5037590000000000 T T T
0. 3763950000000000 0. 4618220000000000 0. 4911670000000000 T T T
0. 4124650000000000 0. 5782730000000000 0. 5659110000000001 T T T
0. 3025220000000000 0. 5752010000000000 0. 4856240000000000 T T T
0. 4228410000000000 0. 5779930000000000 0. 4219170000000000 T T T
0. 5425680000000001 0. 6032500000000000 0. 5752380000000000 T T T

Pathway 36

\$POSCAR 1 Au

1.000000

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0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.5413900000000000	0.5883890000000001	0.5000000000000000	T T T
0.6791990000000000	0.5877910000000000	0.5000000000000000	T T T
0.6100010000000000	0.7029950000000000	0.5000000000000000	T T T
0.6108190000000000	0.4725290000000000	0.5000000000000000	T T T
0.4735870000000000	0.4731960000000000	0.5000000000000000	T T T
0.5423500000000000	0.3531990000000000	0.5000000000000000	T T T
0.4039430000000000	0.3571860000000000	0.5000000000000000	T T T
0.4706060000000000	0.2425900000000000	0.5000000000000000	T T T
0.3388330000000000	0.4732430000000000	0.5000000000000000	T T T
0.4059430000000000	0.5960410000000000	0.5000000000000000	T T T
0.2742580000000000	0.5880910000000000	0.5000000000000000	T T T
0.6733220000000000	0.3553700000000000	0.5000000000000000	T T T
0.4757490000000000	0.7093800000000000	0.5000000000000000	T T T

Au

1.0000000000000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Au

13

Selective dynamics

Direct

0.5409414959171855	0.5877554746478308	0.5159126620774691	T T T
0.6791893470289918	0.5865398716689242	0.5081383914954961	T T T
0.6097087145990374	0.7010715069959521	0.5016365025660162	T T T
0.6092846963789660	0.4726744851606551	0.5022183311675206	T T T
0.4729875734522754	0.4722202861638981	0.5173955749363707	T T T
0.5422184386876017	0.3535109308796319	0.4935879104438189	T T T
0.4041036523561015	0.3573000859523878	0.4988450206376952	T T T
0.4703268048451100	0.2429291746597364	0.4895321656805670	T T T
0.3395943202240210	0.4736183076993008	0.4960709943880868	T T T
0.4063694460794953	0.5956062032760430	0.5064387601227273	T T T
0.2769543922245205	0.5887900552231734	0.4822910388992769	T T T
0.6725316410590136	0.3587643097629875	0.4787738578007658	T T T

0. 4757894771477073 0. 7092198343370664 0. 5091587897841410 T T T

Au

1. 000000000000000

20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

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Au

13

Selective dynamics

Direct

0. 5385491841937524 0. 5873615914382250 0. 5333348488261043 T T T

0. 6786015470992429 0. 5791504517941223 0. 5066562663651921 T T T

0. 6101536593458262 0. 6919622040569724 0. 4934762857152614 T T T

0. 5975646317821920 0. 4755991789870508 0. 4942768871115217 T T T

0. 4691738605313273 0. 4705337129172935 0. 5381178876435800 T T T

0. 5447037149948553 0. 3526866956364301 0. 4904332357815803 T T T

0. 4066234598827290 0. 3580698183362085 0. 4987565881824568 T T T

0. 4718736589089403 0. 2430900110612789 0. 4890044308091940 T T T

0. 3411465358793235 0. 4742665783342321 0. 4917276129349348 T T T

0. 4065124659823057 0. 5947784767572616 0. 5144179866024653 T T T

0. 2828605820250797 0. 5911808371318823 0. 4706018227939662 T T T

0. 6752231791822387 0. 3730829938352941 0. 4736696572280024 T T T

0. 4770135201922046 0. 7082379794483250 0. 5055264900057109 T T T

Au

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20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

