

Supporting Information:

Metallic back contact interface design in photoelectrochemical devices

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We provide in this supporting information further computational details on Density Functional Theory (DFT) calculations performed on the FCC/corundum metal/oxide interfaces. Below we report the convergence parameters for each interface and the relaxed geometries of the converged unit cells of each slab. The converged energy cut-off and k-space grid for each interface are detailed in Table S.1. All geometries are provided in the following format: cell lattice vectors, atom types and number of atoms, atom locations in fractional coordinates, according to VASP standard input.

Table S.1 – Convergence of k-space grids and plane wave energy cut-offs for the examined Mt/M₂O₃ interfaces.

| Interface | Ag/Fe ₂ O ₃ | Al/Fe ₂ O ₃ | Au/Fe ₂ O ₃ | Ir/Fe ₂ O ₃ | Pd/Fe ₂ O ₃ | Pt/Fe ₂ O ₃ | Pt/Cr ₂ O ₃ | Pt/Al ₂ O ₃ |
|-----------|-----------------------------------|-----------------------------------|-----------------------------------|-----------------------------------|-----------------------------------|-----------------------------------|-----------------------------------|-----------------------------------|
| k-grid | 6×6×1 | 8×8×1 | 6×6×1 | 9×9×1 | 8×8×1 | 8×8×1 | 6×6×1 | 6×6×1 |
| cut-off | 650 eV | 700 eV | 700 eV | 650 eV | 750 eV | 850 eV | 650 eV | 650 eV |

The relaxed interface geometries are as follows:

1. Ag/Fe₂O₃/Ag interface geometry:

```
4.4027900000000000 2.5419499999999999 0.0000000000000000
0.0000000000000000 5.0838999999999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 47.0000000000000000
O Fe Ag
15 8 18
0.7092739156189367 0.9826803755452005 0.6178426969101025
0.9314162559587658 0.3739117574167921 0.6178731211416846
0.3182794343580611 0.5961197912803442 0.6178678417315027
0.9566666188531059 0.0088227117500281 0.5698284186751366
0.6581216278090096 0.6192895533879224 0.5698310879708899
0.3461123500479601 0.3205590508504699 0.5698318413480976
0.0173473124109194 0.2856391038912136 0.5208672109105237
0.3208576967897443 0.6777739618397050 0.5208720413371069
0.6251864055670069 0.9817179345957854 0.5208056324579928
0.2969773572413459 0.3443236327762307 0.4718136088079632
0.9851872217640079 0.9550254527182958 0.4718339375234635
0.6858113451836019 0.6430308013718857 0.4719133922059058
0.3267194281977623 0.5903668214695230 0.4237290787228076
0.7123374706896968 0.9817296289082691 0.4237764636773491
```

0.9347344828646769 0.3675354391703394 0.4238377088247276
0.6531674911975358 0.3172060336031350 0.5979603403700722
0.9868787678759148 0.6502264355761795 0.5921218568522377
0.9881216509691910 0.6478558905759044 0.5031816984651556
0.3225029071988956 0.9806145335550838 0.4897088042846605
0.3202376522126826 0.9826170640425858 0.5519893253011574
0.6541842440896986 0.3151298817491082 0.5384196546210376
0.6569969127841446 0.3139616667415766 0.4495820785078024
0.9908327244393149 0.6468792042159848 0.4436344779862296
0.3175741211374827 0.6579569484549523 0.6629901621253680
0.9903653527349547 0.3180164917795096 0.6629927168228562
0.6503868861981630 0.9855002853830612 0.6629843346208375
0.9879383873517043 0.9864968735535626 0.7127839471718502
0.6518445788627432 0.6540735612457809 0.7127773973695497
0.3202480836664847 0.3177128595599612 0.7127704534360504
0.3210499345214188 0.9845026133341293 0.7635785946435121
0.9877382152776590 0.6511725629761145 0.7632886766817464
0.6543082851081863 0.3178931756908483 0.7632988812914405
0.9906313308309933 0.3156448255916970 0.3786225622366430
0.6510006710722180 0.9880470835449984 0.3786508742870183
0.3233962125033045 0.6555605926474328 0.3786479367803182
0.9898785650511854 0.9856612370796469 0.3287520700864448
0.6539525710988272 0.6539485753319525 0.3287488994769419
0.3213777840403651 0.3176235675172876 0.3287681646202003
0.3219886461812393 0.9845472735738170 0.2778142588847956
0.9887205078231602 0.6513482565909712 0.2780922870789340
0.6552762816664597 0.3179208226706578 0.2780997797876950

