

Supporting Information:

Can We Judge an Oxide by its Cover? The Case of Platinum over α -Fe₂O₃ from First Principles

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We provide in this supporting information further computational details on Density Functional Theory (DFT)-type calculations performed for bulk and slab unit cells. Below we report the unit cell relaxed geometries and k-grid and plane-wave energy cut-offs used for each cell. All provided geometries are in the following format:

Cell lattice vectors, atom types and number of atoms, atom locations in fractional coordinates, according to VASP standard input.

1. Pure Fe₂O₃ cell geometries:

Fe₂O₃ SI relaxed geometry – calculated with a 3x3x1 gamma-centered k-grid and a 750 eV plane-wave energy cut-off:

```
4.4147882200000002 2.5488791700000002 0.0000000000000000
0.0000000000000000 5.0977583400000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 24.2761897900000001
```

O Fe

15 8

```
0.7032668212234233 0.9671799607560607 0.6804087998133914
0.9111114517877474 0.3547494843452895 0.6849972014116901
0.3136889725721897 0.5768829115793970 0.6832436196237939
0.9464341897668318 0.0217192343082198 0.5933125456992934
0.6529532989991161 0.6186885057386179 0.5948306546663915
0.3341103678331658 0.3245160804375761 0.5944583849588342
0.0076716931603871 0.2941326676123869 0.4987765329675424
0.3121164993236054 0.6836580128616536 0.5012674801580631
0.6159872220553455 0.9879872287685975 0.5002890423910960
0.2872587291223717 0.3571189947200909 0.4051726471809701
0.9763104136061156 0.9582521764096346 0.4069385994963990
0.6703746490243262 0.6518104091761945 0.4058242746496463
0.2808355293979980 0.6219298606395353 0.3148530135702338
0.6859164372361491 0.0111160709138278 0.3184862354933084
0.8984030614707141 0.3991817723884537 0.3168797726179063
0.6519949143266223 0.3027789221593706 0.6487981623360762
0.9867969338111848 0.6301774632366307 0.6414371928127582
0.9803155925484134 0.6577928590527174 0.4666834995602047
0.3079059564030085 0.9949826311217210 0.4385534835694903
0.3145352220763202 0.9819946946897153 0.5615122004927471
0.6495003145295549 0.3199225084335164 0.5334038566430429
0.6300132687329087 0.3451456547322431 0.3602321742839434
0.9663914830507484 0.6761498635932315 0.3506625752487111
```

