Supporting Information for: Hybrid Catalysis-Reactive Sorption Mechanism for 2-CEES and Sulfur Mustard Dehydrochlorination on Single Metal Atoms on Anatase-TiO_2

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Transition State Calculations

The kinetic barriers calculated in this study were done using transition state theory (TST). All reactant and product structures were first optimized, after which minimum-energy pathways were identified using saddle-point search techniques, namely climbing image nudged elastic band (CI-NEB). In CI-NEB, a series of intermediate images connecting fully optimized initial and final states were generated and linked by spring forces to allow for an even distribution along the reaction coordinate. The images were then optimized simultaneously to obtain the minimum energy path while constraining motion perpendicular to the path. After initial convergence, the highest-energy image was converted to a climbing image by removing the spring forces and inverting the force component along the reaction coordinate, driving this image directly toward the first-order saddle point. The resulting transition states were further refined using the dimer and quasi-Newton methods. The optimized transition states were subsequently verified by vibrational frequency analysis to confirm the presence of a single imaginary frequency.

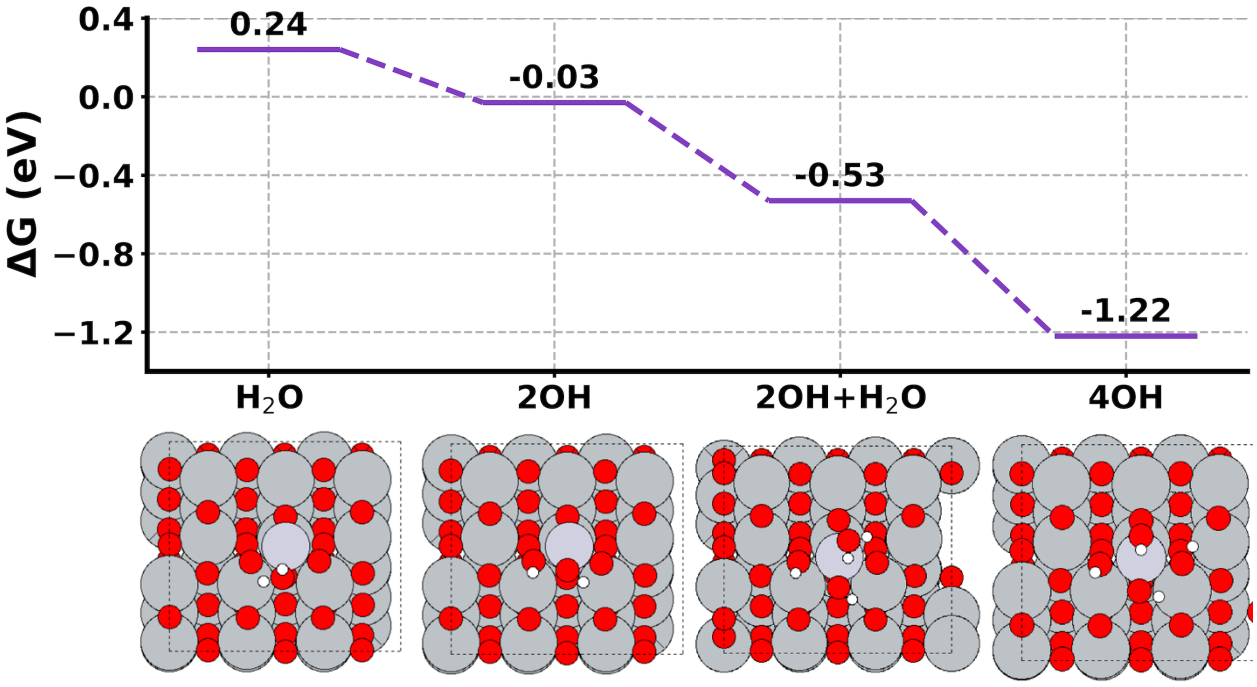

Figure S1. Gibbs free energy profile of sequential adsorption and dissociation of two water molecules on PtO_2 supported on anatase-TiO_2(101). The partial pressure of $H_2O_{(g)}$ is taken as the vapor pressure of water at 298 K assuming vapor-liquid equilibrium.

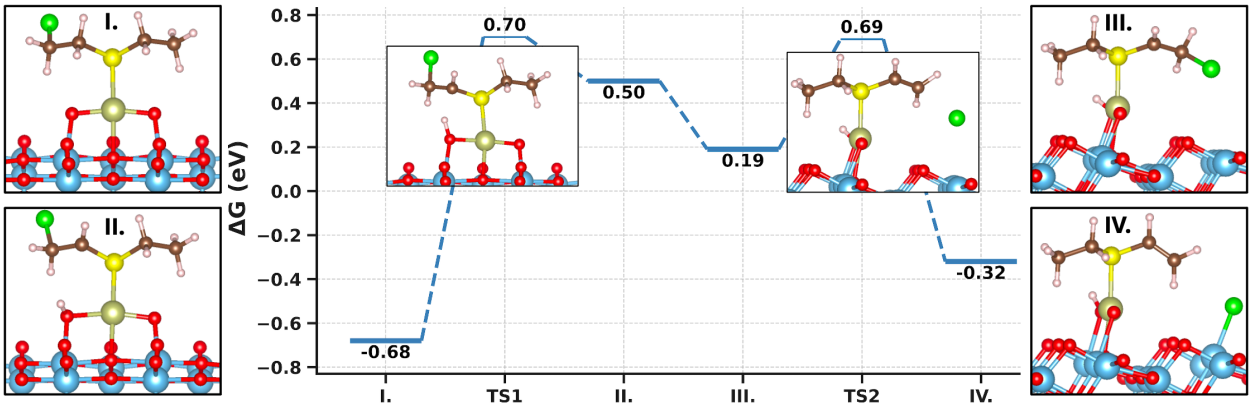

Figure S2. Gibbs free energy profile of 2-CEES decomposition on dry IrO_2 supported on anatase-TiO_2(101) via C–H and C-Cl bond cleavages starting from the most stable adsorption mode. Elementary reaction barriers are indicated by TS1 and TS2 whose structures have been overlaid on the profile. For the free energy calculation T = 298 K, partial pressure of 2-CEES = 0.01 bar, and conversion of 2-CEES into EVS is 50%.

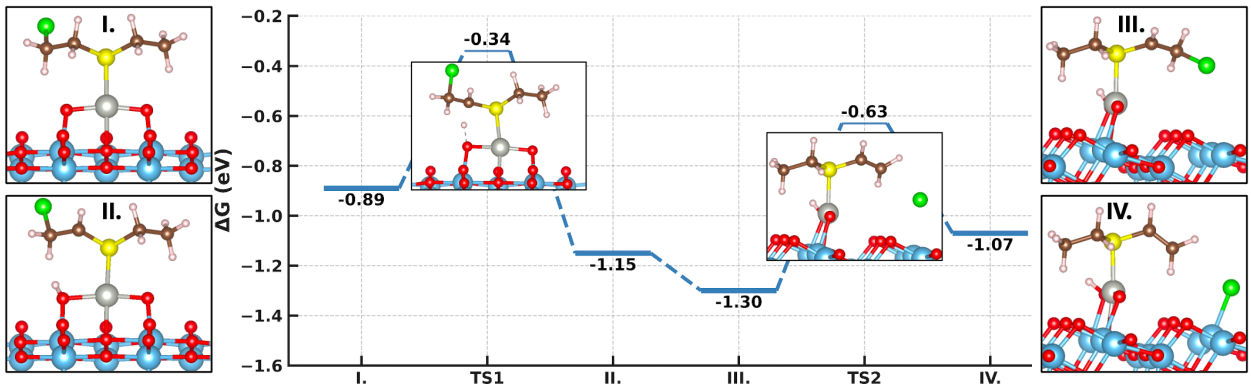

Figure S3. Gibbs free energy profile of 2-CEES decomposition on dry PdO_2 supported on anatase-TiO_2(101) via C–H and C-Cl bond cleavages starting from the most stable adsorption mode. Elementary reaction barriers are indicated by TS1 and TS2 whose structures have been overlaid on the profile. For the free energy calculation T = 298 K, partial pressure of 2-CEES = 0.01 bar, and conversion of 2-CEES into EVS is 50%.

