

Supplementary Information

New routes for improving adhesion at metal/ α -Al₂O₃(0001) interface

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1. Structural information on metal M = Cr, Ni, Ag, and Zn adatoms adsorbed on bare (3O) and (Al) terminations [(3O)M_y and (Al)+M, respectively], and on hydroxylated (Al) termination [(Al)OHM_y], as obtained from VASP calculations at the LDA level, Fig. 5.

(3O)Cr

4.697352000000000

1.0000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.8660254030004244	0.0000000000000000
0.0000000000000000	0.0000000000000000	4.3980452500000000

Al O Cr

10 18 2

Selective dynamics

Direct

0.3391003514708331	0.6840446782289078	0.1877375788380959	T	T	T
0.0058102037260070	0.3506640883756944	0.2011522798011285	T	T	T
0.6725916116500343	0.0171657808598411	0.2885976716790921	T	T	T
0.3393893417933356	0.6837155877471162	0.3121401947007030	T	T	T
0.0061983510573071	0.3502796786417264	0.3930240017248607	T	T	T
0.6729877883638835	0.0168714353047861	0.4163041100917013	T	T	T
0.3397676469648303	0.6834641931662873	0.4972064980099518	T	T	T
0.0065254065158271	0.3501051707353113	0.5207344156165590	T	T	T
0.6732884048486270	0.0167456233628442	0.6081934918659968	T	T	T
0.3399872942163427	0.6834168936402705	0.6216012019992974	T	T	T
0.0246853911265958	0.0287082844411159	0.1427152046606324	T	T	T
0.3088829214015973	0.3696633099591509	0.1427056271324645	T	T	T
0.6837341953896399	0.6539150282648762	0.1427261671289415	T	T	T
0.3365112583201579	0.9948471720346390	0.2476616845802937	T	T	T
0.6501001239558164	0.3756447170845476	0.2476520698684368	T	T	T
0.0309749717324976	0.6812477876541720	0.2476572881571428	T	T	T
0.9791112426173285	0.0164079658885044	0.3524704189421399	T	T	T
0.3670803625044456	0.3233471569733197	0.3524711696035538	T	T	T
0.6722074373523128	0.7112620782783381	0.3524656909179882	T	T	T
0.3120956381497706	0.0438371279971719	0.4568636668302304	T	T	T
0.7000737502436749	0.3507654016887116	0.4568667030147964	T	T	T
0.0070015541224322	0.6558943301547373	0.4568610875404602	T	T	T
0.0290075525025344	0.9916745890421197	0.5616859207818834	T	T	T
0.3425361825491606	0.3725387120954338	0.5616862055922738	T	T	T
0.6481557974911567	0.6860876298316114	0.5616859198260684	T	T	T
0.3702274640222782	0.9978056751945559	0.6666278385243274	T	T	T
0.6543827968768454	0.3387938295993962	0.6666250375496290	T	T	T
0.9953689207466141	0.7136666271249794	0.6666317941869693	T	T	T

0.6724149263866650 0.0174231426861837 0.1161878053268239 T T T
0.0066547218216684 0.3500913221231272 0.6931400351258787 T T T

(Al)+Cr

4.69735200000000
1.0000000000000000 0.0000000000000000 0.0000000000000000
0.5000000000000000 0.8660254030004244 0.0000000000000000
0.0000000000000000 0.0000000000000000 4.3980452500000000

Al O Cr
12 18 2

Selective dynamics

Direct

0.0164171495555632 0.3291585264456706 0.1754355217056089 T T T
0.6828979177338570 0.9960061101049928 0.2551528884201577 T T T
0.3494432258689970 0.6627083073537431 0.2747746641879963 T T T
0.0160925636202001 0.3293468239766134 0.3585325215751083 T T T
0.6827632835154165 0.9960097653311735 0.3816135459492386 T T T
0.3495088202237132 0.6626619165460866 0.4630797859669442 T T T
0.0162031223596418 0.3293191596744567 0.4860942047480156 T T T
0.6828897597045560 0.9960080881641403 0.5675563304455997 T T T
0.3496041673457325 0.6626894528424517 0.5906450481038650 T T T
0.0162921549324562 0.3293716141371053 0.6743947681950677 T T T
0.6830457567368114 0.9960132957834084 0.6940210465895497 T T T
0.3497990122968963 0.6625997197180605 0.7737394940949820 T T T
0.0349381384169420 0.9727319042153368 0.2132457197916669 T T T
0.3541889945177747 0.3479049225951949 0.2132340649486960 T T T
0.6598798838992522 0.6670666847428132 0.2132831069704058 T T T
0.3758254231214587 0.9949778531076360 0.3176207390511019 T T T
0.6816755049308523 0.3040239842948010 0.3176297520176018 T T T
0.9907850903974326 0.6890706844450052 0.3176235804679882 T T T
0.0159474440279540 0.0231973873693234 0.4223243634683370 T T T
0.3224778973269609 0.3291253716914002 0.4223314951636932 T T T
0.7100250968878619 0.6356596028458518 0.4223231417858359 T T T
0.3497623270957959 0.9687816898506786 0.5268444933828074 T T T
0.6556798471186207 0.3563567654288984 0.5268478517092362 T T T
0.0432346865142667 0.6628623573770825 0.5268467687996702 T T T
0.9898615243930258 0.9971295535628867 0.6315412855021529 T T T
0.3749440028759860 0.3029417111234255 0.6315452902728461 T T T
0.6840306690417643 0.6880158111115268 0.6315485471829489 T T T
0.3310966777643720 0.0191051603820140 0.7359081741587310 T T T
0.7062618099164157 0.3247581993291805 0.7359371088770861 T T T
0.0118952670795769 0.6440084163847611 0.7359132151246268 T T T
0.3506875231048348 0.6623428019184822 0.1417166643287843 T T T
0.0170738371583705 0.3290618331585813 0.8074582192537736 T T T

(Al)OHCr

4.69735200000000
1.0000000000000000 0.0000000000000000 0.0000000000000000
0.5000000000000000 0.8660254030004244 0.0000000000000000