2. Al/Fe₂O₃/Al interface geometry:

5.0210599899000004 0.0000000000000000 0.0000000000000000
2.5105279683999999 4.3483666752000003 0.0000000000000000
0.0000000000000000 0.0000000000000000 47.0000000000000000
O Fe Al
15 8 36
0.6873750090000001 0.9761949780000023 0.6208559869999988
0.9594450000000023 0.3538109960000000 0.6208750010000017
0.3101670149999975 0.6253859999999989 0.6208860280000010
0.9610919949999968 0.0046320000000009 0.5705739859999994
0.6576380130000032 0.6270089750000025 0.5705720189999965
0.3386220040000012 0.3236719969999982 0.5705670119999979
0.0133179999999982 0.2908340099999975 0.5207819940000036
0.3191779850000032 0.6795269850000025 0.5207880139999972
0.6246740220000007 0.9853489999999994 0.5207890269999993
0.2994140090000030 0.3432950079999983 0.4709770079999984
0.9804149870000032 0.9658629890000014 0.4709730149999984
0.6768580079999964 0.6468610169999991 0.4709770079999984
0.3278180060000011 0.6167610290000027 0.4207249880000035
0.6784110070000011 0.9944660069999998 0.4206959899999987
0.9500359889999999 0.3454009889999980 0.4206779900000015
0.6525049809999999 0.3183040019999979 0.5983610150000018
0.9857130050000009 0.6519150139999965 0.5927140120000018
0.9857199790000024 0.6517990230000024 0.5025920269999986
0.3189179900000028 0.9854140280000010 0.4893459979999975
0.3192160130000019 0.9851089719999990 0.5521460180000020
0.6522709730000003 0.3185969889999996 0.5389040109999996
0.6522880200000003 0.3186329899999976 0.4488230050000013
0.9853739739999980 0.6522639989999988 0.4431439940000033
0.3194650109999984 0.6624869700000033 0.6572520140000009

0.9891520139999983 0.3070699869999984 0.6571879979999977
 0.6475520130000021 0.9792320130000007 0.6572629810000024
 0.9846050140000031 0.9836220150000017 0.7052149769999971
 0.6607660060000029 0.6447669860000005 0.7052019830000020
 0.3232780100000028 0.3210400039999968 0.7052010299999978
 0.3226769859999976 0.9830530289999970 0.7548810239999995
 0.9893199799999977 0.6497960089999992 0.7546709780000000
 0.6560050249999989 0.3163880110000008 0.7547479870000018
 0.3226589860000004 0.6493459940000008 0.8032590150000019
 0.9891520139999983 0.3165059979999967 0.8032540080000032
 0.6562910079999966 0.9828950169999970 0.8032550220000019
 0.9896799919999992 0.9828140139999988 0.8518990279999983
 0.6556829809999982 0.6497049930000003 0.8518970009999975
 0.3228099939999964 0.3157890140000035 0.8518959880000025
 0.3228549959999967 0.9825760129999992 0.9011260269999966
 0.9894589780000018 0.6492490170000025 0.9011459950000003
 0.6561579700000024 0.3158429859999998 0.9011840220000025
 0.9988449809999977 0.3041279910000014 0.3843500019999979
 0.6434770230000026 0.9874399899999986 0.3842639920000011
 0.3264699879999995 0.6595810060000034 0.3843350109999975
 0.9848020080000026 0.9834259750000029 0.3363580110000015
 0.6608719829999998 0.6459800000000016 0.3363730009999983
 0.3220640119999985 0.3223420079999997 0.3363679950000034
 0.3224259910000029 0.9837970139999968 0.2866950040000020
 0.9890260100000035 0.6505060200000017 0.2868269980000022
 0.6557469959999978 0.3171159919999980 0.2869049910000001
 0.3224900069999990 0.6500110030000030 0.2383700009999998
 0.9888929720000021 0.3171530070000017 0.2383760060000029
 0.6560299989999976 0.9836919899999970 0.2383760060000029
 0.9895359869999965 0.9833400249999968 0.1897359940000030
 0.6555709840000006 0.6504470109999971 0.1897370069999980
 0.3224430080000005 0.3166140020000014 0.1897359940000030
 0.3225620090000021 0.9833269720000004 0.1405249979999965
 0.9892659779999988 0.6499620080000028 0.1404740070000017
 0.6559150220000021 0.3165729939999977 0.1405110059999970