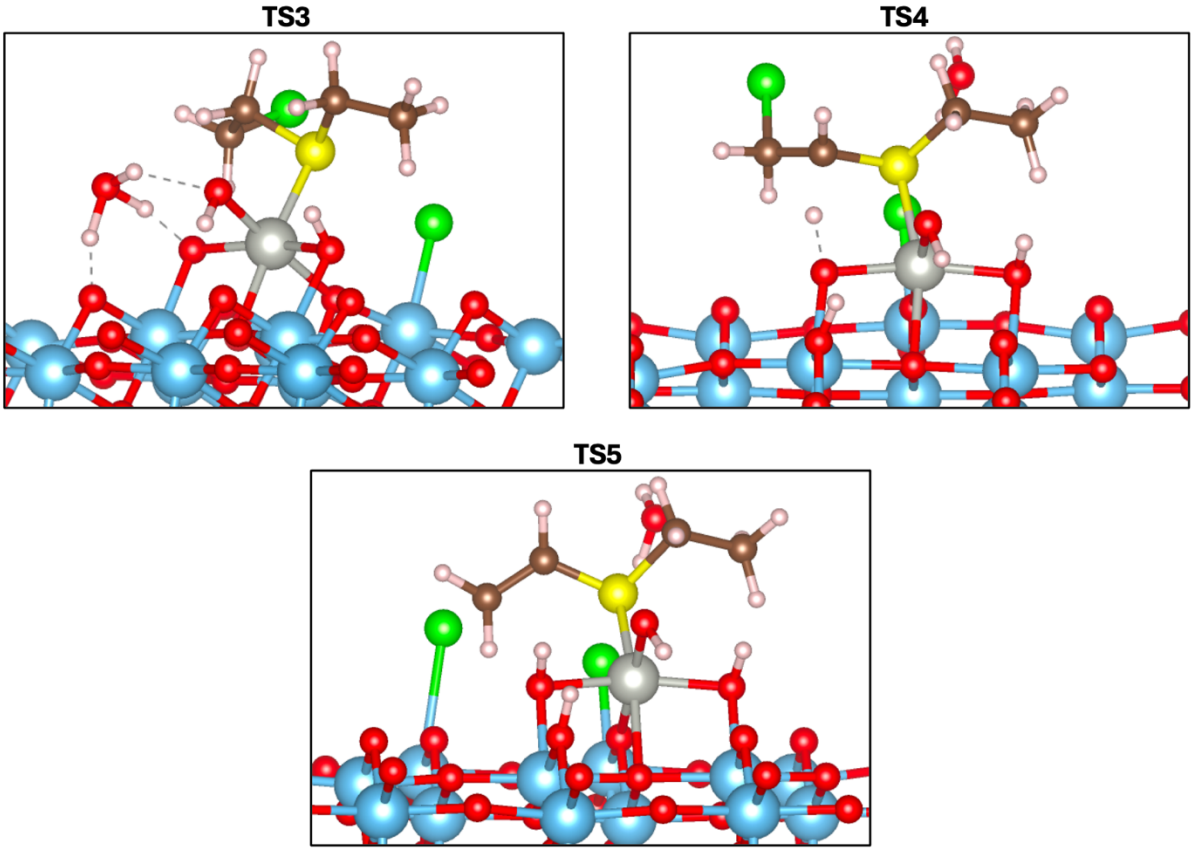

Figure S4. Transition state (TS) structures for Figure 5: Gibbs free energy profile of elementary steps for conversion of two 2-CEES molecules into two $EVS_{(g)}$ molecules on hydroxylated PdO_2 supported on anatase-TiO_2(101). TS3 corresponds to H transfer, TS4 corresponds to dehydrogenation, and TS5 corresponds to dechlorination.

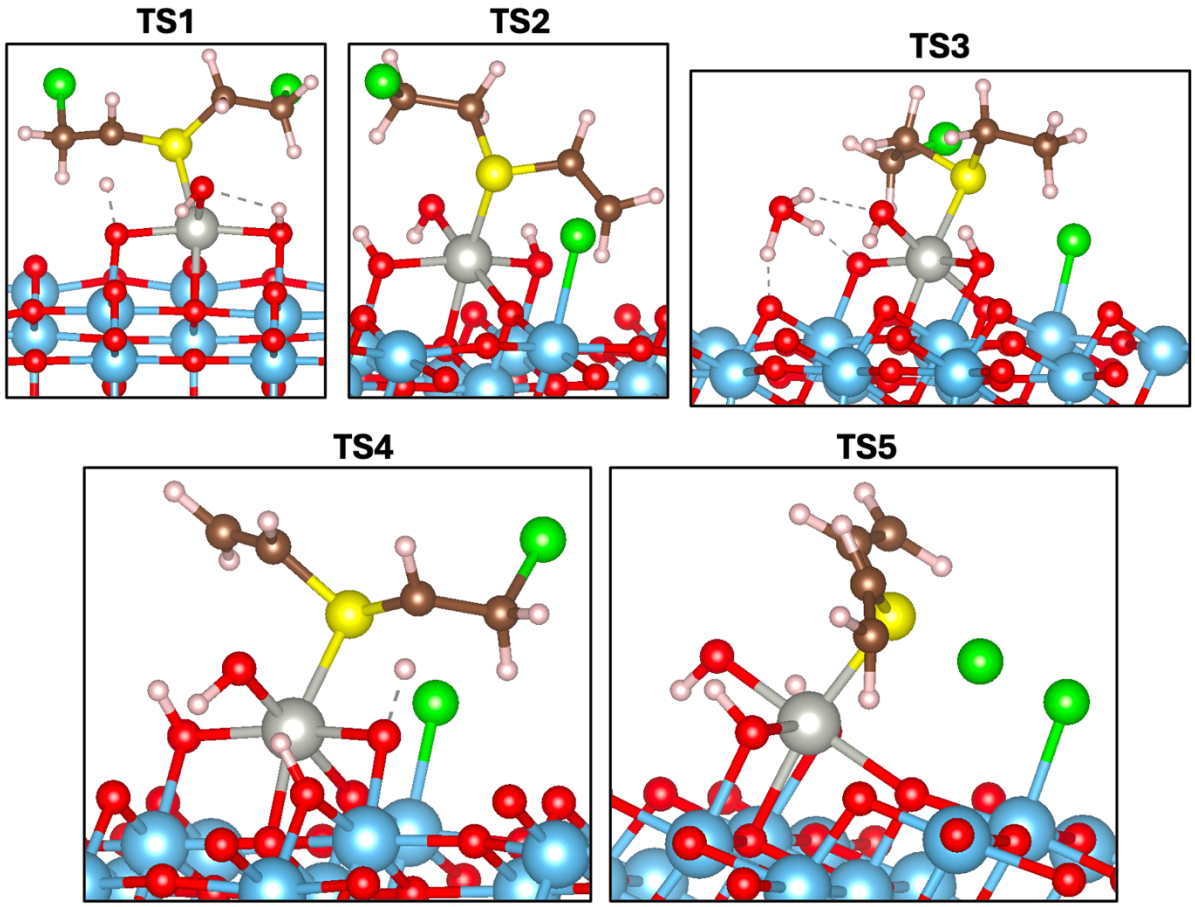

Figure S5. Transition state (TS) structures for Figure 8: Gibbs free energy profile of elementary steps for sulfur mustard conversion into divinyl-sulfide (DVS) on hydroxylated PdO_2 supported on anatase-TiO_2(101). TS1 corresponds to 1st dehydrogenation, TS2 corresponds to 1st dechlorination, TS3 corresponds to H transfer, TS4 corresponds to 2nd dehydrogenation, and TS5 corresponds to 2nd dechlorination.

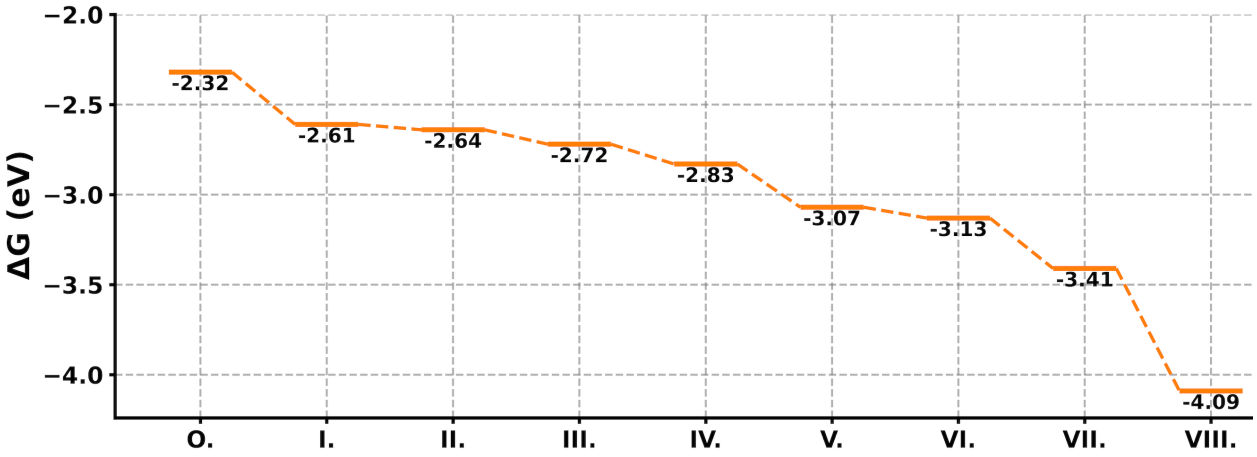

Figure S6. Gibbs free energy profile of elementary steps for a 2nd sulfur mustard molecule conversion into divinyl-sulfide (DVS) on hydroxylated PdO_2 supported on anatase-TiO_2(101). Structure O represents desorbed $DVS_{(g)}$ and H_2O bound to the Pd active site (structure IX in Figure 8). Structure I represents a 2nd sulfur mustard molecule bound to the Pd active site and desorbed DVS (substitution of DVS by the 2nd mustard). Structure VIII represents the 2nd DVS molecule. Structures II to VII are the reaction intermediates: (II-H transfer, III-Dehydrogenation, IV-Rearrangement, V-Dechlorination, VI-H transfer, VII-Dehydrogenation, VIII- Dechlorination). For the free energy calculation T = 298 K, partial pressure of 2-CEES and sulfur mustard = 0.01 bar, and conversion is 50%.

```
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     0.0000000000000000   10.4970798492000004    0.0000000000000000
     0.0000000000000000    0.0000000000000000   30.0000000000000000
   Ti   O    Pt   C    Cl   H    S
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Selective dynamics
Direct
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Figure S7. POSCAR for 2-CEES adsorption on dry PtO_2 supported on anatase-TiO_2(101)