0.0000000000000000 0.0000000000000000 4.3980452500000000

Al O H Cr

12 20 2 2

Selective dynamics

Direct

0.0226934159324451	0.3598051252550051	0.2314687371791108	T	T	T
0.6862965532661452	0.0332034566607382	0.3047992729266224	T	T	T
0.3538835981572810	0.7007319009554821	0.3227088773261752	T	T	T
0.0196920654424149	0.3665421908608560	0.4078774795454491	T	T	T
0.6868450487054893	0.0330605051470989	0.4308046454766122	T	T	T
0.3536532495597096	0.6994035551675257	0.5122507105734780	T	T	T
0.0201548074470549	0.3663830712360039	0.5354644241679963	T	T	T
0.6870116857681056	0.0330457956128061	0.6169146795159082	T	T	T
0.3534095112708637	0.7003793324941632	0.6398379347639329	T	T	T
0.0220294023838116	0.3661746399966067	0.7250034387823554	T	T	T
0.6871113004120599	0.0337518890667273	0.7429166177154931	T	T	T
0.3503880546856621	0.6970765374192617	0.8162755770868223	T	T	T
0.1207268965209419	0.1747918352152104	0.1530650958085508	T	T	T
0.0368401629196995	0.0132785895190699	0.2662733495687935	T	T	T
0.3661003670147692	0.3850283981928723	0.2593197098037269	T	T	T
0.6680971727960646	0.7069257030708712	0.2609327002973291	T	T	T
0.3807049774800407	0.0330117753872717	0.3663497526508905	T	T	T
0.6821552091556884	0.3443958330358235	0.3670093361235859	T	T	T
0.9966315972427763	0.7236088572699482	0.3668462315806376	T	T	T
0.0201372448719385	0.0600480881386967	0.4713949615441553	T	T	T
0.3263535906293287	0.3654887530112015	0.4717009041887896	T	T	T
0.7139172708616999	0.6731051292860893	0.4716239935308380	T	T	T
0.3538383846273232	0.0059977540321183	0.5761388883841395	T	T	T
0.6591414352608815	0.3932181415514901	0.5759796648860780	T	T	T
0.0473436626723075	0.6999003483045582	0.5763303762022848	T	T	T
0.9938217676288801	0.0378986814311810	0.6807189203878111	T	T	T
0.3809950603397378	0.3393884829703733	0.6813704973199903	T	T	T
0.6875636180222178	0.7234325943968501	0.6808636771659939	T	T	T
0.3427493910714549	0.0517912822132782	0.7867872824079281	T	T	T
0.7189447479728501	0.3539414773253540	0.7883494577244358	T	T	T
0.0177241303280716	0.6832742420273988	0.7814906126167410	T	T	T
0.2656963574489395	0.5965984109702970	0.8946745503234103	T	T	T
0.1720927985850412	0.2721086846888809	0.1159883056696140	T	T	T
0.4180610195361792	0.5408485915820841	0.9312841346505244	T	T	T
0.3227504160158385	0.7076348268811691	0.1852802955433231	T	T	T
-0.0011675057429212	0.3965350245497228	0.8623774680740731	T	T	T

(30)Ni_1.5

4.697352000000000

2.0000000000000000 0.0000000000000000 0.0000000000000000

0.5000000000000000 0.8660254030004244 0.0000000000000000

0.0000000000000000 0.0000000000000000 4.3980452500000000

Al O Ni

Selective dynamics

Direct

0.3309173263810789	0.9804845656023603	0.2006436636388758	T	T	T
0.8462303284698640	0.0208634823375605	0.2100333629516143	T	T	T
0.1618189905822418	0.6541420346934234	0.2333666241154740	T	T	T
0.6602073089025220	0.7068236937104646	0.2190034770049447	T	T	T
0.0014266751672303	0.3326118353111241	0.3116994750203164	T	T	T
0.5005977074614059	0.3407155328986004	0.3087623514160126	T	T	T
0.3372493874511817	-0.0001958993046068	0.3311458606974363	T	T	T
0.8305129171045784	0.0076624165794482	0.3347125035585594	T	T	T
0.1687520117090855	0.6669665939863706	0.4150833806144323	T	T	T
0.6668985370202357	0.6731403217463471	0.4142521671221288	T	T	T
0.0017186800237264	0.3341401713562684	0.4381360168582181	T	T	T
0.4998542920661908	0.3403176782656183	0.4373010850516820	T	T	T
0.3313694572848984	0.0074846907240548	0.5212504642801021	T	T	T
0.8380870670641455	0.9996587880890409	0.5176719810364449	T	T	T
0.1680163622395699	0.6665996020328310	0.5436251936749567	T	T	T
0.6671952218632071	0.6746949352378478	0.5406939104320340	T	T	T
0.0084298964146871	0.3004938583450347	0.6333945320250629	T	T	T
0.5068097167739408	0.3531864442854667	0.6190259551874255	T	T	T
0.3377046193126697	0.0268719188014246	0.6517591502374929	T	T	T
0.8224056927668086	0.9864581214982777	0.6423485836010919	T	T	T
0.0398521536961145	0.9331277904571200	0.1656625574260096	T	T	T
0.4935988124651923	0.9939874905955994	0.1632945855837233	T	T	T
0.1470411073147130	0.3353477244332901	0.1650613928084177	T	T	T
0.7292699853997402	0.3745286325295086	0.1586191943071153	T	T	T
0.3829356124774113	0.6205657077837702	0.1472861561853143	T	T	T
0.7878224517831424	0.8051340061130758	0.1578502250136524	T	T	T
0.1845293859565236	0.9874780598803919	0.2687189656218852	T	T	T
0.6805961906470475	0.0134906738801571	0.2695630154106389	T	T	T
0.3322715333625204	0.3101377749688894	0.2689353107531500	T	T	T
0.8353513911356126	0.3212695928011893	0.2705549996862923	T	T	T
0.9835270234308815	0.6982499593359036	0.2716550238686549	T	T	T
0.4896779796590934	0.6935320411881227	0.2660383726232702	T	T	T
0.0013597331187333	0.0280025087160207	0.3742846909667873	T	T	T
0.5008248090819760	0.0315926366190414	0.3731676030704295	T	T	T
0.1556492757097821	0.3324522018646272	0.3731790903860999	T	T	T
0.6519918773087003	0.3417764530208010	0.3742777886556352	T	T	T
0.3479526245234448	0.6437677413710911	0.3734919539754560	T	T	T
0.8483053244184002	0.6441449097870267	0.3749997062090231	T	T	T
0.1677853199927467	0.9757077996613464	0.4792289211473218	T	T	T
0.6672421389068752	0.9793196201235465	0.4781024540241021	T	T	T
0.3206619175042190	0.3635220974093586	0.4789012938992910	T	T	T
0.8203172256339943	0.3631407326802031	0.4773866559370640	T	T	T
0.0166133193120773	0.6655398240826585	0.4781064199900354	T	T	T
0.5129779108898826	0.6748058542157436	0.4792169097178673	T	T	T
0.9880217846399553	0.9938507733998768	0.5828290649202915	T	T	T
0.4841073185150465	0.0198161680301632	0.5836802955685702	T	T	T

0.1789591937774689	0.3137935818670437	0.5863633991762475	T	T	T
0.6850954197864320	0.3090821413535807	0.5807330917484002	T	T	T
0.3363390642109226	0.6971945357339265	0.5834674627856947	T	T	T
0.8332839514972302	0.6860606124963374	0.5818266744349478	T	T	T
0.1750250823652088	0.0133653154329000	0.6891045595572934	T	T	T
0.6287666897602169	0.0742878668840407	0.6867313172160585	T	T	T
0.2856838831324103	0.3867608030851361	0.7051357097889188	T	T	T
0.8807980686700168	0.2022282138410531	0.6945386239674742	T	T	T
0.9393391827783002	0.6328403331565202	0.6937731028537352	T	T	T
0.5215928791675905	0.6720298866205874	0.6873391160694782	T	T	T
0.9387608125955657	0.3687373144929302	0.1471011024127935	T	T	T
0.5834859692849815	0.2305875160102323	0.1411549328499738	T	T	T
0.2160895647400035	0.5767479211692423	0.1182292655970047	T	T	T
0.0851463684324662	0.7767649159125366	0.7112357176146922	T	T	T
0.7298546962110828	0.6386627426894537	0.7052755555185830	T	T	T
0.4525155417778698	0.4306893506916263	0.7341655661674081	T	T	T