3. Au/Fe₂O₃/Au interface geometry:

5.1010174750999999 0.0000000000000000 0.0000000000000000
 2.5505211197000000 4.4176294481999996 0.0000000000000000
 0.0000000000000000 0.0000000000000000 47.0000000000000000
 O Fe Au
 15 8 18
 0.7007558023373548 0.9821673622922376 0.6174967947697709
 0.9412935077738567 0.3648875861001031 0.6175145133787225
 0.3176410093070743 0.6055501215969912 0.6174982197516599
 0.9571090219691385 0.0081995942775634 0.5697144592115748
 0.6588625033241158 0.6198018175083106 0.5697451899537711
 0.3452843193695756 0.3216876186509907 0.5697240586653152
 0.0173294151026511 0.2862426689532711 0.5208732251350483
 0.3211125917425690 0.6788380093067659 0.5208806329456053
 0.6249253845522063 0.9825058085344125 0.5208788334051064
 0.2973627946790458 0.3456643577698131 0.4720112938463288
 0.9838412045380451 0.9571472802570256 0.4719983204515330
 0.6855613129883338 0.6439152389241087 0.4720462362223259
 0.3256415397040158 0.6014680666212300 0.4242340029361742
 0.7022788348947628 0.9841957146859244 0.4242272811158472
 0.9426637763519139 0.3611889469753322 0.4242640565985667
 0.6533605347953824 0.3172552854270450 0.5976848227098017

0.9869575355820643 0.6503576555400414 0.5919555676723078
 0.9880312040492640 0.6489828990168292 0.5034344219531306
 0.3221163269035401 0.9821729896269247 0.4896869885436672
 0.3204166913118769 0.9831251962131446 0.5520578476145985
 0.6542010519254760 0.3159944886325334 0.5383186716659125
 0.6560885238715386 0.3158267504111052 0.4497894230151189
 0.9898796257517404 0.6489248171232518 0.4440601484149056
 0.3171248335204950 0.6567031173287248 0.6625135807803133
 0.9899734108802960 0.3179765376125516 0.6625564885170334
 0.6513408794148603 0.9837735710745790 0.6625541737723211
 0.9889527692052695 0.9856008776064229 0.7127439098117279
 0.6515359920878936 0.6539852284515320 0.7127444026138718
 0.3205355344557219 0.3167558169646654 0.7127388937532473
 0.3210995556906582 0.9846265857929239 0.7652861455345956
 0.9877539004959175 0.6513016781522367 0.7646762668599223
 0.6544627246666437 0.3179496452929769 0.7646548901468648
 0.9909424464429293 0.3143086637246952 0.3791845241305580
 0.6523899868191663 0.9870322427208293 0.3791880818782545
 0.3252663367353961 0.6529569282360441 0.3792206929074737
 0.9910645324396796 0.9847056321815941 0.3289947615501916
 0.6536938992344830 0.6537170187852936 0.3289822924086607
 0.3221099818886231 0.3164366063441193 0.3289989070760200
 0.3220223179253594 0.9847355988623008 0.2764353614244186
 0.9886739847279955 0.6514186599001377 0.2770654092896336
 0.6553906715431381 0.3180412415233960 0.2770445885681312