Fe₂O₃ S2 relaxed geometry - calculated with a 2x3x1 gamma-centered k-grid and a 750 eV plane-wave energy cut-off:

```

8.8295759999999994 0.0000000000000000 0.0000000000000000
0.0000000000000000 5.0977583400000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 24.2761897900000001
O Fe
30 16
0.3564859063406232 0.3349562376726709 0.6834450776406698
0.4638695639306505 0.8436809146338220 0.6814586901072488
0.1659689062359746 0.7501538316880030 0.6851986864046182
0.4722807950073999 0.4743381308024581 0.5948495490455343
0.3199615912950549 0.9363130659759022 0.5932855391041585
0.1639359121954129 0.4894013611556645 0.5951009473179596
0.9975504570700480 0.2894849618962070 0.5007372796027525
0.1490562635922146 0.8351913365257673 0.4993268937340503
0.3010019599349221 0.2899516704930036 0.5000690025192114
0.1343275175061294 0.4954265389371102 0.4068400484714090
0.4793255622159407 0.4548559946592619 0.4051829257873223
0.3327998955162741 0.9851468855301420 0.4050142568952566
0.1601590384860074 0.7566582847819987 0.3186101462346755
0.3520910365627117 0.3498247271954966 0.3165456760969008
0.4643441641342108 0.8566218966171633 0.3150080203239156
0.8564884213170600 0.8349419340051227 0.6834397806522574
0.9638664424666672 0.3436629025991564 0.6814560004336698
0.6659582288741106 0.2501537637708395 0.6851980746939077
0.9722839414806188 0.9743313628913484 0.5948442924367754
0.8199616352506922 0.4362938338005478 0.5932798924023217
0.6639305956016912 0.9893969743310365 0.5950966561524140
0.4975463341851594 0.7894881056374814 0.5007403359354186
0.6490523827747197 0.3351860035009935 0.4993267885079717
0.8009984054767045 0.7899466145054319 0.5000656218051276
0.6343271437355824 0.9954257116001699 0.4068408774650436
0.9793281372766600 0.9548538098129598 0.4051831967402393
0.8328004638696385 0.4851450450637458 0.4050130745345015
0.6601582873688514 0.2566573912972956 0.3186104827871006
0.8520897114554487 0.8498252219632931 0.3165454292371663
0.9643434502485846 0.3566298859264805 0.3150081584068403
0.3229361335472589 0.6473281838043690 0.6497097831711827
0.4899844291627673 0.1489483738725568 0.6391136520508951
0.4826785581329887 0.1347117937481386 0.4662957174557647
0.150745048777335 0.1421293175633664 0.4393075143974059
0.8229439340554876 0.1473159797092691 0.6497003775732111
0.9899889154843180 0.6489627432774654 0.6391125313440966
0.9826894909979416 0.6347176978583278 0.4662947894322258
0.6507432247479343 0.6421260209357840 0.4393067655290750
0.1516391668087991 0.1379548293867856 0.5607851399182309
0.3141620768414484 0.6401101155211038 0.5337953296149962
0.3254452853454524 0.6430588781112760 0.3609538326089137
0.4912006928270003 0.1436060477843739 0.3504099733977881
0.6516390711887681 0.6379530450750366 0.5607842520488191
0.8141636740606444 0.1401012726004041 0.5337938349241043
0.8254446721287536 0.1430633483905268 0.3609526611337941
0.9911979384769580 0.6435959530906104 0.3504084439230226

```

2. Pure Pt cell geometries – slab structures with [111] direction along the z vector, we provide slabs with 6 Pt layers since results were converged at this slab thickness and slabs with more layers can be produced from these:

6 Pt layer S1 relaxed geometry– calculated with a 8x8x1 gamma-centered k-grid and a 850 eV plane-wave energy cut-off:

```

5.6267361641000004  0.0000000000000000  0.0000000000000000
2.8133625273999998  4.8729040702999997  0.0000000000000000
0.0000000000000000  0.0000000000000000  24.1884000000000015
Pt
24
-0.0000048833883087  0.0000040462855170 -0.0004271556033260
-0.0000012986939024  0.5000004487615781 -0.0004260710767443
0.5000039566252645  0.0000016435274606 -0.0004226800794963
0.5000048228472398  0.4999953802781900 -0.0004253261527987
0.3333410381420492  0.3333298980930839  0.0956984004227112
0.3333353484910266  0.8333298664405113  0.0956919359130304
0.8333311052733073  0.3333291719442387  0.0957003118373938
0.8333336978337078  0.8333361805947319  0.0956997422452069
0.1666743558615970  0.1666619395269428  0.1902551629235457
0.1666756068490030  0.6666662685392805  0.1902539863502123
0.6666675147652589  0.1666675470827210  0.1902653882096254
0.6666648972039361  0.6666690534272054  0.1902580288280599
-0.0000008171466622 -0.0000027320328139  0.2845771388509701
-0.0000036769073551  0.5000007897021220  0.2845689147258862
0.4999942543961413 -0.0000014658246163  0.2845798289828265
0.4999931032484659  0.5000036498748900  0.2845795372702162
0.3333263535595399  0.3333393565511631  0.3791368341958505
0.3333320190982731  0.8333320850150286  0.3791430355174622
0.8333313694304125  0.3333388964672312  0.3791367144873997
0.8333341743622458  0.8333294076107443  0.3791350242374795
0.1666649974825692  0.1666682353992518  0.4752579642081792
0.1666562094959378  0.6666690578462944  0.4752605020146706
0.6666696079004494  0.1666573989440241  0.4752623794905482
0.6666722432698137  0.6666698759452296  0.4752604022010762