(Al)+Ni

4.69735200000000

1.0000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.8660254030004244	0.0000000000000000
0.0000000000000000	0.0000000000000000	4.3980452500000000

Al O Ni

12 18 2

Selective dynamics

Direct

0.0154752854881863	0.3300183074005716	0.1787125196352264	T	T	T
0.6832190007463197	0.9956802652003987	0.2553617640486792	T	T	T
0.3497930102961888	0.6628487907563354	0.2739785771375196	T	T	T
0.0163586075488240	0.3293670538087028	0.3585338835856859	T	T	T
0.6830122596171506	0.9960536122622656	0.3816040975937582	T	T	T
0.3496520860509875	0.6626931548589567	0.4630357254825839	T	T	T
0.0162682553643947	0.3293699086613984	0.4861362920671723	T	T	T
0.6828582031898591	0.9960509990097108	0.5675628278047569	T	T	T
0.3495098656816111	0.6627756363187558	0.5906438214113265	T	T	T
0.0159880696754442	0.3294768132662256	0.6751967862505381	T	T	T
0.6827326262002842	0.9964525677612883	0.6938101074656586	T	T	T
0.3499654169677413	0.6621777225999068	0.7704600272029722	T	T	T
0.0317417537196150	0.9758380695427888	0.2132841116878765	T	T	T
0.3538681465078000	0.3445940751863930	0.2135922409122983	T	T	T
0.6621653925499231	0.6675469846273430	0.2134090871027894	T	T	T
0.3760376395926031	0.9944872727680121	0.3175723714935330	T	T	T
0.6815686801883558	0.3044982753931009	0.3175434409264923	T	T	T
0.9916304735766914	0.6890572609770018	0.3175485229852342	T	T	T
0.0160562608911263	0.0233136930981104	0.4223142311700485	T	T	T
0.3226772790679604	0.3290786188278574	0.4223120492629207	T	T	T
0.7102961794418405	0.6356854116430313	0.4223063561989804	T	T	T
0.3498620013555964	0.9687545157344388	0.5268557930873285	T	T	T
0.6556186341504429	0.3564056420068695	0.5268663788197756	T	T	T

0.0432507845100218	0.6630006646903084	0.5268650323769606	T	T	T
0.9897991985510046	0.9977335537336529	0.6316033272842674	T	T	T
0.3742404713479317	0.3030936870893370	0.6316230299056258	T	T	T
0.6843066504659205	0.6876597134365312	0.6316184269101655	T	T	T
0.3341641434070723	0.0160921297354122	0.7358140161334248	T	T	T
0.7035688609394271	0.3246545842128654	0.7358134320598850	T	T	T
0.0117954462448466	0.6474177150606906	0.7356047269587691	T	T	T
0.3481478787639531	0.6577215284280840	0.1465368665974722	T	T	T
0.0196000173842563	0.3314172469164376	0.8026435306803847	T	T	T

(Al)OHNi_0.5

4.69735200000000

2.0000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.8660254030004244	0.0000000000000000
0.0000000000000000	0.0000000000000000	4.3980452500000000

Al O H Ni

24 40 4 2

Selective dynamics

Direct

0.0044140706328014	0.3357587155983474	0.2342322991783392	T	T	T
0.5024771731415127	0.3364048995384959	0.2341563579600023	T	T	T
0.3382005205930239	0.0148178045986394	0.3058986220300036	T	T	T
0.8326501353867490	0.0042014517547196	0.3037539473107724	T	T	T
0.1676905901465161	0.6788875278631372	0.3266150871676946	T	T	T
0.6698094295651680	0.6688820799732687	0.3145376740128881	T	T	T
0.9986106470079170	0.3431861989764589	0.4078418243760854	T	T	T
0.5048673433744354	0.3386020409931804	0.4065951776369426	T	T	T
0.3354025942918656	0.0078035049068895	0.4311190119630924	T	T	T
0.8345005406632041	0.0069554250810022	0.4293457450515744	T	T	T
0.1680626498885846	0.6752128640282188	0.5118657121637578	T	T	T
0.6683885517258166	0.6733679223816468	0.5112309927291915	T	T	T
0.0014504294341333	0.3419822688275835	0.5350961026942561	T	T	T
0.5017749201032761	0.3401349925162418	0.5344654278498273	T	T	T
0.3344328580543918	0.0075461355629696	0.6152151852093741	T	T	T
0.8353419330073791	0.0083685138073147	0.6169840411078062	T	T	T
0.1649864942523724	0.6767267978116300	0.6397322304585248	T	T	T
0.6712294751049800	0.6721408200175107	0.6384768691472346	T	T	T
0.0000577092274858	0.3464456505380878	0.7317909311921365	T	T	T
0.5021709126386791	0.3363982991733146	0.7197136615675898	T	T	T
0.3316787964490728	0.0004660558368843	0.7404378585871818	T	T	T
0.8372118164046863	0.0111299054762413	0.7425694139774058	T	T	T
0.1673792585691202	0.6789080870119958	0.8121755224852518	T	T	T
0.6654700027581076	0.6795338093326394	0.8121044905639101	T	T	T
0.0709372973866436	0.1394085776061427	0.1558424480077782	T	T	T
0.4029410513962648	0.4289787850386281	0.1555830591396652	T	T	T
0.0135992769289932	0.9775514098355998	0.2639130378524051	T	T	T
0.5075372050664677	0.9858921265141022	0.2620163391519843	T	T	T
0.1758884330780304	0.3649284584777551	0.2599038717225610	T	T	T
0.6748513227244461	0.3451773999789491	0.2593731111274069	T	T	T