4. Ir/Fe₂O₃/Ir interface geometry:

4.2603200000000001 2.4596900000000002 0.0000000000000000
 0.0000000000000000 4.9193899999999999 0.0000000000000000
 0.0000000000000000 0.0000000000000000 47.0000000000000000
 O Fe Ir
 15 8 24
 0.6724040211223965 0.9734159136546978 0.6214763079688339
 0.9795949003941189 0.3368132132862911 0.6214811126697342
 0.3091117722715921 0.6437780998761511 0.6214829711135224
 0.9620733152312013 0.0040858452354939 0.5713224261721734
 0.6595683943561212 0.6263570448005353 0.5713260488071228
 0.3398694340463564 0.3238588028314027 0.5713182757116542
 0.0141481550420721 0.2910686775513867 0.5208692431640358
 0.3207791258227672 0.6781362887629214 0.5208663437677643
 0.6270334881860862 0.9848118871022180 0.5208637213407101
 0.3013842091759926 0.3432168381241283 0.4704536526584135
 0.9816132176764185 0.9653228729140864 0.4704473756789511
 0.6793013632428995 0.6454706829999921 0.4704502269740161
 0.3321858268652704 0.6324784132839056 0.4203071860987819
 0.6615252709006114 0.9958887570473536 0.4203066069122983
 0.9689889328233647 0.3251298178303870 0.4203110950945543
 0.6537778358281443 0.3180382157782446 0.5999494611300165
 0.9871749498629327 0.6513630517338242 0.5935732971173096
 0.9873433918783832 0.6513291521141369 0.5018995097071937
 0.3207712391488897 0.9846544062306748 0.4895020501903957
 0.3205087908010924 0.9847617754421663 0.5522552573038837
 0.6539605308107568 0.3180144928801099 0.5398786128761301
 0.6540852770787424 0.3179632641264334 0.4482096223821017
 0.9874778998690985 0.6512596988161903 0.4418108221778496
 0.3170669594935163 0.6487728447368752 0.6626262060878645
 0.9844780361012795 0.3235872559780617 0.6626220489473766
 0.6590407152428170 0.9815248847692999 0.6626175110799792

0.9851878922293835 0.9856716883299868 0.7078457300181142
 0.6539932274208482 0.6496966667510051 0.7078476762351826
 0.3212453908770030 0.3182862646659856 0.7078496968156287
 0.3199523084110325 0.9845773678141114 0.7555843516897482
 0.9866305747488653 0.6512468601786168 0.7551113810440953
 0.6532815797865013 0.3179354025460626 0.7551386338532637
 0.3198961901575359 0.6252696194480905 0.8006765646033287
 0.9606338459743853 0.3439256835814888 0.8006746627737442
 0.6792104029851700 0.9846211115626815 0.8006721352498190
 0.9822428534809120 0.3201403381808845 0.3791471909167612
 0.6568995416878849 0.9874845614304917 0.3791425435826952
 0.3241618108113400 0.6453211408105943 0.3791401178146145
 0.9873925678188726 0.9832125171843984 0.3339172475560162
 0.6560103915270901 0.6504355240140001 0.3339190595249804
 0.3201124814560714 0.3189022529600365 0.3339152258052778
 0.3212985149179275 0.9840883745151388 0.2861897694220019
 0.9879575787315957 0.6507389208181920 0.2866408779712657
 0.6546672955758552 0.3173754858489630 0.2866632878588149
 0.3213443359737198 0.6246172871259716 0.2410942413160910
 0.9619479518607292 0.3435006581239648 0.2410942172425763
 0.6807181593720557 0.9841195524508208 0.2410930362377783