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Au

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Selective dynamics

Direct

0. 5382841831353922 0. 5859369610012239 0. 5458093321013778 T T T

0. 6764717510175094 0. 5675689327123993 0. 5045748627405321 T T T

0. 6122867966924713 0. 6826174751906925 0. 4914613610914049 T T T

0. 5804640885276792 0. 4799778762198335 0. 4780387663871019 T T T

0. 4660806541718275 0. 4692987202593606 0. 5483783045210749 T T T

0. 5489408484322994 0. 3514411990156825 0. 4890482749373259 T T T

0. 4087163022738433 0. 3593116750515617 0. 4973871943322593 T T T

0. 4739857355971543 0. 2440469559514329 0. 4896324057158593 T T T

0. 3421460036284764 0. 4747603543936635 0. 4895560684754370 T T T

0. 4075979645695151 0. 5933245578086426 0. 5204584545071975 T T T

0. 2884035350647162 0. 5940386474884903 0. 4668074464937383 T T T

0. 6773409029702160 0. 3932216248844365 0. 4789742663282813 T T T

0. 4792812339189235 0. 7044555497487750 0. 4998732623683679 T T T
Au

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Au

13

Selective dynamics

Direct

0. 5406195439352490 0. 5818824126996405 0. 5556804271077926 T T T
0. 6728384245724164 0. 5562142684641640 0. 5031243658615454 T T T
0. 6116188106222327 0. 6740783654607719 0. 4888579119968149 T T T
0. 5652206288733944 0. 4848434421631446 0. 4648471533854093 T T T
0. 4659251443996143 0. 4663929299585518 0. 5547726805872110 T T T
0. 5512160029776456 0. 3546530022214219 0. 4894053989052400 T T T
0. 4090607789941034 0. 3602944504282954 0. 4952134228909220 T T T
0. 4773536164159579 0. 2464773762440426 0. 4897238660255986 T T T
0. 3444179756749773 0. 4759213372224139 0. 4871432657415430 T T T
0. 4097443754074588 0. 5900358405373999 0. 5304288503644493 T T T
0. 2980930590332560 0. 5988849699208965 0. 4637250716918422 T T T
0. 6747946442271562 0. 4137165176246499 0. 4852579264979898 T T T
0. 4790969948665920 0. 6966056167768500 0. 4918196589436186 T T T

Au

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Selective dynamics

Direct

0. 5436007027510266 0. 5789731433110470 0. 5640723071115256 T T T
0. 6720551163473925 0. 5584359438727707 0. 5032424775481246 T T T
0. 6007021555823413 0. 6706466405971249 0. 4833092951505776 T T T
0. 5630042952267202 0. 4885403644753617 0. 4640591828933091 T T T
0. 4682549796764638 0. 4621708123346535 0. 5586852815184468 T T T
0. 5495443667104425 0. 3575373456073133 0. 4884914668256571 T T T
0. 4079443244211461 0. 3614575031386513 0. 4924916362598205 T T T
0. 4769310639338541 0. 2480190707022914 0. 4887097596840834 T T T
0. 3483007191669814 0. 4795694386197848 0. 4841091250502154 T T T
0. 4117028387114086 0. 5843754940350711 0. 5478989767475604 T T T
0. 3181462989703180 0. 6092601647253360 0. 4595388218333004 T T T
0. 6725166996951226 0. 4172519826964892 0. 4856130077068140 T T T