0.3242215560355810	0.6838789009424229	0.2663566070896847	T	T	T
0.8297695440586992	0.6778453461480947	0.2597673054935959	T	T	T
0.1801894201993791	0.0150076176621871	0.3666024642256613	T	T	T
0.6822151659439517	-0.0003521851264203	0.3651993493692336	T	T	T
0.3333255189000509	0.3196906910743872	0.3677171509340592	T	T	T
0.8346387549498407	0.3151120381949160	0.3643526328619187	T	T	T
0.9901720285725326	0.6983332629324217	0.3670353677863669	T	T	T
0.4904486236969359	0.6991177376931631	0.3654117116398016	T	T	T
0.0007199363588318	0.0351185355572017	0.4707130319551323	T	T	T
0.5021689350691468	0.0349332506405760	0.4709358046423604	T	T	T
0.1544891915260565	0.3408610570538306	0.4716807621931289	T	T	T
0.6554756757291615	0.3393646028938374	0.4703681528607940	T	T	T
0.3486700188045396	0.6474091651526366	0.4708566821723050	T	T	T
0.8483648251464465	0.6474684034783146	0.4709548552036214	T	T	T
0.1676600525522312	0.9804234256134617	0.5753999393958853	T	T	T
0.6691258327776575	0.9802214078829659	0.5756129853682570	T	T	T
0.3211714383622236	0.3679410669970999	0.5754765826270702	T	T	T
0.8214825309772767	0.3678566082424016	0.5753725256411669	T	T	T
0.0143712140809389	0.6759527411096279	0.5759652604375406	T	T	T
0.5153481858167880	0.6744810679112250	0.5746481354474426	T	T	T
0.9876326118005562	0.0156855017335675	0.6811263166029704	T	T	T
0.4896635799886450	0.0003121774325813	0.6797250837632439	T	T	T
0.1794069954514007	0.3162102061556776	0.6809208939504908	T	T	T
0.6796742659880532	0.3169862655420059	0.6792873410660524	T	T	T
0.3365314809158378	0.6956385406595847	0.6786137686827808	T	T	T
0.8352121006548689	0.7002136539166630	0.6819730724661780	T	T	T
0.1623338769177317	0.0294244375083561	0.7843162293463984	T	T	T
0.6562647301192214	0.0377427027080092	0.7824115807706957	T	T	T
0.3456309963586100	0.3314406582521596	0.7799713547289122	T	T	T
0.8401080996753014	0.3374271362637137	0.7865637209153138	T	T	T
0.9950004453788384	0.6701520634015744	0.7869516187449692	T	T	T
0.4939913120733474	0.6503715548190456	0.7864294968625112	T	T	T
0.2668901891140608	0.5864243525464093	0.8907526719561413	T	T	T
0.5989249933111463	0.8759273681422798	0.8904880575379586	T	T	T
0.1289445825967800	0.1962002000831427	0.1238965532408360	T	T	T
0.4260913156038157	0.2398635222139826	0.1287790393064037	T	T	T
0.2437406700553917	0.7757003657127437	0.9175136503756770	T	T	T
0.5408526345423896	0.8191733958354190	0.9224181652933278	T	T	T
0.1802312915141561	0.7019865436315098	0.1981113030006953	T	T	T
0.4896271932951523	0.3133594244885924	0.8482154558991410	T	T	T

(30)Ag_1.5

4.69735200000000

2.0000000000000000 0.0000000000000000 0.0000000000000000

0.5000000000000000 0.8660254030004244 0.0000000000000000

0.0000000000000000 0.0000000000000000 4.3980452500000000

Al O Ag

20 36 6

Selective dynamics

Direct

0.3240618362856719	0.9878651098776203	0.2061787893397612	T	T	T
0.8438092688471496	0.0257581356577338	0.2096773638965364	T	T	T
0.1735965994153879	0.6432278492677858	0.2231960374750768	T	T	T
0.6554832376296802	0.7078336079235797	0.2212531839136521	T	T	T
0.0022345640230055	0.3358725465460806	0.3103945051077640	T	T	T
0.4989089830715228	0.3391235314771062	0.3103429336812500	T	T	T
0.3352947485680803	0.0007599085403308	0.3324854347891085	T	T	T
0.8331276419843228	0.0061717013146117	0.3339441541597238	T	T	T
0.1675338468959110	0.6696722226413462	0.4144231364308055	T	T	T
0.6676705432791264	0.6708396691225935	0.4145911145880966	T	T	T
0.0009325119145400	0.3364580639576951	0.4377980938938119	T	T	T
0.5010790167641844	0.3376124040168281	0.4379677628863411	T	T	T
0.3333114175613657	0.0065728376651502	0.5199107169845031	T	T	T
0.8354823381684011	0.0011447344155449	0.5184524386018697	T	T	T
0.1697032514742625	0.6682071886229897	0.5420467519032010	T	T	T
0.6663898471261562	0.6714070616407215	0.5419947944156671	T	T	T
0.0131224071076288	0.2995039351576679	0.6311516850286448	T	T	T
0.4950229393129630	0.3641178546220528	0.6291967010777134	T	T	T
0.3445666858401548	0.0194972596611776	0.6462160127078208	T	T	T
0.8248031296969732	0.9815181083804623	0.6427136215109053	T	T	T
0.0264101607815129	0.9196031978521618	0.1628783677992458	T	T	T
0.4893291420023035	0.9427160736106064	0.1604955360096459	T	T	T
0.1680238827881077	0.3337560007629490	0.1636026432413650	T	T	T
0.7270642314909566	0.3940478933541047	0.1578792216154623	T	T	T
0.3270665034433045	0.6504487714216634	0.1639093640388128	T	T	T
0.7721259943767916	0.8469007391649537	0.1524921266805341	T	T	T
0.1796050418608981	-0.0097624119303493	0.2693500350645261	T	T	T
0.6785220345883819	0.0176867336674610	0.2677247275258220	T	T	T
0.3336523560697982	0.3022856253609502	0.2696350332240051	T	T	T
0.8330713940115865	0.3279664914773287	0.2695776347134572	T	T	T
0.9865704469482754	0.6965033201370231	0.2685143424660901	T	T	T
0.4898468010945746	0.6904693484920797	0.2686759185647636	T	T	T
0.0003705394550694	0.0309393741974066	0.3739706191654864	T	T	T
0.5012263300870605	0.0302194658651050	0.3737360939238155	T	T	T
0.1543685247320550	0.3350699827950944	0.3735372293420116	T	T	T
0.6536847109906553	0.3374705188250547	0.3742959094778601	T	T	T
0.3479896133831285	0.6430258712308364	0.3740607860478183	T	T	T
0.8477040803244765	0.6453107373602551	0.3741160109740102	T	T	T
0.1673742778296964	0.9771134041716163	0.4786568118215117	T	T	T
0.6682456099350702	0.9763640418496601	0.4784207929407928	T	T	T
0.3206221966934602	0.3642868682013782	0.4783322640914549	T	T	T
0.8209083709194686	0.3619873917255020	0.4782753576478971	T	T	T
0.0149266845507182	0.6698271030685169	0.4780959381587228	T	T	T
0.5142426452578907	0.6722305368084344	0.4788555351131108	T	T	T
0.9901042142228869	-0.0103833082528395	0.5846632065080135	T	T	T
0.4890313530494273	0.0170869669355015	0.5830468007868573	T	T	T
0.1787762559664286	0.3168758490532765	0.5837285676309331	T	T	T
0.6820520551966160	0.3107915411636279	0.5838807711603944	T	T	T

0.3349670182463996	0.7050584295115596	0.5827583053814045	T	T	T
0.8355532305444534	0.6793028063955406	0.5828241430442069	T	T	T
0.1793118805938259	0.0646406901923524	0.6918994284167975	T	T	T
0.6422066191084633	0.0877603904925044	0.6895204038054378	T	T	T
0.3415442180537535	0.3569514843750078	0.6884823203400414	T	T	T
0.8965067703750369	0.1604831557258314	0.6998648260392911	T	T	T
0.9415752221464828	0.6132833445100178	0.6945332055737989	T	T	T
0.5006131034244684	0.6736033250990174	0.6887764984023124	T	T	T
0.9473561485504597	0.3814753878330822	0.1403514902513630	T	T	T
0.5514493519833721	0.2724261091748355	0.1403031189074404	T	T	T
0.1923862392372119	0.6055168699578597	0.0796158646784290	T	T	T
0.1171467572544185	0.7349945183250552	0.7120752612728317	T	T	T
0.7212779618528179	0.6258302777190488	0.7120612356293544	T	T	T
0.4762779827425812	0.4019139643925144	0.7727686041697156	T	T	T

(Al)+Ag

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1.0000000000000000	0.0000000000000000	0.0000000000000000
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0.0000000000000000	0.0000000000000000	4.3980452500000000