```
Ti  O Pt  C Cl  H  S  O  H
   1.00000000000000
    11.6086997986000000    0.0000000000000000    0.0000000000000000
     0.0000000000000000   10.4970798492000004    0.0000000000000000
     0.0000000000000000    0.0000000000000000   30.0000000000000000
   Ti   O    Pt   C    Cl   H    S    O    H
    48    98     1     4     1     9     1     1     2
Selective dynamics
Direct
  0.5006996977415312  0.1226303397709572  0.0308348817084223   F   F   F
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  0.4982751631253209  0.5402131298761882  0.3800775200982815   T   T   T
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  0.3351961858245648  0.0519928046564737  0.3894223938278100   T   T   T
  0.3338478865793429  0.1854733264711786  0.2954998343153192   T   T   T
  0.3225263331315910  0.3283707339836199  0.4173107753721528   T   T   T
  0.5006977989396262  0.3950558257726016  0.0504933171525792   F   F   F
  0.4999330569646375  0.8140740497838191  0.4083634371556900   T   T   T
  0.8340243141044184  0.1226482355139069  0.0307980139515251   F   F   F
  0.8335786928661761  0.4021588425862823  0.2651331380878234   T   T   T
  0.8335745586351783  0.5482814151677592  0.3848937515787035   T   T   T
  0.6673735281712538  0.6231742660465827  0.0310847702734023   F   F   F
  0.6673951759417196  0.0481725313389545  0.3888096164299600   T   T   T
  0.6672102903909255  0.1846291484843854  0.2932659463333199   T   T   T
  0.6766241359365230  0.3233182891401287  0.4120004940651627   T   T   T
  0.8339804263420234  0.3950105172548319  0.0504908085087479   F   F   F
  0.8335211784891066  0.8182224354954573  0.4064685834845911   T   T   T
  0.1673963672531045  0.1226654081311054  0.0308197627108626   F   F   F
  0.1677983311255273  0.4021748364213629  0.2651172441593074   T   T   T
  0.1672469949031171  0.5477681529038325  0.3844583593693280   T   T   T
  0.0007263314815944  0.6228463858092255  0.0309515503156916   F   F   F
  0.0015433950065945  0.0456095513127396  0.3875221854552114   T   T   T
  0.0008357578091112  0.1832172418649743  0.2901577265052513   T   T   T
 -0.0000216970416797  0.3194331524115483  0.4054873884877560   T   T   T
  0.1674312504078657  0.3950208983825121  0.0505129066471497   F   F   F
  0.1693122236125967  0.8183295395697201  0.4065366735857001   T   T   T
  0.5004422555829128  0.2606305215457437  0.1472362610752844   T   T   T
  0.3335546693858786  0.9079880098478873  0.2668299387754016   T   T   T
  0.3338534530539774  0.0426226377680375  0.1739690178107987   T   T   T
  0.5004224987531377  0.6858824930412041  0.2878632757536969   T   T   T
  0.8338411091215537  0.2613464731449517  0.1475071242267942   T   T   T
  0.6678383318046897  0.9064570375423606  0.2666510916084371   T   T   T
  0.6672926056649904  0.0423252899385640  0.1731849036234862   T   T   T
  0.8337013860993039  0.6835378634353103  0.2888738180282919   T   T   T
  0.1674687004729145  0.2613187960816431  0.1475398476954921   T   T   T
  0.0007627100417719  0.9037832561341325  0.2661409035873009   T   T   T
  0.0006306145963632  0.0415669077123069  0.1720563638582190   T   T   T
  0.1678642328973381  0.6838901492913173  0.2888068778218262   T   T   T
  0.3337248410126658  0.7646543924683140  0.1479332787268943   T   T   T
  0.3340496263033970  0.8954046178637896  0.0510558284607043   F   F   F
  0.5003813029786151  0.5432392804865687  0.1707973182219182   T   T   T
  0.6674938872389039  0.7637452590620887  0.1479656147592959   T   T   T
  0.6673697039057487  0.8953863539000935  0.0510144758035480   F   F   F
  0.8337272593093744  0.5420132312396527  0.1712516775103028   T   T   T
  0.0006939179915054  0.7623065862702039  0.1477940910120975   T   T   T
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0.0007108818663752	0.8951314846780249	0.0506837988146742	F	F	F
0.1678450156274837	0.5421596560654997	0.1712615323273975	T	T	T
0.5006495162805134	0.2232300783651386	0.2887539201932872	T	T	T
0.5014348993201039	0.3667709155105835	0.4154243645846377	T	T	T
0.3340608422739209	0.4347500569770943	0.0492537621692151	F	F	F
0.3358327900126816	0.8622395333535228	0.4152591986094478	T	T	T
0.3348322512096134	0.0088942953209510	0.3206020149970806	T	T	T
0.3359631030421834	0.1586747135877926	0.4394695280975657	T	T	T
0.5007293049093207	0.2184841558815336	0.0825058595281405	F	F	F
0.4985906792695330	0.6405347376686298	0.4365400675411609	T	T	T
0.5007079090333875	0.5747900337452734	0.0243574470876453	F	F	F
0.5012334138514104	0.9987697719050973	0.3911969657891293	T	T	T
0.3340489994025546	0.0743763215772404	0.0241986002383783	F	F	F
0.3341913723909275	0.3660275398142652	0.2699017454337296	T	T	T
0.3343333594378899	0.5020059557780676	0.3815910342161810	T	T	T
0.3341879658059526	0.7800918013219302	0.0021772415827357	F	F	F
0.3347318139632635	0.2222747607807195	0.3591676710720635	T	T	T
0.5007091085999136	0.2795535314299684	0.0017775871505918	F	F	F
0.5002756810751159	0.7226953344946977	0.3561825834382297	T	T	T
0.8337613116083467	0.2226092432512034	0.2884935772814796	T	T	T
0.8381609824131537	0.3684551911352769	0.4109903067866230	T	T	T
0.6673456418459622	0.4347311450016207	0.0492304192247275	F	F	F
0.6662861434703193	0.8628409129670870	0.4150230081827523	T	T	T
0.6666862647451361	0.0100189662596027	0.3202890797105212	T	T	T
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0.8340225507848231	0.2184562882131900	0.0824675952741032	F	F	F
0.8331575522346391	0.6605473572404759	0.4345847915099980	T	T	T
0.8340017310513801	0.5746942132115365	0.0242903919570736	F	F	F
0.8332978726191554	0.0065322752820910	0.3896363664979277	T	T	T
0.6673462887887567	0.0743685216712393	0.0241764804384488	F	F	F
0.6671180911288873	0.3646106463913054	0.2688449206904185	T	T	T
0.6665406301596252	0.5024797332835449	0.3845562435128574	T	T	T
0.6674038655757499	0.7800676015289767	0.0021396817594521	F	F	F
0.6659174329855209	0.2239917474497002	0.3582397905318512	T	T	T
0.8339983198822054	0.2795543115580585	0.0017489980147616	F	F	F
0.8325143162028888	0.7258700926054892	0.3544725646686181	T	T	T
0.1674466010226690	0.2227181640268102	0.2883233200020039	T	T	T
0.1605856149597250	0.3694331590190845	0.4115334090668649	T	T	T
0.0007073033921188	0.4346424832735067	0.0491818976677934	F	F	F
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0.0012198958886010	0.0093997964761427	0.3192436158182277	T	T	T
0.9998835667343271	0.1636297067939107	0.4354605958309083	T	T	T
0.1674625023756704	0.2184840320475629	0.0824889304489673	F	F	F
0.1690163237629520	0.6599035755353772	0.4344361885676223	T	T	T
0.1674389389043753	0.5747081516329970	0.0243156673899705	F	F	F
0.1688920418612672	0.0073229342322843	0.3904232787768863	T	T	T
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0.0004840912781059	0.3638681315232040	0.2678981898686709	T	T	T
0.0000583160452432	0.5104929153722007	0.3863210268971980	T	T	T
0.0007941924944674	0.7797634528032376	0.0019151049756942	F	F	F
0.0012566752682518	0.2222516096314883	0.3550186194453193	T	T	T
0.1674887040323156	0.2795668261471747	0.0017706688979260	F	F	F
0.1689364585226854	0.7263343956620357	0.3544583063070884	T	T	T
0.5006557638464041	0.0798771617571317	0.1699408729109685	T	T	T
0.3344790433461499	0.7221222102168533	0.2868782073273754	T	T	T