0. 4672964388067994 0. 6837626256034708 0. 4797786616705406 T T T

Au

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Selective dynamics

Direct

0. 5433559367025697 0. 5808824737204425 0. 5790629484144640 T T T

0. 6741323259268707 0. 5582751822305883 0. 5279932733512521 T T T

0. 5963911647197152 0. 6474104188554730 0. 4632341122868694 T T T

0. 5611369644647870 0. 5108619308669061 0. 4566315156202360 T T T

0. 4697509472006312 0. 4667034700604317 0. 5571494721552225 T T T

0. 5442699305791759 0. 3756238636999260 0. 4796674145640271 T T T

0. 4048206569975461 0. 3665192738978165 0. 4916944823438624 T T T

0. 4825676629147321 0. 2594421682776061 0. 4787104369807744 T T T

0. 3498110069172385 0. 4859585515806599 0. 4886778680179589 T T T

0. 4082637900983270 0. 5869070153239784 0. 5731349663100052 T T T

0. 3327741582171441 0. 6169268334194882 0. 4624170954694072 T T T

0. 6653871276256358 0. 4287945969816100 0. 4892116000281556 T T T

0. 4673383276356688 0. 6156947495745965 0. 4524148144577529 T T T

Au

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Au

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Selective dynamics

Direct

0. 5487275828849935 0. 5674423960848584 0. 5806588346638035 T T T

0. 6725544606867707 0. 5536224391395534 0. 5226305392519007 T T T

0. 5888675193207932 0. 6498225446685489 0. 4723457095857350 T T T

0. 5536493647368216 0. 5201635301762981 0. 4433182130998810 T T T

0. 4702387392478469 0. 4578946896408156 0. 5824571042253355 T T T

0. 5218901259978033 0. 3913653915834540 0. 4657182970838697 T T T

0. 3943910492607918 0. 3676773674181873 0. 5091823453622242 T T T

0. 4825037405605547 0. 2683769835173553 0. 5004202092404493 T T T

0. 4141497576630705 0. 4918360567623877 0. 4554311478999389 T T T

0. 4145897741825778 0. 5810836192370714 0. 5743269827529595 T T T

0. 3282407141408496 0. 5992160045306867 0. 4723703808285922 T T T

0. 6501686938751396 0. 4292218876326924 0. 4748482956858625 T T T

0. 4600284774420193 0. 6222776372291784 0. 4462919403194633 T T T
Au
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Au

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Selective dynamics

Direct

0. 5489689254834398 0. 5596912765144367 0. 5741732950654075 T T T
0. 6691322114987037 0. 5412786267645255 0. 5128545110070509 T T T
0. 5917866549763168 0. 6524520817767879 0. 4764596098054034 T T T
0. 5548650479314405 0. 5250295506723709 0. 4330442089621359 T T T
0. 4850586928707439 0. 4416282098548826 0. 5754674590167080 T T T
0. 5057524970774625 0. 4021317453828459 0. 4326569267103270 T T T
0. 3933948817689135 0. 3675338823236898 0. 5038004136352294 T T T
0. 5173623516180657 0. 3103003326005548 0. 5317690658491043 T T T
0. 4084984305513798 0. 4947976514711212 0. 4465215617627695 T T T
0. 4150606079740521 0. 5592816721355818 0. 5732690543289829 T T T
0. 3309893835097396 0. 6047595987501662 0. 4756093229275032 T T T
0. 6170951253593735 0. 4160395618017733 0. 5097283658713977 T T T
0. 4620351893804038 0. 6250763573690975 0. 4546462050580294 T T T

\$POSCAR 1 Au

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13

Selective dynamics

Direct

0. 5357150000000001 0. 5738070000000000 0. 5768980000000000 T T T
0. 6375940000000000 0. 5165230000000000 0. 5027440000000000 T T T
0. 5955990000000000 0. 6508310000000000 0. 4794500000000000 T T T
0. 5423990000000000 0. 5463960000000000 0. 4068010000000000 T T T
0. 5158440000000000 0. 4418080000000000 0. 5834790000000000 T T T
0. 5214640000000000 0. 4187600000000000 0. 4404560000000000 T T T
0. 4003340000000000 0. 3938860000000000 0. 5131840000000000 T T T
0. 5096710000000000 0. 3128130000000000 0. 5305460000000000 T T T
0. 4140100000000000 0. 5020450000000000 0. 4251330000000000 T T T
0. 4085680000000000 0. 5243660000000000 0. 5636400000000000 T T T
0. 3316110000000000 0. 5982800000000000 0. 4775450000000000 T T T
0. 6274570000000000 0. 3847540000000000 0. 5235800000000000 T T T
0. 4597340000000000 0. 6357320000000000 0. 4765440000000000 T T T