Al O Ag

12 18 2

Selective dynamics

Direct

0.0159253481311181	0.3291824680127914	0.1879404899861032	T	T	T
0.6827655092150529	0.9957386146224485	0.2564359327715911	T	T	T
0.3493804772764738	0.6625459580392837	0.2713731669844011	T	T	T
0.0161256647247884	0.3292890593180170	0.3586762451922724	T	T	T
0.6828040666338858	0.9960055723743253	0.3816326590517280	T	T	T
0.3496359252058433	0.6626764236608864	0.4628864141918931	T	T	T
0.0163764321549415	0.3293023488354385	0.4862559444537073	T	T	T
0.6830796588329399	0.9960343006001435	0.5675044214973090	T	T	T
0.3498182713916562	0.6627085096628766	0.5904747495887235	T	T	T
0.0166255535350268	0.3293245666373320	0.6778181225250308	T	T	T
0.6832969894440752	0.9961268324349575	0.6927275488632724	T	T	T
0.3501530068748125	0.6628183956234843	0.7611646783709421	T	T	T
0.0276276351263102	0.9741328037540286	0.2132987540297628	T	T	T
0.3593764002806618	0.3406824623041055	0.2133502254237567	T	T	T
0.6609468164846650	0.6725679915154328	0.2133041020634390	T	T	T
0.3748466102574347	0.9933835912504237	0.3173874566537131	T	T	T
0.6801882906998696	0.3063162140618096	0.3174145217162244	T	T	T
0.9931880698036049	0.6880160471701698	0.3173987618502114	T	T	T
0.0156387372380649	0.0235031062276043	0.4222973988053245	T	T	T
0.3226912490509110	0.3286246312183732	0.4223422157549797	T	T	T
0.7104885476940263	0.6357451453394002	0.4223127675257939	T	T	T
0.3503572141152552	0.9684478689535004	0.5268500477137674	T	T	T
0.6555023684115856	0.3563014434022174	0.5268429617996321	T	T	T
0.0432774210259245	0.6633309552116203	0.5268350348097642	T	T	T
0.9910662169141786	-0.0014238938046880	0.6317759249845581	T	T	T

0.3727493962647349	0.3038991733150319	0.6317598672527420	T	T	T
0.6856629236637150	0.6856116515099087	0.6317960383021749	T	T	T
0.3384899345585538	0.0179889852076209	0.7359406468157159	T	T	T
0.7051619049699156	0.3192699430979352	0.7358743937201513	T	T	T
0.0067188964065448	0.6511980378914457	0.7358217134474114	T	T	T
0.3489531931766647	0.6601335044374681	0.1193039371437007	T	T	T
0.0163098499201319	0.3315327631274111	0.8299662589503140	T	T	T

(Al)OHAg

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0.0000000000000000 0.0000000000000000 4.3980452500000000

Al O H Ag

12 20 2 2

Selective dynamics

Direct

0.0432950018668876	0.3536439315645694	0.2366834048332649	T	T	T
0.7086253909081890	0.0250333406129428	0.3057712412936340	T	T	T
0.3749338935210531	0.6906948689671566	0.3208014579220659	T	T	T
0.0411994106647029	0.3574739437390875	0.4079982105298825	T	T	T
0.7077188226766040	0.0239994872901903	0.4308930467098548	T	T	T
0.3740339738954646	0.6909246959426056	0.5121574143752810	T	T	T
0.0404381710432986	0.3579199377044162	0.5355542903324420	T	T	T
0.7066912404239361	0.0247731885823228	0.6167844400402558	T	T	T
0.3733538683521260	0.6916096179430795	0.6397028445789417	T	T	T
0.0398433945380390	0.3580862930689932	0.7268553945926328	T	T	T
0.7076635822267576	0.0244894448117279	0.7419358591711998	T	T	T
0.3706584217565592	0.6899735482283660	0.8110205411676219	T	T	T
0.0116816107020128	0.3059888189279363	0.1505756600437138	T	T	T
0.0563536791305381	0.9993396799938594	0.2639438023322782	T	T	T
0.3895421778435448	0.3688402811774623	0.2603437765463923	T	T	T
0.6903554476508873	0.6998699672675244	0.2632545018067844	T	T	T
0.3999853491469096	0.0232998554067834	0.3665163796711752	T	T	T
0.7047191774426196	0.3351231041822587	0.3667012814500410	T	T	T
0.0192967066471965	0.7149231205155857	0.3668747929820526	T	T	T
0.0403162227317182	0.0517397216596223	0.4715085959384524	T	T	T
0.3474977657529621	0.3565298849978760	0.4717083091844216	T	T	T
0.7349110611505054	0.6641354892977276	0.4716069671173102	T	T	T
0.3740108691756632	0.9973385705569200	0.5761372280589256	T	T	T
0.6793879511895256	0.3846970732909156	0.5759946359801447	T	T	T
0.0671628126724855	0.6920643355320877	0.5761461450015233	T	T	T
0.0143228820347900	0.0280985880748261	0.6809985944915766	T	T	T
0.3977266005037734	0.3329262264611543	0.6811612870245156	T	T	T
0.7087956129112882	0.7136168690774980	0.6807900583950754	T	T	T
0.3640682453427573	0.0428683753723647	0.7844393446184625	T	T	T
0.7321250601557736	0.3437847561266025	0.7873167314039478	T	T	T
0.0295709266813233	0.6767878317882818	0.7837378690234473	T	T	T
0.2908566361206582	0.7212522223444751	0.8971122197623771	T	T	T

0.0904442364703257	0.4129197205495032	0.1205887516006854	T	T	T
0.4760924034563345	0.6431318082980013	0.9272019333439232	T	T	T
0.3942261870137074	0.7156993666463833	0.1714262975445209	T	T	T
0.0821836724897977	0.3395794648044586	0.8762292526448192	T	T	T

(30)Zn_1.5

4.69735200000000					
2.0000000000000000	0.0000000000000000	0.0000000000000000			
0.5000000000000000	0.8660254030004244	0.0000000000000000			
0.0000000000000000	0.0000000000000000	4.3980452500000000			