5. Pd/Fe₂O₃/Pd interface geometry:

4.2951300000000003 2.4797899999999999 0.0000000000000000
 0.0000000000000000 4.9595799999999999 0.0000000000000000
 0.0000000000000000 0.0000000000000000 47.0000000000000000
 O Fe Pd
 15 8 24
 0.6815486872084406 0.9752987049190054 0.6202068564330006
 0.9678728984421952 0.3461740707795542 0.6201967949796128
 0.3106221939307332 0.6325478138593326 0.6202058741882510
 0.9593960878525039 0.0050250648801295 0.5709648155353477
 0.6598050792739940 0.6246439616962789 0.5709696787680656
 0.3398708248306832 0.3250234880728300 0.5709688833266355
 0.0138260587730556 0.2907323793952443 0.5207940408236311
 0.3195762073666160 0.6793398013374130 0.5207958466994640
 0.6251992696989817 0.9850824307359218 0.5207942758563746
 0.2994549176600643 0.3453426729696503 0.4706275379597571
 0.9794958926778605 0.9648776842755851 0.4706278013646141
 0.6798788870450707 0.6450013019368299 0.4706242528026507
 0.3292589855350059 0.6227279976943834 0.4213728117522635
 0.6727243995771275 0.9943652776551488 0.4213646416413255
 0.9576414514614555 0.3378040474862019 0.4213757841382204
 0.6532057646204450 0.3181040015744685 0.5997538046490263
 0.9864708019426303 0.6514803986344830 0.5934401681216741
 0.9862005136262155 0.6517285499808239 0.5020915651868805
 0.3195642025524990 0.9850847702622261 0.4893412471448286
 0.3196274943960091 0.9849491557904173 0.5522644825296439
 0.6528892976893772 0.3183664494942207 0.5395228403960388
 0.6530251837614998 0.3183834983866021 0.4481654099945231
 0.9864166283187430 0.6516902055511409 0.4418457013720669
 0.3175103895975226 0.6513380944268334 0.6618829730238076
 0.9879908578892440 0.3201470825218777 0.6618723354469225
 0.6568432298043447 0.9809514973682525 0.6618866347366890
 0.9902600771906691 0.9840938613167012 0.7088309700616975
 0.6522686931973070 0.6524603513474645 0.7088302243645472
 0.3218224819168682 0.3145029382919375 0.7088302508418565
 0.3221842672992850 0.9831139364998833 0.7559558473462786

0.9888243541760318 0.6498243370967671 0.7557123606572986
 0.6554702188433410 0.3164710094847933 0.7557239800433777
 0.3226776028330036 0.6491291084838551 0.8032288188646035
 0.9895191631524085 0.3161074167082987 0.8032164558972710
 0.6565052963866194 0.9823035693942401 0.8032231528405944
 0.9847132652068922 0.3173619503162115 0.3797006382877584
 0.6534967195502617 0.9877231044526056 0.3796857046049098
 0.3237065340132759 0.6486468245380408 0.3796942005650337
 0.9905260512254657 0.9838748650692395 0.3327330741626966
 0.6523856902127889 0.6534204587462966 0.3327344520307207
 0.3209012823914676 0.3153214144462240 0.3327343720408464
 0.3219188989842436 0.9837895301019088 0.2855775101150542
 0.9885690794196904 0.6504597159675214 0.2858357033080878
 0.6552352012575042 0.3171274008239422 0.2858375031617371
 0.3227015410761851 0.6497219126381282 0.2383053408364475
 0.9889039818964278 0.3168181653420703 0.2382991673945725
 0.6560172942379765 0.9835324472490612 0.2383062137032468