Pathway 37

\$POSCAR 1 Au

1.000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

13

Selective dynamics

Direct

0.5413900000000000	0.5883890000000001	0.5000000000000000	T T T
0.6791990000000000	0.5877910000000000	0.5000000000000000	T T T
0.6100010000000000	0.7029950000000000	0.5000000000000000	T T T
0.6108190000000000	0.4725290000000000	0.5000000000000000	T T T
0.4735870000000000	0.4731960000000000	0.5000000000000000	T T T
0.5423500000000000	0.3531990000000000	0.5000000000000000	T T T
0.4039430000000000	0.3571860000000000	0.5000000000000000	T T T
0.4706060000000000	0.2425900000000000	0.5000000000000000	T T T
0.3388330000000000	0.4732430000000000	0.5000000000000000	T T T
0.4059430000000000	0.5960410000000000	0.5000000000000000	T T T
0.2742580000000000	0.5880910000000000	0.5000000000000000	T T T
0.6733220000000000	0.3553700000000000	0.5000000000000000	T T T
0.4757490000000000	0.7093800000000000	0.5000000000000000	T T T

Au

1.0000000000000000

20.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.0000000000000000	0.0000000000000000
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Au

13

Selective dynamics

Direct

0.5399362596042701	0.5879879855009947	0.4887785212139832	T T T
0.6789675832525947	0.5852552690942359	0.4957135516578394	T T T
0.6094069722889570	0.6948567115140012	0.5280549711970717	T T T
0.6089532815284328	0.4735329739764926	0.4758688024885990	T T T
0.4717447020952724	0.4734341359341004	0.4729135208884382	T T T
0.5436475104244164	0.3559346700244960	0.4970147399333409	T T T
0.4059396973081850	0.3591151978987910	0.5048771891210847	T T T
0.4750812919606393	0.2506383773805033	0.5365487204925028	T T T
0.3380950747337975	0.4727688198432874	0.4924339668563791	T T T
0.4048686123233279	0.5951871197751201	0.4960281081603077	T T T
0.2732216605092762	0.5872287388339283	0.5004521277175638	T T T
0.6746847087616310	0.3593447584052104	0.4878746837222361	T T T

0. 4754531603981089 0. 7047142114410937 0. 5234410965505910 T T T

Au

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20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

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Au

13

Selective dynamics

Direct

0. 5375404298690075 0. 5850533528085901 0. 4813465701918316 T T T

0. 6753710914280558 0. 5646655594216546 0. 5066968781399683 T T T

0. 6136787112292338 0. 6765902701895815 0. 5417400115283412 T T T

0. 6009279958445014 0. 4735958483107094 0. 4432667615608434 T T T

0. 4656301215840599 0. 4742345853223162 0. 4520613934183382 T T T

0. 5471512727715671 0. 3639322508489781 0. 4994420595029335 T T T

0. 4089764642846309 0. 3640572902905373 0. 5080878811376929 T T T

0. 4827352841704204 0. 2656829461290337 0. 5576134727006642 T T T

0. 3349722050421229 0. 4724443886677395 0. 4862362223740841 T T T

0. 4030945819154791 0. 5947036128461840 0. 4923393867553086 T T T

0. 2715326183616515 0. 5878108124698425 0. 4964862666864566 T T T

0. 6792015759500498 0. 3819422729872915 0. 4978646117793871 T T T

0. 4791881660830920 0. 6952857726399488 0. 5368184842241304 T T T

Au

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20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