Al O Zn
20 36 6

Selective dynamics

Direct

0.3351578900262570	-0.0058254334745984	0.2065476687386106	T	T	T
0.8330128805621285	0.0129215048885211	0.2083579442853615	T	T	T
0.1688502472278811	0.6639298751691444	0.2289847177051320	T	T	T
0.6632168101786570	0.6845391950658983	0.2168879864357659	T	T	T
-0.0002540317673417	0.3377064545306765	0.3111907960216129	T	T	T
0.5019227078106894	0.3368891092100678	0.3099301822138920	T	T	T
0.3358352248173951	0.0015775261072491	0.3329676142434852	T	T	T
0.8327899281843388	0.0060118197760974	0.3329400516881870	T	T	T
0.1676678928288835	0.6694091623744874	0.4147410304634767	T	T	T
0.6676490080701273	0.6713418444426871	0.4142403912849282	T	T	T
0.0010720411756679	0.3359642785046049	0.4381377613753982	T	T	T
0.5010703395809650	0.3378867870230872	0.4376508057502040	T	T	T
0.3328690918606276	0.0057303691469100	0.5194331600177616	T	T	T
0.8359428322179034	0.0012340901667338	0.5194423719540066	T	T	T
0.1667539534850918	0.6703524209475976	0.5424621399568332	T	T	T
0.6689810270992859	0.6695121652934368	0.5411885861835490	T	T	T
0.0053498529167911	0.3227527339410233	0.6355096606157689	T	T	T
0.4997761158432928	0.3431719264749857	0.6233606579433310	T	T	T
0.3334559465834555	0.0130656966901098	0.6458720950366520	T	T	T
0.8354668446199343	-0.0055949760004184	0.6440327844948180	T	T	T
0.0159684108317444	0.9391281009894362	0.1633841376135524	T	T	T
0.4972041351870570	0.9620740692722860	0.1613912283782812	T	T	T
0.1756285728398956	0.3302955917446625	0.1618508804663457	T	T	T
0.6990545495430459	0.3569358374893979	0.1616514259175121	T	T	T
0.3213999377195013	0.6726513370636376	0.1640845548391993	T	T	T
0.7988152017606625	0.7459990656901597	0.1613987507519710	T	T	T
0.1792216498650473	0.0031997911631218	0.2685752816525884	T	T	T
0.6787048965906174	0.0065976210098112	0.2691267067063928	T	T	T
0.3328777105903312	0.3104236137450430	0.2696663216426244	T	T	T
0.8368908831628088	0.3150027361733197	0.2681445700496873	T	T	T
0.9894399016656747	0.6932739125729908	0.2695737639608712	T	T	T
0.4883244503569020	0.6934396439064231	0.2681447035422729	T	T	T
0.0005079724239812	0.0301529165484483	0.3739569976096885	T	T	T
0.5007823824422688	0.0316780490638629	0.3739525410854308	T	T	T
0.1547652899389053	0.3345023169608702	0.3739573792664595	T	T	T

0.6539618272315142	0.3383777709165078	0.3738981170823413	T	T	T
0.3476130017250599	0.6434762731313551	0.3737057293061964	T	T	T
0.8481424572795189	0.6445088063225332	0.3741593482441402	T	T	T
0.1679092056424700	0.9756771117122622	0.4784582320634545	T	T	T
0.6682052640030328	0.9772124893661983	0.4784420220130774	T	T	T
0.3211192648040906	0.3638531342634629	0.4786954048127500	T	T	T
0.8205696357882653	0.3627975163088523	0.4782281415740578	T	T	T
0.0147752623800708	0.6689396051534361	0.4784698527343404	T	T	T
0.5139291181527353	0.6728629816055333	0.4784248754307822	T	T	T
0.9899445564948588	0.0005932579926688	0.5832803100617209	T	T	T
0.4894492854320540	0.0039119476601754	0.5838009152328496	T	T	T
0.1803202885008039	0.3138562547614567	0.5842608455607801	T	T	T
0.6792155593700039	0.3139912155051109	0.5828266151700837	T	T	T
0.3358014437123832	0.6968607284462378	0.5827367899545162	T	T	T
0.8318465027138650	0.6921752594678190	0.5842244494820370	T	T	T
0.1713576290366225	0.0451966831328046	0.6910055537348849	T	T	T
0.6524697869561140	0.0683686758802028	0.6889697063318334	T	T	T
0.3470553463423511	0.3350023606561019	0.6882279994825818	T	T	T
0.8697186736647810	0.2612297270245790	0.6909714471860567	T	T	T
0.9692978843746195	0.6504118976533849	0.6907759267210303	T	T	T
0.4929535720523288	0.6775276235067360	0.6907238437652645	T	T	T
-0.0277575880179606	0.3569409047916597	0.1502551069436258	T	T	T
0.5296516797691625	0.2997479520982650	0.1455250673337266	T	T	T
0.1789931793771244	0.6388902726146599	0.1057151247869547	T	T	T
0.1386994438243922	0.7078138230515025	0.7068154421251415	T	T	T
0.6964706975656760	0.6503934313432151	0.7022203803958946	T	T	T
0.4893372447144294	0.3686937545441706	0.7466226866173343	T	T	T

(Al)OHZn_0.5

4.697352000000000

2.0000000000000000 0.0000000000000000 0.0000000000000000

0.5000000000000000 0.8660254030004244 0.0000000000000000

0.0000000000000000 0.0000000000000000 4.3980452500000000

Al O H Zn

24 40 4 2

Selective dynamics

Direct

-0.0002857223557365	0.3330630599892228	0.2352674603506802	T	T	T
0.5053408777561976	0.3349592825624179	0.2358702005408273	T	T	T
0.3375776600462381	0.0135450965565485	0.3053953299970338	T	T	T
0.8337328023856000	0.0034786146358525	0.3044419874038104	T	T	T
0.1676317444134474	0.6800998682935344	0.3255343814071773	T	T	T
0.6693773131714571	0.6699937135521086	0.3155086539767403	T	T	T
0.9990877362526087	0.3430829604387149	0.4079373315354916	T	T	T
0.5040589689404688	0.3401586311475061	0.4066469890143106	T	T	T
0.3355049022062018	0.0076580993048641	0.4307558552156782	T	T	T
0.8343799012966328	0.0078966131458827	0.4296798952179541	T	T	T
0.1680353439531544	0.6749598705768036	0.5118423029193003	T	T	T
0.6680390048549014	0.6742406821329658	0.5111873698492839	T	T	T