0.3341717967825294	0.8677544066452418	0.2006161605218586	T	T	T
0.5001624093381154	0.3673010165961826	0.1994219285523767	T	T	T
0.5034652269131495	0.5121644037267954	0.3161450231189251	T	T	T
0.5008005475783179	0.8677352018266854	0.2690769725478679	T	T	T
0.3340379406546745	0.2231072670559902	0.1508611855948187	T	T	T
0.3338778699936830	0.0795472824316759	0.2397358648345019	T	T	T
0.5007507797904911	0.4334412812573385	0.1185960717235649	T	T	T
0.5001423760968856	0.5790922898821310	0.2366159077115274	T	T	T
0.8338790990826734	0.0795744174139236	0.1694913619575809	T	T	T
0.6669634057695734	0.7225435470509753	0.2867562217913859	T	T	T
0.6673218137323604	0.8679875447494343	0.2005050254872766	T	T	T
0.8334494265108149	0.3670641402998602	0.1995908011213360	T	T	T
0.8351370338685986	0.5117640355926015	0.3174222660324468	T	T	T
0.8339315613456318	0.8671490436597623	0.2689491568416845	T	T	T
0.6671170385234363	0.2231916861861525	0.1507675776952076	T	T	T
0.6675272204979326	0.0795796241042887	0.2393302588956703	T	T	T
0.8340445974432955	0.4335432827404595	0.1186696252786603	T	T	T
0.8331579651070163	0.5781107637316025	0.2370197623571982	T	T	T
0.1672448496482365	0.0796223283142648	0.1696540609917538	T	T	T
0.0005642368916610	0.7218878487240180	0.2864124188463381	T	T	T
0.0005488534879468	0.8673578368306786	0.2000241803039799	T	T	T
0.1681240349731405	0.3671315740636913	0.1996448022346938	T	T	T
0.1633846994575906	0.5122446554355004	0.3172582881670138	T	T	T
0.1673642889242140	0.8671056612501380	0.2688415021069042	T	T	T
0.0006262852729628	0.2230899707706863	0.1506036511788187	T	T	T
0.0003268342810802	0.0781768148722020	0.2381175893528016	T	T	T
0.1672682281291429	0.4334584447979701	0.1186963719868509	T	T	T
0.1685991664730694	0.5782739647257679	0.2369552263442671	T	T	T
0.5006934580584428	0.9350405989188815	0.0496932592300823	F	F	F
0.3340577937616961	0.5795396671307477	0.1680922221945792	T	T	T
0.3340947839824011	0.7189221860353214	0.0828425009930811	F	F	F
0.5006827171200285	0.7248539923585200	0.1507102672113180	T	T	T
0.3339047900487890	0.9350931869349397	0.1196641667654654	T	T	T
0.8340406046899460	0.9349139215369533	0.0495568998044718	F	F	F
0.6672209282454686	0.5795641650781208	0.1682559179965178	T	T	T
0.6673675098228316	0.7188948654106966	0.0828061453563009	F	F	F
0.8339518737512924	0.7242107378239605	0.1507495414615778	T	T	T
0.6672439441669086	0.9349640023484898	0.1195144374966737	T	T	T
0.1673516720937158	0.9349303605052057	0.0495816536762632	F	F	F
0.0006717289741561	0.5793093519092043	0.1684881652988283	T	T	T
0.0007264128441875	0.7186515520999706	0.0826216172703127	F	F	F
0.1673015880396185	0.7243652844475122	0.1507742860543800	T	T	T
0.0006821104262736	0.9343978018509514	0.1190682583538950	T	T	T
0.6727625732566094	0.4260732495397380	0.4746627284810425	T	T	T
0.3284058732783988	0.4317703520991060	0.4689657989965791	T	T	T
0.4962263322414483	0.4646965643113847	0.4759194370028385	T	T	T
0.3388457402214872	0.5114468953701730	0.5615448451891053	T	T	T
0.5762311313498160	0.5112923714587436	0.5785717649694879	T	T	T
0.2348773610049830	0.5828046711909642	0.5439609485750700	T	T	T
0.6950136543600467	0.5683490659590541	0.5702748231671186	T	T	T
0.2271251478932111	0.7410437449404573	0.5666398487305231	T	T	T
0.6957981998935916	0.6710927718982498	0.5770528026562645	T	T	T
0.3449110962474264	0.5176459577329491	0.5980146270189713	T	T	T
0.7575744242307212	0.5225504805941662	0.5925828145575828	T	T	T
0.5432110553651390	0.5351037000410032	0.6118945296234838	T	T	T

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0.5733911254983811  0.4075279043595536  0.5740531386320602   T   T   T
0.2352041182146408  0.5906156802382974  0.5075383061741442   T   T   T
0.1564434529366915  0.5327751420587494  0.5543537613552743   T   T   T
0.7232469370798131  0.5526122998709327  0.5357887778716492   T   T   T
0.3366946151691475  0.4114530385134612  0.5507737702695615   T   T   T
0.4723973936198612  0.5784049166515218  0.5397191172357677   T   T   T
0.4999408129571849  0.3067336782322311  0.5121899438682220   T   T   T
0.6705919813118278  0.3558387080930814  0.4964405619871360   T   T   T
0.4573583000038336  0.2425690966218889  0.4948815787072540   T   T   T
```

Figure S8. POSCAR for 2-CEES adsorption on hydroxylated PtO_2 supported on anatase-TiO_2(101)