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Au

13

Selective dynamics

Direct

0. 5358555744235943 0. 5758642986701359 0. 4831854027642695 T T T

0. 6680499825986936 0. 5409078670544308 0. 5136410578000921 T T T

0. 6184809228416200 0. 6576869207611798 0. 5504461070331699 T T T

0. 5934326719902299 0. 4719361305526801 0. 4182792289361855 T T T

0. 4600822514948738 0. 4746762964789373 0. 4343865835044284 T T T

0. 5517980943097240 0. 3773961548548178 0. 5046091165237254 T T T

0. 4128386951132024 0. 3733742673759710 0. 5122275292141593 T T T

0. 4902239213572014 0. 2869030337797436 0. 5759454661764936 T T T

0. 3318502705999012 0. 4720026306809004 0. 4768641589361837 T T T

0. 4011804307344004 0. 5915499878959927 0. 4944494737546691 T T T

0. 2696871524516855 0. 5886625873040601 0. 4889463421321962 T T T

0. 6839217910496614 0. 4075266336703454 0. 4981191493037432 T T T

0. 4825987607164960 0. 6815121515583448 0. 5489003839206930 T T T

Au

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20. 0000000000000000 0. 0000000000000000 0. 0000000000000000

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Au

13

Selective dynamics

Direct

0. 5341404806658129 0. 5491846263313308 0. 5025668960699680 T T T

0. 6710536740508908 0. 5405726383595704 0. 5091699548221266 T T T

0. 6063573479590977 0. 6486949910119882 0. 5491891904849220 T T T

0. 5962917627662474 0. 4679423096766686 0. 4085757703107795 T T T

0. 4620508856844885 0. 4721442812039235 0. 4153486992606035 T T T

0. 5556306718427952 0. 3871374204789054 0. 5083192200610485 T T T

0. 4191540645237245 0. 4009361651834416 0. 5231664215332579 T T T

0. 4863074155967732 0. 3081822446447270 0. 5872944325639624 T T T

0. 3299572144337740 0. 4747174664602540 0. 4575050370627859 T T T

0. 4030860699114271 0. 5749562365851357 0. 5067969119821356 T T T

0. 2743050698718177 0. 5940316296533553 0. 4857357003033261 T T T

0. 6889941665635784 0. 4083658562051354 0. 4909211394813224 T T T

0. 4726716961174555 0. 6731330942299362 0. 5554106260637652 T T T

Au

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Au

13

Selective dynamics

Direct

0. 5409754551309340 0. 5185612413950992 0. 5189233866664839 T T T

0. 6713504568573512 0. 5500199263286513 0. 5091676874235790 T T T

0. 5819879424280001 0. 6432386838160876 0. 5391674913064493 T T T

0. 5962882813009129 0. 4594791692917474 0. 4000787175570165 T T T

0. 4642344192269802 0. 4703673421925279 0. 4083655020941828 T T T

0. 5564894725286390 0. 3787617671128564 0. 5023924628530824 T T T

0. 4297562465479363 0. 4247430414061308 0. 5359103856544286 T T T

0. 4769894035000817 0. 3089496364623995 0. 5804718674416405 T T T

0. 3338530159366184 0. 4789945280055113 0. 4540802440428569 T T T

0. 4153337480185396 0. 5647655924569588 0. 5185025172213793 T T T

0. 2908737033597736 0. 6016293020402684 0. 4874188645364510 T T T

0. 6872214722819437 0. 4169549708216644 0. 4924549920606934 T T T

0. 4546469028763940 0. 6835337586820601 0. 5530658811417544 T T T

Au

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Au

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Selective dynamics

Direct

0. 5549042197215924 0. 4938756668078689 0. 5502160680401351 T T T

0. 6666808832342359 0. 5620261088684168 0. 5023734091461449 T T T

0. 5555303004424299 0. 6310894094256519 0. 5292369674407135 T T T

0. 5944935491969299 0. 4803255847763968 0. 4094918087481255 T T T

0. 4623993308297533 0. 4678936973188261 0. 4128963860315412 T T T

0. 5491656307492397 0. 3718191666069364 0. 4773400296199892 T T T