6. Pt/Fe₂O₃/Pt interface geometry:

4.3174200000000003 2.4926599999999999 0.0000000000000000
 0.0000000000000000 4.9853199999999998 0.0000000000000000
 0.0000000000000000 0.0000000000000000 47.0000000000000000
 O Fe Pt
 15 8 36
 0.6751735851342318 0.9749593629931397 0.6198849762614742
 0.9742343331083276 0.3402386738195133 0.6198706655653297
 0.3098295860155247 0.6394046959046591 0.6198808470682238
 0.9594006485898561 0.0052131539296880 0.5707106095810346
 0.6588226426851165 0.6254148072766057 0.5707168783076142
 0.3393269073322571 0.3247691834498312 0.5707164959382069
 0.0134769884146522 0.2907588450239729 0.5207858004166610
 0.3189590803437810 0.6798163004103444 0.5207878709296310
 0.6243948703316562 0.9852863375419645 0.5207860899366139
 0.2990136554150737 0.3450408955649138 0.4708582972370721
 0.9794493282271617 0.9652220575363870 0.4708614338550063
 0.6788058645283357 0.6457716828965729 0.4708525238494303
 0.3294368407924182 0.6298031146005272 0.4216973065773928
 0.6651559890982952 0.9951507685949750 0.4216829176138432
 0.9641643917782474 0.3307490200129806 0.4216942546585472
 0.6528133567573633 0.3183328844066651 0.5992150304045651
 0.9860259187742955 0.6517070799848383 0.5928974790093307
 0.9856205005434262 0.6519586119340985 0.5023136133743193
 0.3190132989911234 0.9853381752765102 0.4893877210798578
 0.3190777804958458 0.9851901625977533 0.5521822788989752
 0.6522901121583544 0.3186125984009109 0.5392527815887647
 0.6525719686427607 0.3186645653115150 0.4486715225836875
 0.9860095361217134 0.6519566851540546 0.4423583728667069
 0.3180824235288782 0.6500638396093947 0.6617163744796386
 0.9865854306243023 0.3211946740437313 0.6617083583241197
 0.6578857605547483 0.9814963540773576 0.6617253639852194
 0.9899736569123263 0.9844223087263160 0.7089420975161360
 0.6531065999176349 0.6515405599054063 0.7089437883544178
 0.3227834115058528 0.3147739121695210 0.7089334859745549
 0.3229782244639452 0.9824264172154926 0.7566200458886314
 0.9896578577359563 0.6490725280538641 0.7565981828640247
 0.6562808022345976 0.3157305889654012 0.7566825039606258
 0.3231649968960539 0.6492549466696715 0.8041267962562344
 0.9904366973811207 0.3152662747725330 0.8041216608881072

0.6565466830209346 0.9819675619136845 0.8041247007072414
 0.9902445399464881 0.9825171120076845 0.8512902107677860
 0.6566153480841024 0.6493433357385072 0.8512789789321076
 0.3234290936966886 0.3158145876181138 0.8512708964996847
 0.3234142505560627 0.9829527666295590 0.8992430685815265
 0.9900423309185129 0.6491951742986615 0.8991694107615800
 0.6567252017968670 0.3159734074354645 0.8991553983217742
 0.9836892196222067 0.3189271319972917 0.3798668535436462
 0.6549248125098472 0.9875050079538426 0.3798516941316876
 0.3232787274258797 0.6479402777458034 0.3798651513718099
 0.9905823170817740 0.9833792570343007 0.3326301663354769
 0.6537020686251012 0.6530619144712446 0.3326332153773919
 0.3208231658317473 0.3162996159668268 0.3326409055655972
 0.3226721693783858 0.9832258303518415 0.2849591687386095
 0.9893632030331645 0.6498308292562882 0.2848977129151393
 0.6559816063983988 0.3165215904397769 0.2849817458569532
 0.3232427326678504 0.6498853424865700 0.2374443755264579
 0.9898751423815568 0.3159424832409385 0.2374462992112640
 0.6559624596539422 0.9831665828289857 0.2374468819165543
 0.9899401114626016 0.9833318005563996 0.1902927468778728
 0.6563234153838025 0.6501571855040140 0.1902808455467024
 0.3230878520756164 0.3166417724024413 0.1902999479996836
 0.3231282444018433 0.9837615869607319 0.1423363301164144
 0.9898658223465020 0.6501016690561059 0.1424226558208517
 0.6565213356648627 0.3165948292738321 0.1424132124821824