```
Ti  O Ir  C Cl  H  S  O  H
   1.00000000000000
    11.6086997986000000    0.0000000000000000    0.0000000000000000
     0.0000000000000000   10.4970798492000004    0.0000000000000000
     0.0000000000000000    0.0000000000000000   30.0000000000000000
   Ti   O    Ir   C    Cl   H    S    O    H
    48    98     1     4     1     9     1     1     2
Selective dynamics
Direct
  0.5006996977415312  0.1226303397709572  0.0308348817084223   F   F   F
  0.5003581643667470  0.4047876038110109  0.2648832170243695   T   T   T
  0.5002811352331652  0.5508635748960971  0.3830601510633468   T   T   T
  0.3340726779424870  0.6232038428029796  0.0311184620879388   F   F   F
  0.3338524883303453  0.0538600635403834  0.3870513293876350   T   T   T
  0.3334777072983423  0.1884582924133556  0.2930900376751267   T   T   T
  0.3230133580247666  0.3298950175849468  0.4127119343956799   T   T   T
  0.5006977989396262  0.3950558257726016  0.0504933171525792   F   F   F
  0.5002302264514029  0.8228063842763419  0.4058400896558787   T   T   T
  0.8340243141044184  0.1226482355139069  0.0307980139515251   F   F   F
  0.8334242034545700  0.4058993794859730  0.2651231569126263   T   T   T
  0.8337911221929379  0.5546575532227751  0.3850034307940258   T   T   T
  0.6673735281712538  0.6231742660465827  0.0310847702734023   F   F   F
  0.6665828461227510  0.0538361719083333  0.3870573462703900   T   T   T
  0.6672592344700683  0.1884225668718261  0.2930622731933781   T   T   T
  0.6775417832835792  0.3297418010019203  0.4126658590779508   T   T   T
  0.8339804263420234  0.3950105172548319  0.0504908085087479   F   F   F
  0.8328748143667520  0.8250512924469785  0.4056792417106496   T   T   T
  0.1673963672531045  0.1226654081311054  0.0308197627108626   F   F   F
  0.1672998400941206  0.4058977601744665  0.2651329880055351   T   T   T
  0.1667350880403936  0.5546279000842648  0.3850020416612002   T   T   T
  0.0007263314815944  0.6228463858092255  0.0309515503156916   F   F   F
  0.0002580811268586  0.0519744847845356  0.3867315768799496   T   T   T
  0.0003583621336109  0.1863861667977010  0.2894163319774695   T   T   T
  0.0002433818595897  0.3251849302891883  0.4049767400155211   T   T   T
  0.1674312504078657  0.3950208983825121  0.0505129066471497   F   F   F
  0.1676383239067669  0.8249952579632225  0.4057432435477255   T   T   T
  0.5005309828802855  0.2626119079970726  0.1474532410395509   T   T   T
  0.3335616296329458  0.9093743124062323  0.2659815710225549   T   T   T
  0.3338669323698530  0.0440008867840549  0.1729010759518855   T   T   T
  0.5003370789930921  0.6878702219242683  0.2881127421627366   T   T   T
  0.8337480480092151  0.2628049928023894  0.1474746421506723   T   T   T
  0.6671433683269515  0.9093561117314211  0.2659718787528184   T   T   T
  0.6672254786693006  0.0439669835887412  0.1728768931366938   T   T   T
  0.8332286855942032  0.6868781080316102  0.2885677903637148   T   T   T
  0.1673070284137954  0.2628217822020094  0.1474928450345804   T   T   T
  0.0003424340247919  0.9067786395027876  0.2657348403181873   T   T   T
  0.0005382395831970  0.0429661653889164  0.1716330142136595   T   T   T
  0.1674478824503993  0.6868980079702329  0.2885866743433724   T   T   T
  0.3338409495712907  0.7647608294528159  0.1478352201701554   T   T   T
  0.3340496263033970  0.8954046178637896  0.0510558284607043   F   F   F
  0.5005234489138324  0.5435015536251177  0.1710601543193160   T   T   T
  0.6671792845701396  0.7647472194393797  0.1478117687781253   T   T   T
  0.6673697039057487  0.8953863539000935  0.0510144758035480   F   F   F
  0.8335315031173783  0.5432234079940697  0.1710876282744741   T   T   T
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0.0005089110062160	0.7633376719340129	0.1476925726408859	T	T	T
0.0007108818663752	0.8951314846780249	0.0506837988146742	F	F	F
0.1675075504983208	0.5432513225722145	0.1711038269949753	T	T	T
0.5003777938028686	0.2262327128990057	0.2888753475208066	T	T	T
0.5003395373472767	0.3699753452545479	0.4127247816030662	T	T	T
0.3340608422739209	0.4347500569770943	0.0492537621692151	F	F	F
0.3340363351718994	0.8711316682056488	0.4128074368442921	T	T	T
0.3345553700957786	0.0135816932465705	0.3195970466069888	T	T	T
0.3341085385325883	0.1620436274864192	0.4377451829115044	T	T	T
0.5007293049093207	0.2184841558815336	0.0825058595281405	F	F	F
0.5001515666685349	0.6630190888102349	0.4340140207206930	T	T	T
0.5007079090333875	0.5747900337452734	0.0243574470876453	F	F	F
0.5002279804345854	0.0120931101051900	0.3896743242217914	T	T	T
0.3340489994025546	0.0743763215772404	0.0241986002383783	F	F	F
0.3338158212186674	0.3688897682444834	0.2692107144044512	T	T	T
0.3335522573483383	0.5093072016900715	0.3851801376795341	T	T	T
0.3341879658059526	0.7800918013219302	0.0021772415827357	F	F	F
0.3302322552628000	0.2287620804663294	0.3577784928371152	T	T	T
0.5007091085999136	0.2795535314299684	0.0017775871505918	F	F	F
0.5003216393406806	0.7294467298660701	0.3540087507830188	T	T	T
0.8337682357345514	0.2252772699473291	0.2872442328661032	T	T	T
0.8386923501440393	0.3749517963401018	0.4115988522604455	T	T	T
0.6673456418459622	0.4347311450016207	0.0492304192247275	F	F	F
0.6664518006951388	0.8711509677170973	0.4128298325603049	T	T	T
0.6659585805636036	0.0135653653790810	0.3195895779728015	T	T	T
0.6662965397114737	0.1620587698097918	0.4377337950997786	T	T	T
0.8340225507848231	0.2184562882131900	0.0824675952741032	F	F	F
0.8323575143590914	0.6677907530518294	0.4342761443135809	T	T	T
0.8340017310513801	0.5746942132115365	0.0242903919570736	F	F	F
0.8334743325828228	0.0132270800093650	0.3887510755376486	T	T	T
0.6673462887887567	0.0743685216712393	0.0241764804384488	F	F	F
0.6669355200916403	0.3688930388297705	0.2692028442975158	T	T	T
0.6669845724134720	0.5093636575749031	0.3851938077582476	T	T	T
0.6674038655757499	0.7800676015289767	0.0021396817594521	F	F	F
0.6703523652708669	0.2287481999520032	0.3577658136085352	T	T	T
0.8339983198822054	0.2795543115580585	0.0017489980147616	F	F	F
0.8330251268625335	0.7309446911958359	0.3540282307429238	T	T	T
0.1669581018505180	0.2252574016994204	0.2872379809536167	T	T	T
0.1618125218885116	0.3750103232575963	0.4116814549439278	T	T	T
0.0007073033921188	0.4346424832735067	0.0491818976677934	F	F	F
0.0002500577535947	0.8727261329380999	0.4125411544134539	T	T	T
0.0002944241097109	0.0140127368942324	0.3186342376116890	T	T	T
0.0002920499230484	0.1696669699205165	0.4348384768507905	T	T	T
0.1674625023756704	0.2184840320475629	0.0824889304489673	F	F	F
0.1682758400534194	0.6676690177297147	0.4343392309469900	T	T	T
0.1674389389043753	0.5747081516329970	0.0243156673899705	F	F	F
0.1670080527888543	0.0131665077577450	0.3887604241733502	T	T	T
0.0007041830368095	0.0743033877040133	0.0240616126602333	F	F	F
0.0003864314497834	0.3683515221868748	0.2680080552620502	T	T	T
0.0002786684238577	0.5162886699849786	0.3864620820255493	T	T	T
0.0007941924944674	0.7797634528032376	0.0019151049756942	F	F	F
0.0003489960273348	0.2286543542873067	0.3543034090885719	T	T	T
0.1674887040323156	0.2795668261471747	0.0017706688979260	F	F	F
0.1675177515005477	0.7309220242202135	0.3540775062475510	T	T	T
0.5005536951710784	0.0808621700031162	0.1693593978617089	T	T	T

0.3337801480479649	0.7250839414911082	0.2861034858429917	T	T	T
0.3336639476699293	0.8697355489523034	0.2002665398149114	T	T	T
0.5004880788190716	0.3685842108107208	0.1997059281670731	T	T	T
0.5002870043174067	0.5155737194162581	0.3172574117080233	T	T	T
0.5003582297908238	0.8704913316636947	0.2686154934598812	T	T	T
0.3339300724938700	0.2248248461667288	0.1506698582584007	T	T	T
0.3341405476658859	0.0823320789591513	0.2388187471308918	T	T	T
0.5005901968163835	0.4343933495192500	0.1186079740815692	T	T	T
0.5004298175328679	0.5804777738283683	0.2367443964303602	T	T	T
0.8338430869042202	0.0806657573365619	0.1690743620712035	T	T	T
0.6668946995512983	0.7250566372420890	0.2860800039159894	T	T	T
0.6672489554925407	0.8697264908889903	0.2002501993802547	T	T	T
0.8332626832328235	0.3689270784505539	0.1995607089682119	T	T	T
0.8348854025840178	0.5157254363963956	0.3174953018554373	T	T	T
0.8335871700402522	0.8704494623277590	0.2686809547897976	T	T	T
0.6671625842435058	0.2248197974468794	0.1506576270769284	T	T	T
0.6669297430796917	0.0823091171018760	0.2388035329417866	T	T	T
0.8339423504265022	0.4344749605934348	0.1185320009589858	T	T	T
0.8333063747456518	0.5807070355816683	0.2367839693926075	T	T	T
0.1672465070753770	0.0806927389968194	0.1691069416027334	T	T	T
0.0003399522955777	0.7249057121650136	0.2860249989140098	T	T	T
0.0004695082281977	0.8690561448931069	0.1998465544743957	T	T	T
0.1677470667899960	0.3689514362860970	0.1995779484698471	T	T	T
0.1658131773747698	0.5157321792547817	0.3175132745201454	T	T	T
0.1671183974809943	0.8704407754476720	0.2686821899387611	T	T	T
0.0005450115844465	0.2247302008185960	0.1504940415960580	T	T	T
0.0003880529595182	0.0807817130068788	0.2374909564023457	T	T	T
0.1672518732848731	0.4345015031593346	0.1185521917976696	T	T	T
0.1675034870699806	0.5807288561776911	0.2368029430972668	T	T	T
0.5006934580584428	0.9350405989188815	0.0496932592300823	F	F	F
0.3339409614777689	0.5805201150713974	0.1682076456092181	T	T	T
0.3340947839824011	0.7189221860353214	0.0828425009930811	F	F	F
0.5005267837554106	0.7258542071125117	0.1508528002450075	T	T	T
0.3339579592231449	0.9356001488730472	0.1193273523495293	T	T	T
0.8340406046899460	0.9349139215369533	0.0495568998044718	F	F	F
0.6670984980554128	0.5805051153747043	0.1681880659986173	T	T	T
0.6673675098228316	0.7188948654106966	0.0828061453563009	F	F	F
0.8337850549988775	0.7255424583772837	0.1506810509466354	T	T	T
0.6671662101473471	0.9355734280453748	0.1193050138730940	T	T	T
0.1673516720937158	0.9349303605052057	0.0495816536762632	F	F	F
0.0005130889128959	0.5803159749779641	0.1682680192274879	T	T	T
0.0007264128441875	0.7186515520999706	0.0826216172703127	F	F	F
0.1672604917808000	0.7255409580993247	0.1506920982654516	T	T	T
0.0005962430946182	0.9350542387293815	0.1188532198933620	T	T	T
0.6604210922110408	0.4085134712330517	0.4738080152030240	T	T	T
0.3400550851662841	0.4083884963931549	0.4737894722746245	T	T	T
0.5004672332769473	0.4218086227461068	0.4810517043287648	T	T	T
0.3729809469922112	0.4034822106959096	0.5767734185099416	T	T	T
0.6170310865428122	0.4034120925461269	0.5803466846775214	T	T	T
0.2632612983084768	0.4788617530909336	0.5691528553150671	T	T	T
0.7276792829816261	0.4790273519472886	0.5738754422525518	T	T	T
0.2602237772273183	0.6212481477720340	0.6022125166658192	T	T	T
0.7217760354730399	0.5732973450900880	0.5895863383334538	T	T	T
0.3893219521538438	0.3894203757457976	0.6125042610232982	T	T	T
0.7993875257845189	0.4270050464210499	0.5893765327396014	T	T	T