0.0014917795856290	0.3415212502561613	0.5351466031422270	T	T	T
0.5014541052918887	0.3409291357145370	0.5345001636734442	T	T	T
0.3340477891083405	0.0080559987811668	0.6155668377594509	T	T	T
0.8351874214413086	0.0078441531953561	0.6166487641285676	T	T	T
0.1655525067294905	0.6754822457683818	0.6397054508285878	T	T	T
0.6705524531146271	0.6725370734791536	0.6383971299886682	T	T	T
0.0004247596200017	0.3451781363891949	0.7308408408507934	T	T	T
0.5020690308663430	0.3354130284015928	0.7207987415957596	T	T	T
0.3322122732872000	0.0017951024716739	0.7409255781477827	T	T	T
0.8360848836222310	0.0116374463540367	0.7418747568897043	T	T	T
0.1645219534566649	0.6801402552917541	0.8104940265780088	T	T	T
0.6701650989976866	0.6819035164380305	0.8110098494290724	T	T	T
0.0567812922648429	0.1390937249769576	0.1552069179249841	T	T	T
0.4127556673746260	0.4102148966865491	0.1547365298066806	T	T	T
0.0134704133975875	0.9741761409596902	0.2646707685388796	T	T	T
0.5076608490096982	0.9855072250032176	0.2620861187041598	T	T	T
0.1737930382384646	0.3602685107260430	0.2573824025321061	T	T	T
0.6773141772365773	0.3452202945800897	0.2597493207035459	T	T	T
0.3262615004570631	0.6838234268691833	0.2655710685113271	T	T	T
0.8278249231424432	0.6809482018214837	0.2600222687122855	T	T	T
0.1802651990529206	0.0151188146949112	0.3662264008140487	T	T	T
0.6819350188404407	0.0012012885514453	0.3654137918233757	T	T	T
0.3327631375926398	0.3208343168967642	0.3667538594917440	T	T	T
0.8342857628069136	0.3162745813088089	0.3650574688442331	T	T	T
0.9907239719542814	0.6974162138177433	0.3669671554714200	T	T	T
0.4906649383823994	0.7004862358784951	0.3658837916086410	T	T	T
0.0009292129171134	0.0352354348009041	0.4707889604170270	T	T	T
0.5016044532973015	0.0361282078629087	0.4708434080110967	T	T	T
0.1548133606444120	0.3403436695572780	0.4715449758136155	T	T	T
0.6550694621789146	0.3399698797210418	0.4706107244440678	T	T	T
0.3482528230411492	0.6477285686605720	0.4707079193415454	T	T	T
0.8483865570712603	0.6479969997487881	0.4710603505452164	T	T	T
0.1678970243443498	0.9796880855671766	0.5755062284162455	T	T	T
0.6685942708854364	0.9805679210697359	0.5755444036096201	T	T	T
0.3212349887446043	0.3681045237201426	0.5756303438022028	T	T	T
0.8211655279424881	0.3677898974875197	0.5752734072463044	T	T	T
0.0144831799907686	0.6757737113372023	0.5757283613263168	T	T	T
0.5147382440871591	0.6753698642942257	0.5747777423621458	T	T	T
0.9877774798945067	0.0142589940302867	0.6809260318388853	T	T	T
0.4893715774459920	0.0005628545673686	0.6800650311728965	T	T	T
0.1790191189352083	0.3149845358426184	0.6804564607345199	T	T	T
0.6789892244194424	0.3181267142397599	0.6793662753871109	T	T	T
0.3369327646483034	0.6946574150558620	0.6795612748214050	T	T	T
0.8354274760042232	0.6991651714529591	0.6812780736976117	T	T	T
0.1622502955474691	0.0296293779534027	0.7842757763310289	T	T	T
0.6562377962528433	0.0409565455470398	0.7816109117539624	T	T	T
0.3435263516453776	0.3313696529703503	0.7807479797563386	T	T	T
0.8420799193485786	0.3339373803500921	0.7863012243655971	T	T	T
0.9925134059515458	0.6699634972688840	0.7865904523235643	T	T	T

0.4960482544688206	0.6549064999920660	0.7888946231812644	T	T	T
0.2573381381749362	0.6052037061405859	0.8916169444901567	T	T	T
0.6136679032138438	0.8752792006548910	0.8910528094602338	T	T	T
0.0940479174635504	0.2084532765532775	0.1176012196597660	T	T	T
0.4394763870659396	0.2097248365133354	0.1311425415035863	T	T	T
0.2312743541902187	0.8063491065506418	0.9148464714175706	T	T	T
0.5789859922162920	0.8037522841463886	0.9290864854519508	T	T	T
0.1878131621188441	0.6889540611067192	0.1936068866259376	T	T	T
0.4821041519712906	0.3256137597460698	0.8527300720417872	T	T	T

(Al)+Zn

4.69735200000000

1.0000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.8660254030004244	0.0000000000000000
0.0000000000000000	0.0000000000000000	4.3980452500000000

Al O Zn

12 18 2

Selective dynamics

Direct

0.0107234261823419	0.3332949530157026	0.2441230671465074	T	T	T
0.6805675747308784	-0.0052205965335614	0.3071005861683018	T	T	T
0.3491417859204149	0.6612747770344958	0.3205939982630995	T	T	T
0.0162589585832703	0.3293599668111231	0.4092933454740305	T	T	T
0.6833562306019230	-0.0041096854557232	0.4319248630860789	T	T	T
0.3501290453778935	0.6625685043473749	0.5131090456974852	T	T	T
0.0168942407355801	0.3288198092780141	0.5366959287564307	T	T	T
0.6835618569536883	-0.0043994076132538	0.6178981397272311	T	T	T
0.3505128286184332	0.6622188471138362	0.6405231160825243	T	T	T
0.0171968501500331	0.3304921009174307	0.7291422993212805	T	T	T
0.6856712981288123	-0.0027742057466676	0.7427498854008621	T	T	T
0.3556381274709681	0.6585581264384930	0.8058388694046407	T	T	T
0.0213951307454647	0.9700547540979837	0.2600901120343772	T	T	T
0.3581651865843562	0.3400332050410793	0.2656681694929310	T	T	T
0.6523723913788755	0.6768378860772420	0.2644289263414151	T	T	T
0.3718930589757729	-0.0072624482349794	0.3678906611868378	T	T	T
0.6829944315581967	0.3045792045329309	0.3675147225913796	T	T	T
0.9930804807308732	0.6888168441544987	0.3676801846786065	T	T	T
0.0152963262244962	0.0236149657684621	0.4729201578486448	T	T	T
0.3232209945794128	0.3286641488882179	0.4725796612259371	T	T	T
0.7111782907574129	0.6354733162944443	0.4726238831148261	T	T	T
0.3516884118470316	0.9677647710724729	0.5769239148620863	T	T	T
0.6558614778383816	0.3559371053104468	0.5772100898865415	T	T	T
0.0437894903003053	0.6627250545788733	0.5772757394726350	T	T	T
0.9947143767889937	-0.0011126642193379	0.6819463688085337	T	T	T
0.3736101828939000	0.3027756212812912	0.6821437213508783	T	T	T
0.6835410600454882	0.6871456683938876	0.6823294813686726	T	T	T
0.3447395230336617	0.0218794034714155	0.7897330978400142	T	T	T
0.7140118427283157	0.3152255728286692	0.7854454517022221	T	T	T
0.0083575876504175	0.6517307001297152	0.7840884060244492	T	T	T

0.1004307879567356 0.6805685808934635 0.1598447649957453 T T T
0.2552353234110523 0.3154805950447959 0.8894327428849100 T T T

2. Structural information on (3O)/Zn, (Al)/Zn and (Al)/Cr/Zn interfaces, as obtained from VASP calculations at the LDA level, Fig. 7.

(Al)/Zn

1.0000000000000000
4.7355004340000004 0.0000000000000000 0.0000000000000000
-2.3677502170000002 4.1010636749999998 0.0000000000000000
0.0000000000000000 0.0000000000000000 35.6763996398312244

Al O Zn
14 21 27

Direct

-0.0000000000000000 0.0000000000000000 0.1025056438708051
-0.0000000000000000 0.0000000000000000 0.8974943561291949
-0.0000000000000000 -0.0000000000000000 0.1965083039485343
-0.0000000000000000 -0.0000000000000000 0.8034916960514585
-0.0000000000000000 -0.0000000000000000 0.0322209196735358
-0.0000000000000000 -0.0000000000000000 0.9677790803264642
0.6666669999999998 0.3333330000000032 0.1525782074067263
0.6666669999999998 0.3333330000000032 0.8474217925932737
0.6666669999999998 0.3333330000000032 0.0360390952771480
0.6666669999999998 0.3333330000000032 0.9639609047228520
0.3333330000000032 0.6666669999999998 0.0870753203797199
0.3333330000000032 0.6666669999999998 0.9129246796202800
0.3333330000000032 0.6666669999999998 0.1598982403511551
0.3333330000000032 0.6666669999999998 0.8401017596488448
0.3115250221626902 0.0017419533762413 0.0642662438302076
0.3115250221626902 0.0017419533762413 0.9357337561697853
0.9982580466237587 0.3097830687864417 0.0642662438302076
0.9982580466237587 0.3097830687864417 0.9357337561697853
0.6902169312135582 0.6884749778373027 0.0642662438302076
0.6902169312135582 0.6884749778373027 0.9357337561697853
0.9904307632361166 0.3475151132786166 0.1850933759262580
0.9904307632361166 0.3475151132786166 0.8149066240737491
0.3382083912167192 0.2709660464124886 0.0000000000000000
0.6524848867213835 0.6429146499574956 0.1850933759262580
0.6524848867213835 0.6429146499574956 0.8149066240737491
0.7290339535875113 0.0672413448042260 0.0000000000000000
0.3570853500425045 0.0095692367638834 0.1850933759262580