7. Pt/Al₂O₃/Pt interface geometry:

4.8389499999999996 0.0000000000000000 0.0000000000000000
 2.4194700000000000 4.1906499999999998 0.0000000000000000
 0.0000000000000000 0.0000000000000000 47.0000000000000000
 O Al Pt
 15 8 36
 0.6771759781171663 0.9794841022625769 0.6068901098392397
 0.9687793519543556 0.3463880819623785 0.6068839594896902
 0.3105325644208733 0.637935277773973 0.6068912938006666
 0.9579959523613598 0.0114447322212493 0.5613666425656715
 0.6557500207749991 0.6275009804554778 0.5613541711345472
 0.3420027786607619 0.3254145414384225 0.5613517660605937
 0.0133353735307631 0.2929483300891110 0.5150042943077925
 0.3179503165114267 0.6838009229506062 0.5150094502664903
 0.6227351416080837 0.9882984621481871 0.5150109111956603
 0.2942729687237792 0.3495040643347817 0.4686724355957079
 0.9805193693429811 0.9654175959660967 0.4686585985244932
 0.6784026438451108 0.6514626902256115 0.4686580695012206
 0.3260155368492538 0.6304375392085370 0.4231391799490019
 0.6676362704440194 0.9973083608196004 0.4231344583236401
 0.9594418449738349 0.3387589131879534 0.4231404103425322
 0.6521465678242369 0.3216573514775679 0.5876428138122678
 0.9856584106070738 0.6546049009243086 0.5821522251126079
 0.9845377062115889 0.6553079853430214 0.4979429826221726
 0.3178537905714190 0.9884402143789751 0.4860738714156208
 0.3181941965125559 0.9882492386494280 0.5439684923647855
 0.6516535220318050 0.3215759398540423 0.5321009806033572
 0.6509117078022196 0.3224652815630431 0.4478791179799878
 0.9846643515768098 0.6555862239792697 0.4423755545144092
 0.3173104839648672 0.6515856597082633 0.6487721407863924
 0.9832170033808102 0.3256943180213960 0.6487750547130757
 0.6571776310282599 0.9857572306170785 0.6487856449897947

0.9856251041691626 0.9882971189047863 0.6975390297111005
 0.6524079732510663 0.6536812668173360 0.6975405260639445
 0.3202282579978413 0.3205155633381792 0.6975447426712819
 0.3199499976808823 0.9874755945115086 0.7464268870550879
 0.9866406438942802 0.6541545256153201 0.7469566890581835
 0.6533044358406054 0.3208361373546300 0.7471344502574022
 0.3201380890431296 0.6546697026957777 0.7963429523375868
 0.9879500873434285 0.3201860725116073 0.7963428724974451
 0.6534302833767893 0.9868964950051788 0.7963420373814324
 0.9878747393313919 0.9867263038000131 0.8455065845635436
 0.6541398842136186 0.6535466658537002 0.8455074803349787
 0.3210766154124049 0.3198019348392748 0.8455078818525099
 0.3218363981548482 0.9858504456028010 0.8953014819408339
 0.9885219313959414 0.6525030702889154 0.8952652611511096
 0.6551911719095291 0.3191660846871004 0.8952658369842637
 0.9802514147607226 0.3246786536607088 0.3812377515798939
 0.6542391349942762 0.9906003943008767 0.3812165990611408
 0.3201601938491136 0.6505369396179712 0.3812358841126082
 0.9856634837666470 0.9874198612297960 0.3324816389104261
 0.6524615507541052 0.6552045121119084 0.3324805894187830
 0.3177893867787803 0.3220575719867430 0.3324765313181118
 0.3194379434461219 0.9880529543119227 0.2835909135148543
 0.9861212208985268 0.6547658728655903 0.2828846984057121
 0.6527698541140202 0.3214312828370618 0.2830638369752037
 0.3205460208439220 0.6549409739033545 0.2336849498106467
 0.9872479445281224 0.3204863862160885 0.2336850668306258
 0.6527609229695132 0.9882950371934914 0.2336851485576805
 0.9876806101598481 0.9874818250341191 0.1845356371845767
 0.6539709247423683 0.6543996035975453 0.1845365110743737
 0.3208092029993760 0.3206728457466431 0.1845326791131902
 0.3217074475887012 0.9868203777637784 0.1347498124891617
 0.9883772503338853 0.6534865158524789 0.1347766027366258
 0.6550413128266466 0.3201512893793842 0.1347736662342235