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0.5937821783653346  0.3943598460034859  0.6157508154943716   T   T   T
0.6209165443888789  0.3084673956674731  0.5651025370068292   T   T   T
0.2531551326735238  0.5063255995420278  0.5341290897062313   T   T   T
0.1889732653180101  0.4211278190712391  0.5791792938432955   T   T   T
0.7474299955444086  0.4908023138730551  0.5383542348056541   T   T   T
0.3680191899047210  0.3110425543445199  0.5597502783286034   T   T   T
0.4973637798900049  0.4896153180195542  0.5546406817679437   T   T   T
0.4999152834215898  0.1991590913997068  0.4976641551747364   T   T   T
0.5683218164349771  0.1744133788436197  0.4787283292409952   T   T   T
0.4321110990035610  0.1743640023160910  0.4783816575464689   T   T   T
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Figure S9. POSCAR for 2-CEES adsorption on hydroxylated IrO_2 supported on anatase-TiO_2(101)

```
Ti  O Pd  C Cl  H  S  O  H
   1.00000000000000
    11.6086997986000000    0.0000000000000000    0.0000000000000000
     0.0000000000000000   10.4970798492000004    0.0000000000000000
     0.0000000000000000    0.0000000000000000   30.0000000000000000
   Ti   O    Pd   C    Cl   H    S    O    H
    48    98     1     4     1     9     1     1     2
Selective dynamics
Direct
  0.5006996977415312  0.1226303397709572  0.0308348817084223   F   F   F
  0.5002744497744891  0.4043609114282954  0.2649205335125916   T   T   T
  0.5001213704335491  0.5514993850712464  0.3829463736638333   T   T   T
  0.3340726779424870  0.6232038428029796  0.0311184620879388   F   F   F
  0.3340600223057611  0.0546356761089481  0.3872056948363213   T   T   T
  0.3332251473018198  0.1885704603864147  0.2936353582641245   T   T   T
  0.3228914589898849  0.3319177751185679  0.4135694767751991   T   T   T
  0.5006977989396262  0.3950558257726016  0.0504933171525792   F   F   F
  0.5001863012898822  0.8226086815458272  0.4061498794461299   T   T   T
  0.8340243141044184  0.1226482355139069  0.0307980139515251   F   F   F
  0.8333095175152825  0.4059520579706817  0.2652703747485149   T   T   T
  0.8343443869784332  0.5554689085264122  0.3851545441890677   T   T   T
  0.6673735281712538  0.6231742660465827  0.0310847702734023   F   F   F
  0.6663562985228239  0.0546531774906036  0.3871938076778824   T   T   T
  0.6672757088917813  0.1884765699230633  0.2935812222773010   T   T   T
  0.6775004781339308  0.3319861179299698  0.4134098437770816   T   T   T
  0.8339804263420234  0.3950105172548319  0.0504908085087479   F   F   F
  0.8326015955641878  0.8255680531626375  0.4059486708693738   T   T   T
  0.1673963672531045  0.1226654081311054  0.0308197627108626   F   F   F
  0.1672244175917018  0.4060060299091397  0.2652692077165102   T   T   T
  0.1661489503254984  0.5554589629459541  0.3851544521196124   T   T   T
  0.0007263314815944  0.6228463858092255  0.0309515503156916   F   F   F
  0.0002440310383545  0.0522578147452503  0.3869764453454902   T   T   T
  0.0002780517504073  0.1864094317852514  0.2896385522350778   T   T   T
  0.0002169670563841  0.3255056320334518  0.4051821356270520   T   T   T
  0.1674312504078657  0.3950208983825121  0.0505129066471497   F   F   F
  0.1677935628203883  0.8255420270076095  0.4059998527461778   T   T   T
  0.5005094921845428  0.2625678487802749  0.1474871255806190   T   T   T
  0.3335044775761226  0.9095480830107352  0.2661059499121168   T   T   T
  0.3338287010346070  0.0439895425502653  0.1731591783896864   T   T   T
  0.5002866004821676  0.6879938063728513  0.2880903147921570   T   T   T
  0.8337007680236773  0.2628007887361832  0.1475427117022172   T   T   T
  0.6670742501337922  0.9094879714537883  0.2660842707060634   T   T   T
  0.6672220181945298  0.0439947881772688  0.1731214711135184   T   T   T
  0.8331241663456754  0.6870204518376961  0.2887424036749672   T   T   T
  0.1673407989629615  0.2627955767045541  0.1475628771927310   T   T   T
  0.0003107964565353  0.9068704383380122  0.2659229202984777   T   T   T
  0.0005194105906652  0.0429380803841745  0.1717572472205834   T   T   T
  0.1674440205110809  0.6870318451591197  0.2887566109793088   T   T   T
  0.3338045591082568  0.7648957975221822  0.1478620999384486   T   T   T
  0.3340496263033970  0.8954046178637896  0.0510558284607043   F   F   F
  0.5005449043131170  0.5436850304803450  0.1711363516093670   T   T   T
  0.6672338606859317  0.7649071780112300  0.1478318622991228   T   T   T
  0.6673697039057487  0.8953863539000935  0.0510144758035480   F   F   F
  0.8335149502972160  0.5432547787901840  0.1712098436414349   T   T   T
  0.0005147536019892  0.7633448000040348  0.1477537716576566   T   T   T
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0.0007108818663752	0.8951314846780249	0.0506837988146742	F	F	F
0.1675390809036626	0.5432702511868192	0.1712152292807569	T	T	T
0.5002629602142309	0.2261686062612087	0.2890930218585745	T	T	T
0.5001574128359213	0.3692121480563762	0.4120721807862870	T	T	T
0.3340608422739209	0.4347500569770943	0.0492537621692151	F	F	F
0.3342908519837656	0.8711701949879391	0.4131664106912438	T	T	T
0.3345027893844445	0.0130557791490407	0.3198336119511858	T	T	T
0.3356430417789537	0.1624991997541935	0.4382667820759486	T	T	T
0.5007293049093207	0.2184841558815336	0.0825058595281405	F	F	F
0.5001158557640044	0.6616699436680216	0.4341065037529032	T	T	T
0.5007079090333875	0.5747900337452734	0.0243574470876453	F	F	F
0.5002150375380139	0.0117953661144017	0.3898116324411796	T	T	T
0.3340489994025546	0.0743763215772404	0.0241986002383783	F	F	F
0.3337225933768983	0.3689792803402898	0.2695090067170972	T	T	T
0.3333097042039292	0.5101031845963002	0.3858492381336443	T	T	T
0.3341879658059526	0.7800918013219302	0.0021772415827357	F	F	F
0.3296511122823998	0.2279800310913897	0.3580214697258293	T	T	T
0.5007091085999136	0.2795535314299684	0.0017775871505918	F	F	F
0.5002848062195917	0.7296113596209416	0.3542237129576017	T	T	T
0.8338044403241356	0.2252097419538727	0.2872866347829216	T	T	T
0.8390547119352757	0.3758950694395752	0.4117044871548736	T	T	T
0.6673456418459622	0.4347311450016207	0.0492304192247275	F	F	F
0.6661414131616751	0.8712511197605367	0.4131980178770338	T	T	T