```

6 Pt layer S2 relaxed geometry - calculated with a 6x8x1 gamma-centered k-grid and a 850 eV plane-wave energy cut-off:

```

8.4401102066000000  0.0000000000000000  0.0000000000000000
0.0000000000000000  4.8728899955999996  0.0000000000000000
0.0000000000000000  0.0000000000000000  26.7332999999999998
Pt
36
0.9936585365948858  0.3118447048694293  0.4162836596253570
0.3271984384179589  0.3115902432326791  0.4162908443067863
0.6602934730315155  0.3113903849285578  0.4162842579456338
0.1603036552745465  0.8114008767833383  0.4162849324204529
0.4936592449400052  0.8118326949284693  0.4162881882357112
0.8271940222658856  0.8115807570909226  0.4162819270764899
0.1613974696582403  0.4781809492046918  0.5030936765693568
0.4947497227686242  0.4783308901674346  0.5030976031649246
0.8279920956556666  0.4782695217834316  0.5030888856076245
0.9947454732067129  0.9783193271253126  0.5030959518611411
0.3279902125397598  0.9782925891907510  0.5030952824062283
0.6613971171556017  0.9781756110795712  0.5030891095503378
0.9950491405743520  0.6440296162707639  0.5884352157914208
0.3283700117158546  0.6440567065897653  0.5884389325576080
0.6617284546574709  0.6440487482495030  0.5884485749709825
0.1617157546315084  0.1440317562422138  0.5884489852016870
0.4950622067368755  0.1440354977547926  0.5884304429436398
0.8283786835280793  0.1440153360286160  0.5884401142525419
0.9952528616768319  0.3108051509848835  0.6734736711851141

```

0.3285200703973956 0.3108553151692135 0.6734635341667570
0.6619030657507494 0.3109353226741547 0.6734662271498308
0.1619079669679735 0.8109024634688993 0.6734662208879030
0.4952471411478783 0.8108064540473734 0.6734610202416746
0.8285273296564597 0.8108369461573233 0.6734684714661157
0.1618798685159604 0.4768557323516518 0.7587803043273809
0.4952317874126351 0.4768994166126816 0.7587719505550936
0.8285444633242705 0.4769223720073299 0.7587810055797846
0.9952397034670852 0.9768946422365374 0.7587802951739988
0.3285456615922300 0.9769140416768849 0.7587774872763191
0.6618682426981763 0.9768888169586205 0.7587773015788173
0.9948587265925966 0.6442926881577193 0.8456262470492177
0.3281791225122959 0.6442773382883047 0.8456123653573542
0.6615087897383702 0.6442970897240841 0.8455915258444691
0.1615247134709605 0.1443068136306209 0.8455979079977070
0.4948518056943243 0.1442744152731024 0.8456144872959683
0.8281749660303106 0.1442787690603851 0.8456133923786027

3. Interface geometries –we provide cells with 6 Pt layers and 4 stoichiometric units of Fe₂O₃. Other thicknesses can be produces from these:

Pt/Fe₂O₃ S1 relaxed geometry - calculated with a 8x8x1 gamma-centered k-grid and a 850 eV plane-wave energy cut-off:

4.6438495955999999 2.6811183324000001 0.0000000000000000
0.0000000000000000 5.3622472520000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 46.0000000000000000
O Fe Pt
15 8 48
0.7278733790115055 0.9824238548110742 0.6082019111321699
0.9071503669657872 0.4062884477587687 0.6081375866292476
0.3044192142433459 0.5856047816869108 0.6082289862457699
0.9555610776103975 0.0170455479201976 0.5587819753731722
0.6451484907529377 0.6331009199269033 0.5587530935239542
0.3396173926907835 0.3230099305019749 0.5587807990230971
0.0090070264338777 0.2956584197651537 0.5104642253500487
0.3133017529815305 0.6870731515807051 0.5104612635326191
0.6175506785310318 0.9914853602738347 0.5104710507272543
0.2871812726875547 0.3493954559758379 0.4621482997519593
0.9815229257536302 0.9651129959510101 0.4621631330789882
0.6712518952254456 0.6597971358120276 0.4621756693292909
0.3216966439091067 0.5784108527925156 0.4127358502022958
0.7183736241643572 0.0003499058231853 0.4127599010352014
0.8990461038625384 0.3972874160866269 0.4128018228494739
0.6465488351808517 0.3246478931089101 0.5858213570933728
0.9801408462428753 0.6579889055673789 0.5803873903505377
0.9798445918488881 0.6582187307654195 0.4946649335638895
0.3132320751269475 0.9916012411719919 0.4790659276622264
0.3132704878339752 0.9912496547698595 0.5418743575129668
0.6465633595660307 0.3248219612744521 0.5262762061157531
0.6462084610942398 0.3252677199936258 0.4405509463876456
0.9799139479602204 0.6584438585606591 0.4351410522840951
0.3134389271215881 0.9881964899930082 0.6521674934656829
0.3128550572323050 0.4944658812011582 0.6507376339676867
0.8076197633051905 0.9883385833031895 0.6507743386138500
0.8197241194383977 0.4824181929477334 0.6507258826022522
0.6514644243315075 0.3307384363828163 0.7032140813567054
0.6511952171710860 0.8291160343325501 0.7038230134044170
0.1532427805527234 0.3305178236490605 0.7036195702333785
0.1497089062467083 0.8323407096798334 0.7038652827607805
0.4865989238013526 0.1680239607615519 0.7567921747673694

0.4872318300909342 0.6677337982834715 0.7568846529950335
 0.9867418946984117 0.1677949897664348 0.7568516417573932
 0.9869807280009439 0.6678911256734850 0.7564137572181622
 0.3203259065351460 0.0009555504687739 0.8098455749685343
 0.3201630203054222 0.5011838975585192 0.8096522459629227
 0.8202456830829732 0.0008142489457157 0.8097085068638989
 0.8206700406223746 0.5010505159965390 0.8096862067098698
 0.6534490951515366 0.3335250730563359 0.8625172520578630
 0.6535777584852056 0.8334609620897737 0.8627196766216443
 0.1533933429488812 0.3336712053551025 0.8627043070651794
 0.1533676143077187 0.8335119192132225 0.8627133383881826
 0.4870692304254050 0.1678084755226266 0.9157628906469313
 0.4871999118899808 0.6672984996079236 0.9157752878157979
 0.9867163590529699 0.1677196100718774 0.9157800676412293
 0.9870193195440464 0.6675891469278312 0.9160179304293479
 0.3133085114945473 0.9891004626979054 0.3690220983169326
 0.3139268545088214 0.4943382818708386 0.3702314417787278
 0.8072351154192958 0.9904222080146496 0.3702015516912525
 0.8186001021787419 0.4831468045945400 0.3702241283788794
 0.6514608025424593 0.3307916068100738 0.3172564982540678
 0.6512422434905574 0.8288800003735020 0.3173760678136048
 0.1534617049505513 0.3306784039038320 0.3175743205403023
 0.1494051245096912 0.8325986509165801 0.3173469898568158
 0.4865360700747985 0.1677371726783576 0.2642057263599469
 0.4871619189576251 0.6675839704394733 0.2641346956246906
 0.9868543955901927 0.1674714072874437 0.2641685101591449
 0.9869598752313209 0.6676488301881847 0.2646904433205108
 0.3203151997429217 0.0010801072333564 0.2113073581585496
 0.3200877205060664 0.5013764247723245 0.2113666786703590
 0.8202363803046779 0.0008698581594118 0.2113137102731955
 0.8207126849165363 0.5011338047997995 0.2113489823999117
 0.6533581628694662 0.3337138636582395 0.1585743029215578
 0.6535913031662659 0.8335990391998394 0.1583612838434405
 0.1532503390670144 0.3339511720389723 0.1583780040513147
 0.1532143386794402 0.8336467629875344 0.1583692493739051
 0.4870958671819920 0.1675925757936128 0.1053563581215471
 0.4872320200022386 0.6671748673137543 0.1053465865060659
 0.9868480156152728 0.1674947929493911 0.1053390168692232
 0.9870977049788507 0.6674069186508333 0.1050024496469177