8. Pt/Cr₂O₃/Pt interface geometry:

4.3123500000000003 2.4897399999999998 0.0000000000000000
 0.0000000000000000 4.9794700000000001 0.0000000000000000
 0.0000000000000000 0.0000000000000000 47.0000000000000000
 O Cr Pt
 15 8 36
 0.6735821544111928 0.9775002727831605 0.6164109016745059
 0.9735658624508119 0.3383971818049432 0.6163982748137329
 0.3126388499771693 0.6383587354902573 0.6164084343223664
 0.9569896455047555 0.0066592313953464 0.5684333391624037
 0.6605551338820277 0.6223623317645490 0.5684418674997858
 0.3414072034869022 0.3258536238182970 0.5684409565950901
 0.0159532290504956 0.2886102712407279 0.5192947007097501
 0.3195976240562786 0.6814994124603970 0.5192961180503772
 0.6230479327483494 0.9851473425887320 0.5192942460237973
 0.2978305383602375 0.3477595584441104 0.4701371949620281
 0.9787144647615946 0.9633050870368365 0.4701385847786952
 0.6822345225469064 0.6442900481837057 0.4701305193898051
 0.3269722212054376 0.6313912629919969 0.4221388481588733
 0.6663004978655067 0.9921858262631744 0.4221316311969261
 0.9662320631744450 0.3314612701811868 0.4221435271614524
 0.6531489911917276 0.3182101359007987 0.5962606236141781
 0.9864448583695875 0.6515614577006090 0.5917787813392223
 0.9862035590993727 0.6517666793613657 0.4989468224957037

0.3195499774390882 0.9851133354088191 0.4902972671553627
0.3195830245430145 0.9850278956429293 0.5482602449315053
0.6528869517371660 0.3183894644227294 0.5396099894148065
0.6530533337572280 0.3184122801351492 0.4467870481568639
0.9863970493331706 0.6517413188671313 0.4423045794595524
0.3188027637618092 0.6451833945643628 0.6587610383185662
0.9818984091485135 0.3250737689394754 0.6587499732317639
0.6618534998385428 0.9821599367855001 0.6587667789160889
0.9880387713557326 0.9841833737921917 0.7063499893202376
0.6546702093078878 0.6496755418730373 0.7063461573899588
0.3224481103590335 0.3163488986434544 0.7063479175441145
0.3224357321238713 0.9828279572195697 0.7535891003316095
0.9891193904286553 0.6494928149427608 0.7540620510907061
0.6557751594641559 0.3161827110656716 0.7541066737474296
0.3229410929371141 0.6501625328400635 0.8012536136268054
0.9904865993360517 0.3149480253264798 0.8012546318758282
0.6552706860597723 0.9826387104145624 0.8012502261469123
0.9894774647938149 0.9826913994543460 0.8483396172620132
0.6567171775178267 0.6490651948009898 0.8483410275893561
0.3231280343272189 0.3162792635758649 0.8483413202577239
0.3232679112663348 0.9829169583218160 0.8963764980347690
0.9899288627850638 0.6496091734040021 0.8963447764524872
0.6566039097096379 0.3162522037289435 0.8963740693011459
0.9796938825741819 0.3235225816355651 0.3798191599113423
0.6596605974325627 0.9866128256076436 0.3798030674656587
0.3226267579626878 0.6436190121953231 0.3798133952221363
0.9885906698230471 0.9832468396893361 0.3322191842922706
0.6551813941101656 0.6510254695157727 0.3322211132782940
0.3206900996522535 0.3177190809932497 0.3322212354162986
0.3221595717756358 0.9835645037383642 0.2849824001730497
0.9888471432532029 0.6502046712147802 0.2844670730805774
0.6554913801499751 0.3168977883718327 0.2845104192108465
0.3225530750771384 0.6509938452125184 0.2373268840915159
0.9902264003586794 0.3157835380673788 0.2373261341406732
0.6550364853864892 0.9833084095991111 0.2373294950642659
0.9892119166907349 0.9834559829795282 0.1902317583710484
0.6564308815640061 0.6498678726320009 0.1902297794756294
0.3228152517057552 0.3170557966561276 0.1902311230893474
0.3230017777188081 0.9836783863093714 0.1421732370519209
0.9896843463926857 0.6503648912978903 0.1421754823047223
0.6563478948984525 0.3170174507041352 0.1422100968560898