0.6657952428821621	0.0129965658048853	0.3198239107777626	T	T	T
0.6646334622544897	0.1627336135235599	0.4382201338620932	T	T	T
0.8340225507848231	0.2184562882131900	0.0824675952741032	F	F	F
0.8329049481661522	0.6682749883426593	0.4345360059046124	T	T	T
0.8340017310513801	0.5746942132115365	0.0242903919570736	F	F	F
0.8332515651409312	0.0138176204431118	0.3891545705109802	T	T	T
0.6673462887887567	0.0743685216712393	0.0241764804384488	F	F	F
0.6668502870508151	0.3688867143890028	0.2694871865690156	T	T	T
0.6670517813421420	0.5101279968960195	0.3859045135372403	T	T	T
0.6674038655757499	0.7800676015289767	0.0021396817594521	F	F	F
0.6708470894441320	0.2279800472282538	0.3579592587267979	T	T	T
0.8339983198822054	0.2795543115580585	0.0017489980147616	F	F	F
0.8329297339858418	0.7315314905571271	0.3542630702399123	T	T	T
0.1667814959853498	0.2252731839716323	0.2872717144033389	T	T	T
0.1613112491014647	0.3760001905116236	0.4118266698268353	T	T	T
0.0007073033921188	0.4346424832735067	0.0491818976677934	F	F	F
0.0001826058743477	0.8732479614202282	0.4127311388049712	T	T	T
0.0004112479391404	0.0140881767659361	0.3189005645833354	T	T	T
0.0002257755039120	0.1701639237268503	0.4350964282100769	T	T	T
0.1674625023756704	0.2184840320475629	0.0824889304489673	F	F	F
0.1675640700684667	0.6681935634205979	0.4345936223620320	T	T	T
0.1674389389043753	0.5747081516329970	0.0243156673899705	F	F	F
0.1671680035236083	0.0137423902402861	0.3892095798078673	T	T	T
0.0007041830368095	0.0743033877040133	0.0240616126602333	F	F	F
0.0002889138510552	0.3687879658585574	0.2684071286743402	T	T	T
0.0002234252491092	0.5171887511116827	0.3864707604786542	T	T	T
0.0007941924944674	0.7797634528032376	0.0019151049756942	F	F	F
0.0003929772826177	0.2287811999457799	0.3545268081768479	T	T	T
0.1674887040323156	0.2795668261471747	0.0017706688979260	F	F	F
0.1675352813630148	0.7315362218991456	0.3543031916099837	T	T	T
0.5005294048014751	0.0808851698084267	0.1695037250535418	T	T	T
0.3337562985401558	0.7250907829445141	0.2863440522929715	T	T	T

0.3336605437353579	0.8695379457148344	0.2003744411231129	T	T	T
0.5004467908920783	0.3685327653617176	0.1998097595815440	T	T	T
0.5002513803775795	0.5155607670755107	0.3174335455867087	T	T	T
0.5003015127073440	0.8702534613396147	0.2685730469188313	T	T	T
0.3339192902297444	0.2248245617014532	0.1508055340032774	T	T	T
0.3339587665720315	0.0821317334031065	0.2390619641327916	T	T	T
0.5006094161887680	0.4343575276813220	0.1186894953775403	T	T	T
0.5003979724898344	0.5803602725096870	0.2368660366914275	T	T	T
0.8338353269205300	0.0807226050458174	0.1692135068549664	T	T	T
0.6668365569231360	0.7250480131218553	0.2862818195054947	T	T	T
0.6672838780897631	0.8695505861732256	0.2003472665669054	T	T	T
0.8332489786130342	0.3689311754572966	0.1997262862493866	T	T	T
0.8343758697085566	0.5160020474014835	0.3177529831818036	T	T	T
0.8335246602844660	0.8705618478282753	0.2687992810718597	T	T	T
0.6671450221898630	0.2248402878914093	0.1507898149264781	T	T	T
0.6668787096829725	0.0820999530110476	0.2390374656327045	T	T	T
0.8338416811979953	0.4344029844001386	0.1186262184663467	T	T	T
0.8333056366212589	0.5807578488907091	0.2369634765981035	T	T	T
0.1672013811406569	0.0807293296601244	0.1692375049801122	T	T	T
0.0002919929075313	0.7251257347793171	0.2862914227490407	T	T	T
0.0005104003240750	0.8690425018546417	0.1999598404311455	T	T	T
0.1676955282172982	0.3689565219559087	0.1997337218679691	T	T	T
0.1659717069337971	0.5160329912578663	0.3177561599841627	T	T	T
0.1671039828663345	0.8704988331618803	0.2687742163640844	T	T	T
0.0005337043487856	0.2247149728048508	0.1505490937669327	T	T	T
0.0003435856728530	0.0807720108059808	0.2376639324617957	T	T	T
0.1673512804311476	0.4344005922660998	0.1186397859821821	T	T	T
0.1674816939653811	0.5808207481409884	0.2369683787059859	T	T	T
0.5006934580584428	0.9350405989188815	0.0496932592300823	F	F	F
0.3339657086475398	0.5805736552596759	0.1683416917598862	T	T	T
0.3340947839824011	0.7189221860353214	0.0828425009930811	F	F	F
0.5005380750762823	0.7257866645406661	0.1508250941341109	T	T	T
0.3339000812462777	0.9356036494196486	0.1194096160793797	T	T	T
0.8340406046899460	0.9349139215369533	0.0495568998044718	F	F	F
0.6670920813631054	0.5805835500200650	0.1683301287231676	T	T	T
0.6673675098228316	0.7188948654106966	0.0828061453563009	F	F	F
0.8338274931006158	0.7254965140341286	0.1507261573161558	T	T	T
0.6672115749325658	0.9356054136050064	0.1193814025462321	T	T	T
0.1673516720937158	0.9349303605052057	0.0495816536762632	F	F	F
0.0005147734907537	0.5803071066285370	0.1683734262574720	T	T	T
0.0007264128441875	0.7186515520999706	0.0826216172703127	F	F	F
0.1672363930595009	0.7254865694126864	0.1507258647903985	T	T	T
0.0005513197500285	0.9350458809921350	0.1189350958625082	T	T	T
0.6648910708803004	0.4048865289419338	0.4745292654278095	T	T	T
0.3351702260648517	0.4047406379851211	0.4745833532274635	T	T	T
0.5001890922232167	0.4127080926733582	0.4797999793857969	T	T	T
0.3734251520550698	0.4044127159589389	0.5756022681668320	T	T	T
0.6166594704834926	0.4045756793169757	0.5791475431639952	T	T	T
0.2636137492228487	0.4804684868793467	0.5688920396918105	T	T	T
0.7274461254437613	0.4807672721168746	0.5737184530271430	T	T	T
0.2622378566525075	0.6215552561536332	0.6026540857434219	T	T	T
0.7212069779895716	0.5741649380041051	0.5899880535969783	T	T	T
0.3916306683275765	0.3904478942538510	0.6112037788776395	T	T	T
0.7984374547857809	0.4277466878676043	0.5892784580998329	T	T	T
0.5914560016239881	0.3949795469601468	0.6143157177914101	T	T	T

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0.6227913550032750  0.3095018922144215  0.5641322988325040   T   T   T
0.2525713187265981  0.5088172398842314  0.5340299636922979   T   T   T
0.1897153254166901  0.4224337342027808  0.5791101990413100   T   T   T
0.7480292884857526  0.4938043340138554  0.5383462314170708   T   T   T
0.3662466122673342  0.3115993701925755  0.5589174095370266   T   T   T
0.4973781585188747  0.4872705645083245  0.5523414501361086   T   T   T
0.5002013028190397  0.2020820072986938  0.4957260324426376   T   T   T
0.5694726840087686  0.1774593539745186  0.4762580416207154   T   T   T
0.4311742606088449  0.1769185535130227  0.4762045438716274   T   T   T
```