0. 4341240612175815 0. 4200664338350162 0. 5437456512085015 T T T

0. 4743070650689343 0. 2939551454390915 0. 5536544059435640 T T T

0. 3367032027785796 0. 4843527697350368 0. 4704481976605696 T T T

0. 4381277734659174 0. 5572510902286579 0. 5287317691407870 T T T

0. 3264723939448876 0. 6188643263415350 0. 4863179820566015 T T T

0. 6704509716328894 0. 4262990659190705 0. 5173972319627276 T T T

0. 4366411377693834 0. 6921804945927928 0. 5181500930006171 T T T

Au

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Au

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Selective dynamics

Direct

0. 5576785477289958 0. 4925783405171494 0. 5704700210700446 T T T

0. 6736415779844107 0. 5525888981742665 0. 5185532069585638 T T T

0. 5586762611556449 0. 6233789783924046 0. 5137443985853712 T T T

0. 5772239442741653 0. 5124989641841085 0. 4253498743705786 T T T

0. 4462726009989471 0. 4878097303300055 0. 4175007323413085 T T T

0. 5349957226444377 0. 3892105541382257 0. 4593117265632917 T T T

0. 4420487317679706 0. 4197956221420220 0. 5620224663294408 T T T

0. 4818114710947036 0. 2954569401986075 0. 5366887036540338 T T T

0. 3336563703645628 0. 4742318292567997 0. 4983100990528612 T T T

0. 4400174433248304 0. 5559163000447659 0. 5455610830194807 T T T

0. 3547254353082466 0. 5947928414176938 0. 4429107683688538 T T T

0. 6578574810165704 0. 4178272120650871 0. 5162559601823702 T T T

0. 4413949355987758 0. 6839127426145689 0. 4933209595037921 T T T
Au
1. 000000000000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

Au

13

Selective dynamics

Direct

0. 5681442208546299 0. 5056688799229838 0. 5833232689046839 T T T
0. 6799624760139257 0. 5597387945492340 0. 5221108374033602 T T T
0. 5630939900297557 0. 6274168059081117 0. 5072720482264530 T T T
0. 5840695781698709 0. 5133393579243866 0. 4319425994988145 T T T
0. 4540032109789620 0. 4991149151342995 0. 4110689216914755 T T T
0. 5262235342044165 0. 3918887687029363 0. 4606447115590258 T T T
0. 4638244590381079 0. 4232716652629060 0. 5846298142783947 T T T
0. 4198212425999247 0. 3206235198878308 0. 5084737721575115 T T T
0. 3588394612357256 0. 4422042783964785 0. 4930258715243451 T T T
0. 4461101066829027 0. 5526587146874854 0. 5482980032351293 T T T
0. 3454829896838020 0. 5710110553796447 0. 4546028521133790 T T T
0. 6508935615202780 0. 4226673453552360 0. 5124659902729058 T T T
0. 4395316921479699 0. 6703948525680162 0. 4821413091345256 T T T

\$POSCAR 1 Au

1. 000000
20. 0000000000000000 0. 0000000000000000 0. 0000000000000000
0. 0000000000000000 20. 0000000000000000 0. 0000000000000000
0. 0000000000000000 0. 0000000000000000 20. 0000000000000000

13

Selective dynamics

Direct

0. 5546940000000000 0. 5411220000000000 0. 5769650000000000 T T T
0. 6831190000000000 0. 5450430000000001 0. 5224520000000000 T T T
0. 5931689999999999 0. 6461980000000001 0. 4946260000000000 T T T
0. 5768580000000000 0. 5217800000000000 0. 4350030000000000 T T T
0. 4475920000000000 0. 5151440000000000 0. 4017130000000000 T T T
0. 5119939999999999 0. 4016290000000000 0. 4435850000000000 T T T
0. 4905310000000000 0. 4203600000000000 0. 5810630000000000 T T T
0. 4301640000000000 0. 3171220000000000 0. 5140140000000000 T T T
0. 3725750000000000 0. 4349160000000000 0. 4889740000000000 T T T
0. 4212330000000000 0. 5381470000000000 0. 5705470000000000 T T T
0. 3357920000000000 0. 5645120000000000 0. 4655740000000000 T T T
0. 6207460000000000 0. 4230140000000000 0. 5293400000000000 T T T
0. 4615340000000000 0. 6310110000000000 0. 4761440000000000 T T T