Pt/Fe₂O₃ S2 relaxed geometry - calculated with a 6x8x1 gamma-centered k-grid and a 850 eV plane-wave energy cut-off:

8.6348400000000005 0.0000000000000000 0.0000000000000000
 0.0000000000000000 4.9853199999999998 0.0000000000000000
 0.0000000000000000 0.0000000000000000 47.0000000000000000
 O Fe Pt
 30 16 72
 0.3376038867607249 0.3125582934556519 0.6198884919607650
 0.4870783824901395 0.8274420041203854 0.6198725701358612
 0.1548750934188519 0.7942430146066997 0.6198864597710028
 0.4796472678526271 0.4848663614103401 0.5706903150176927
 0.3294310645244707 0.9548002164710354 0.5706959173809665
 0.1696432194063604 0.4945100649235670 0.5706958225083270
 0.0067041843376430 0.2975053396980840 0.5207825108317081
 0.1594652464026325 0.8392500862137169 0.5207846034936452
 0.3122011554810129 0.2974926750577609 0.5207834804100884
 0.1495022381674573 0.4946608580552692 0.4708742587900758
 0.4896464850896933 0.4549079722830811 0.4708774004372884
 0.3394419664241184 0.9850980886916147 0.4708677123771494

0.1647178602406640 0.7945522171329813 0.4216944989978018
0.3325358727798502 0.3277770764423735 0.4216823329952106
0.4820636157515068 0.8128050320861036 0.4216908674202173
0.8376003109007542 0.8125518347847773 0.6198885314544142
0.9870767891416676 0.3274332810615519 0.6198728868795556
0.6548772304989612 0.2942572721210865 0.6198858970184773
0.9796472814473844 0.9848644148013008 0.5706905844285117
0.8294321856163549 0.4547977294365424 0.5706960593104355
0.6696434997472238 0.9945105738008664 0.5706957603711516
0.5067042908675177 0.7975060695047418 0.5207825752446027
0.6594657496587715 0.3392501244415129 0.5207846458368479
0.8122013115628732 0.7974920190023838 0.5207834509630587
0.6495020497214128 0.9946615479860412 0.4708742339629666
0.9896461148055025 0.9549050807908728 0.4708773403714730
0.8394421952133158 0.4850946231864981 0.4708674627005109
0.6647195438192526 0.2945485590368051 0.4216934300133133
0.8325340824169132 0.8277663679564000 0.4216822995348366
0.9820669244244513 0.3127986095538446 0.4216914919891792
0.3264002272610114 0.6447544969275611 0.5991963748576765
0.4929903760933954 0.1447246637922674 0.5928981831955724
0.4927946849874161 0.1447633016449856 0.5023113775494465
0.1594860699192822 0.1448441590107805 0.4894034151453326
0.8264014381188431 0.1447498855871459 0.5991965811437794
0.9929906130944843 0.6447196934795016 0.5928986831897092
0.9927951609735999 0.6447636829069481 0.5023112158551015
0.6594867336355534 0.6448439424641421 0.4894033736320154
0.1595256213324205 0.1447280835192899 0.5521673541067145
0.3261271220166932 0.6447510632297195 0.5392568585747810
0.3262730008376025 0.6449524509790265 0.4486709100397590
0.4929776591863941 0.1449748626648244 0.4423695278792863
0.6595264278316719 0.6447278715978584 0.5521673151234197
0.8261268089270004 0.1447509789704782 0.5392569063876351
0.8262737660493400 0.1449457412260813 0.4486708061504316
0.9929777707456537 0.6449699546289125 0.4423693258299792
0.9933443833504185 0.3144272848029175 0.6616980329514703
0.3288866727420086 0.3103337248882596 0.6617126929117063
0.6590379184570736 0.3092713601426880 0.6617042938987154
0.1590380705384575 0.8092529203662906 0.6617051411669976
0.4933453028408010 0.8144484457742891 0.6616971925827499
0.828880693330825 0.8103292105856283 0.6617127714499844
0.1614289835371565 0.4762135254859245 0.7089330534102913
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