Figure S10. POSCAR for 2-CEES adsorption on hydroxylated PdO_2 supported on anatase-TiO_2(101)

```
Ti  O Pd  C Cl  H  S  O  H
   1.00000000000000
    11.6086997986000000    0.0000000000000000    0.0000000000000000
     0.0000000000000000   10.4970798492000004    0.0000000000000000
     0.0000000000000000    0.0000000000000000   30.0000000000000000
   Ti   O    Pd   C    Cl   H    S    O    H
    48    98     1     4     2     8     1     1     2
Selective dynamics
Direct
  0.5006996977415312  0.1226303397709572  0.0308348817084223   F   F   F
  0.5004484004407784  0.4000573113919596  0.2637740243517147   T   T   T
  0.4983482799041515  0.5407418396895899  0.3800664038717055   T   T   T
  0.3340726779424870  0.6232038428029796  0.0311184620879388   F   F   F
  0.3351367907532092  0.0519066635727035  0.3893572690688465   T   T   T
  0.3339913660415443  0.1854561791359565  0.2953432561406470   T   T   T
  0.3236727584993503  0.3281933176787512  0.4170080921643282   T   T   T
  0.5006977989396262  0.3950558257726016  0.0504933171525792   F   F   F
  0.5001088273210863  0.8143441617462943  0.4081438611107455   T   T   T
  0.8340243141044184  0.1226482355139069  0.0307980139515251   F   F   F
  0.8336764025779709  0.4021693661589292  0.2651050334097131   T   T   T
  0.8336106000308793  0.5479795307703981  0.3848862895497689   T   T   T
  0.6673735281712538  0.6231742660465827  0.0310847702734023   F   F   F
  0.6674768628982505  0.0484563649532791  0.3888433603979495   T   T   T
  0.6673530214346519  0.1846927988269807  0.2933747135189109   T   T   T
  0.6764567514440397  0.3236277104967524  0.4122898338367038   T   T   T
  0.8339804263420234  0.3950105172548319  0.0504908085087479   F   F   F
  0.8334193311370567  0.8180254457244365  0.4065586863238011   T   T   T
  0.1673963672531045  0.1226654081311054  0.0308197627108626   F   F   F
  0.1679259826730714  0.4021745420544243  0.2650652348904594   T   T   T
  0.1674175946022180  0.5476297106369461  0.3843870880374991   T   T   T
  0.0007263314815944  0.6228463858092255  0.0309515503156916   F   F   F
  0.0014798910677117  0.0455757214688319  0.3874848996638688   T   T   T
  0.0009430659969322  0.1832292337982425  0.2901215926048267   T   T   T
  0.0002828211606663  0.3195040027286565  0.4055021147613627   T   T   T
  0.1674312504078657  0.3950208983825121  0.0505129066471497   F   F   F
  0.1693571402750097  0.8182484100093912  0.4064650769775128   T   T   T
  0.5005541044055084  0.2606236636652161  0.1472410512377626   T   T   T
  0.3337079823187943  0.9078974774181615  0.2668097819419833   T   T   T
  0.3339413770471974  0.0425982117918646  0.1739061044040234   T   T   T
  0.5006367024098979  0.6858737858811990  0.2877671636429411   T   T   T
  0.8339151294162198  0.2613582046741764  0.1474944684634359   T   T   T
  0.6679832880753366  0.9065751408984516  0.2666247971092605   T   T   T
  0.6673994460220736  0.0423490333152744  0.1732079753281026   T   T   T
  0.8337580874842220  0.6835561509236578  0.2889006785687632   T   T   T
  0.1675453040037587  0.2613010442838607  0.1475226432524278   T   T   T
  0.0008461078933618  0.9037486024688842  0.2661020720200019   T   T   T
  0.0006978544095079  0.0415573131813469  0.1720248077609761   T   T   T
  0.1679766847815058  0.6839042546025683  0.2887519220157880   T   T   T
  0.3338262522134093  0.7645809473751568  0.1479261102870795   T   T   T
  0.3340496263033970  0.8954046178637896  0.0510558284607043   F   F   F
  0.5004886395348399  0.5432216864242214  0.1707670506583404   T   T   T
  0.6675708244325489  0.7637844588194477  0.1479445398339353   T   T   T
  0.6673697039057487  0.8953863539000935  0.0510144758035480   F   F   F
  0.8337861151287520  0.5420184914342198  0.1712525207189572   T   T   T
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0.1679245011175100	0.5421821340963212	0.1712254574193110	T	T	T
0.5007988288682836	0.2232163523406354	0.2887328601223626	T	T	T
0.5010508510500442	0.3672526534532581	0.4153908752474882	T	T	T
0.3340608422739209	0.4347500569770943	0.0492537621692151	F	F	F
0.3358911635890093	0.8623901728048250	0.4150976114347881	T	T	T
0.3349455379951481	0.0089723577889620	0.3205566470474504	T	T	T
0.3361428775652189	0.1589605381796844	0.4393884348668045	T	T	T
0.5007293049093207	0.2184841558815336	0.0825058595281405	F	F	F
0.4986062348950416	0.6406649725319469	0.4360794159645541	T	T	T
0.5007079090333875	0.5747900337452734	0.0243574470876453	F	F	F
0.5012386350755733	0.9993194166049243	0.3911254130256900	T	T	T
0.3340489994025546	0.0743763215772404	0.0241986002383783	F	F	F
0.3343276918835971	0.3660363554628063	0.2698602822462537	T	T	T
0.3342900274528680	0.5020380745604858	0.3814342199331244	T	T	T
0.3341879658059526	0.7800918013219302	0.0021772415827357	F	F	F
0.3349181006231665	0.2224332828476119	0.3591067743767961	T	T	T
0.5007091085999136	0.2795535314299684	0.0017775871505918	F	F	F
0.5003590215829667	0.7230740622961692	0.3559624947258356	T	T	T
0.8338721122235748	0.2225363220117369	0.2884458973242512	T	T	T
0.8382561106828120	0.3683554030127004	0.4110885581384634	T	T	T
0.6673456418459622	0.4347311450016207	0.0492304192247275	F	F	F
0.6662320363948941	0.8627812830584117	0.4148250978700557	T	T	T
0.6668262074787261	0.0100987933619109	0.3202959771041904	T	T	T
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0.8340225507848231	0.2184562882131900	0.0824675952741032	F	F	F
0.8329508936780118	0.6601479553206093	0.4345997556496325	T	T	T
0.8340017310513801	0.5746942132115365	0.0242903919570736	F	F	F
0.8333097117682141	0.0064809416750374	0.3896620976367322	T	T	T
0.6673462887887567	0.0743685216712393	0.0241764804384488	F	F	F
0.6672816339732602	0.3645845533880828	0.2688281640477759	T	T	T
0.6666000428929073	0.5022493404447891	0.3846100407167685	T	T	T
0.6674038655757499	0.7800676015289767	0.0021396817594521	F	F	F
0.6658649972834577	0.2241340376862207	0.3583354907810847	T	T	T
0.8339983198822054	0.2795543115580585	0.0017489980147616	F	F	F
0.8326273673443431	0.7257487202558667	0.3545241793339152	T	T	T
0.1675874718771513	0.2227289390725009	0.2882873120860444	T	T	T
0.1612915576506670	0.3696729899239860	0.4118835668027884	T	T	T
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0.0011997370310615	0.8660467410592743	0.4127650564638023	T	T	T
0.0013025058528018	0.0094667268679959	0.3192081857206340	T	T	T
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0.1674625023756704	0.2184840320475629	0.0824889304489673	F	F	F
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0.0007041830368095	0.0743033877040133	0.0240616126602333	F	F	F
0.0005797071186311	0.3638437397684101	0.2678396765031285	T	T	T
0.0002594288241564	0.5101329014821386	0.3863078115767015	T	T	T
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0.1674887040323156	0.2795668261471747	0.0017706688979260	F	F	F
0.1690046549604430	0.7262676259207089	0.3544018850229185	T	T	T
0.5007423526642993	0.0798769996799178	0.1699182012586600	T	T	T

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0.8340277617351843	0.8671399436962500	0.2689383709139457	T	T	T
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0.8332672133575657	0.5781113121226801	0.2370295859514994	T	T	T
0.1673326480000594	0.0796009183619204	0.1696200400167222	T	T	T
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0.1682326122301323	0.3671233314409106	0.1996095948773578	T	T	T
0.1633157240210197	0.5121840476668860	0.3171979976845622	T	T	T
0.1675115692875393	0.8671037831878680	0.2688013348152465	T	T	T
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0.1687772363000242	0.5782855459487732	0.2369027313201508	T	T	T
0.5006934580584428	0.9350405989188815	0.0496932592300823	F	F	F
0.3341474319983209	0.5795247387037092	0.1680516537183319	T	T	T
0.3340947839824011	0.7189221860353214	0.0828425009930811	F	F	F
0.5007659527694354	0.7248707414436607	0.1507025164325257	T	T	T
0.3339618896374642	0.9350918381027481	0.1196478248960078	T	T	T
0.8340406046899460	0.9349139215369533	0.0495568998044718	F	F	F
0.6673041716677534	0.5795605418284689	0.1682331472286453	T	T	T
0.6673675098228316	0.7188948654106966	0.0828061453563009	F	F	F
0.8340208194927113	0.7242089720644025	0.1507399595456493	T	T	T
0.6673090550593676	0.9349686496896802	0.1195143097010390	T	T	T
0.1673516720937158	0.9349303605052057	0.0495816536762632	F	F	F
0.0007510041917978	0.5792902513470827	0.1684738353640240	T	T	T
0.0007264128441875	0.7186515520999706	0.0826216172703127	F	F	F
0.1673770830299565	0.7243608813973401	0.1507582857150998	T	T	T
0.0007309515510166	0.9343746790459201	0.1190514809249349	T	T	T
0.6722328926410412	0.4236286697626849	0.4749157503605468	T	T	T
0.3295560597551900	0.4307104883554338	0.4693203906934168	T	T	T
0.4955739518506870	0.4633373903445170	0.4755202867107684	T	T	T
0.3384492879450996	0.5173273356244037	0.5611196635604381	T	T	T
0.5749724523929516	0.5183624468605657	0.5770892666621431	T	T	T
0.2338752082909110	0.5866299897212919	0.5430620571025503	T	T	T
0.6947327449723746	0.5694239402300658	0.5674379979682874	T	T	T
0.2268557115431233	0.7471426935010794	0.5636061530027382	T	T	T
0.7027651513918445	0.7374892694514907	0.5770805828760617	T	T	T
0.3448765933175591	0.5262296006522655	0.5975264016326292	T	T	T
0.7566535539833853	0.5238498358827999	0.5899636774056062	T	T	T

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0.2332039812713971  0.5903892260557767  0.5065715886765578   T   T   T
0.1559200600217867  0.5376876955596910  0.5545326846823758   T   T   T
0.7206166318591827  0.5516511228505662  0.5328062922992900   T   T   T
0.3369419412424190  0.4165452016828071  0.5512055693642890   T   T   T
0.4704413202851874  0.5843838559974768  0.5384388695417603   T   T   T
0.4989524424052388  0.3097880624839147  0.5130845985183506   T   T   T
0.6656722238191438  0.3523471142293813  0.4961667650551125   T   T   T
0.4556959048072504  0.2455267296937051  0.4960486954102530   T   T   T
```

Figure S11. POSCAR for sulfur mustard adsorption on hydroxylated PdO_2 supported on anatase-TiO_2(101)