0.3570853500425045	0.0095692367638834	0.8149066240737491
0.9327586551957741	0.6617916087832807	0.0000000000000000
0.0229825033742963	0.6647550134832122	0.1252471734428900
0.0229825033742963	0.6647550134832122	0.8747528265571100
0.3352449865167877	0.3582284898910744	0.1252471734428900
0.3352449865167877	0.3582284898910744	0.8747528265571100
0.6417715101089255	0.9770174966257038	0.1252471734428900
0.6417715101089255	0.9770174966257038	0.8747528265571100
0.9991917583536107	0.3438853601395148	0.2575218108880327
0.6561146398604852	0.6553063982141101	0.2575218108880327
0.3446936017858970	0.0008082416463893	0.2575218108880327
0.3333333333333357	0.6666666666666643	0.3195121063645024
-0.0000000000000000	0.0000000000000000	0.3213109028741292
0.6666666666666643	0.3333333333333357	0.3193942356748009
0.9999716865473307	0.3347616591983901	0.3805578674608269
0.6652383408016099	0.6652100273489477	0.3805578674608269
0.3347899726510522	0.0000283134526693	0.3805578674608269
0.3333333333333357	0.6666666666666643	0.4403109960533311
-0.0000000000000000	0.0000000000000000	0.4405408885082351
0.6666666666666643	0.3333333333333357	0.4402927774509034
0.0000435912103772	0.3334376805220871	0.5000000000000000
0.6665623194779130	0.6666059106882831	0.5000000000000000
0.3333940893117169	0.9999564087896228	0.5000000000000000
0.3333333333333357	0.6666666666666643	0.5596890039466688
-0.0000000000000000	0.0000000000000000	0.5594591114917649
0.6666666666666643	0.3333333333333357	0.5597072225490967
0.9999716865473307	0.3347616591983901	0.6194421325391731
0.6652383408016099	0.6652100273489477	0.6194421325391731
0.3347899726510522	0.0000283134526693	0.6194421325391731
0.3333333333333357	0.6666666666666643	0.6804878936354977
-0.0000000000000000	0.0000000000000000	0.6786890971258709
0.6666666666666643	0.3333333333333357	0.6806057643251990
0.9991917583536107	0.3438853601395148	0.7424781891119672
0.6561146398604852	0.6553063982141101	0.7424781891119672
0.3446936017858970	0.0008082416463893	0.7424781891119672

(3O)/Zn

1.0000000000000000		
4.7355004340000004	0.0000000000000000	0.0000000000000000
-2.3677502170000002	4.1010636749999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	32.8785631314693276

Al O Zn
12 21 27

Direct

-0.0000000000000000	-0.0000000000000000	0.1118141833253549
-0.0000000000000000	-0.0000000000000000	0.8881858166746451
-0.0000000000000000	-0.0000000000000000	0.0350198526094203
-0.0000000000000000	-0.0000000000000000	0.9649801473905797
0.6666669999999998	0.3333330000000003	0.1646119797038546

0.6666669999999968 0.3333330000000032 0.8353880202961527
0.6666669999999968 0.3333330000000032 0.0390252083964011
0.6666669999999968 0.3333330000000032 0.9609747916035989
0.3333330000000032 0.6666669999999968 0.0938404279625205
0.3333330000000032 0.6666669999999968 0.9061595720374795
0.3333330000000032 0.6666669999999968 0.1723040498630998
0.3333330000000032 0.6666669999999968 0.8276959501369001
0.3118532400346448 0.0022264585033828 0.0696508783324429
0.3118532400346448 0.0022264585033828 0.9303491216675572
0.9977735414966173 0.3096267815312692 0.0696508783324429
0.9977735414966173 0.3096267815312692 0.9303491216675572
0.6903732184687308 0.6881467599653551 0.0696508783324429
0.6903732184687308 0.6881467599653551 0.9303491216675572
0.9923513259804883 0.3632854294263718 0.2023398259590634
0.9923513259804883 0.3632854294263718 0.7976601740409366
0.3380733059593085 0.2712005499003475 -0.0000000000000000
0.6367145705736281 0.6290648965541332 0.2023398259590634
0.6367145705736281 0.6290648965541332 0.7976601740409366
0.7287994500996525 0.0668717560589563 -0.0000000000000000
0.3709351034458667 0.0076486740195116 0.2023398259590634
0.3709351034458667 0.0076486740195116 0.7976601740409366
0.9331282439410438 0.6619266940406916 -0.0000000000000000
0.0230915299368153 0.6645939506372853 0.1357432116303115
0.0230915299368153 0.6645939506372853 0.8642567883696886
0.3354060493627146 0.3584985792995345 0.1357432116303115
0.3354060493627146 0.3584985792995345 0.8642567883696886
0.6415014207004656 0.9769084700631776 0.1357432116303115
0.6415014207004656 0.9769084700631776 0.8642567883696886
-0.0000000000000000 -0.0000000000000000 0.2292474658605163
0.6666666666666643 0.3333333333333357 0.2485974654537722
0.3333333333333357 0.6666666666666643 0.2530531708530087
0.3236588174172025 0.3106799775605179 0.3086592846086904
0.9870211601433154 0.6763411825827975 0.3086592846086904
0.6893200224394820 0.0129788398566917 0.3086592846086904
-0.0000000000000000 -0.0000000000000000 0.3725254410361252
0.6666666666666643 0.3333333333333357 0.3724669587880620
0.3333333333333357 0.6666666666666643 0.3714238867727209
0.3338022183645797 0.3344350170483856 0.4360208743190439
0.0006327986837987 0.6661977816354203 0.4360208743190439
0.6655649829516144 0.9993672013162013 0.4360208743190439
-0.0000000000000000 -0.0000000000000000 0.5000000000000000
0.6666666666666643 0.3333333333333357 0.5000000000000000
0.3333333333333357 0.6666666666666643 0.5000000000000000
0.3338022183645797 0.3344350170483856 0.5639791256809560
0.0006327986837987 0.6661977816354203 0.5639791256809560
0.6655649829516144 0.9993672013162013 0.5639791256809560
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(Al)/Cr/Zn

1.0000000000000000
4.7355004340000004 0.0000000000000000 0.0000000000000000
-2.3677502170000002 4.1010636749999998 0.0000000000000000
0.0000000000000000 0.0000000000000000 32.9424800794594930

Al O Zn Cr
14 21 9 18

Direct

0.0000000000000000 0.0000000000000000 0.1112430161287989
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