Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary information

A DFT study of the adsorption energy and the electronic interactions of SO_2 molecule on CoP hydrotreating catalyst

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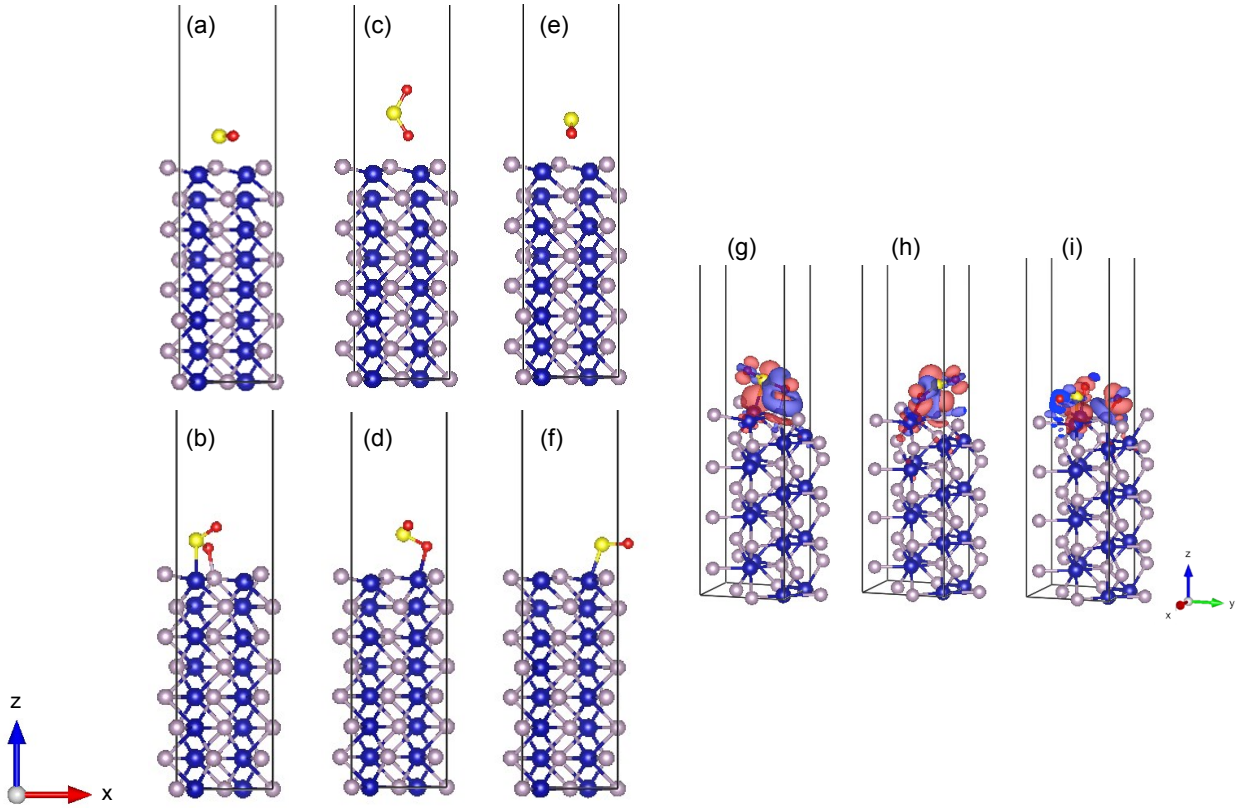

Figure S1. Initial and relaxed structures for SO_2 adsorbed on (100) surface with (a,b) parallel molecular configuration, (c,d) perpendicular molecular configuration, (e,f) and perpendicular molecule with two oxygen atoms facing the surface. Charge density difference for relaxed structures starting with SO_2 (g) parallel, (h), perpendicular, and (h) perpendicular with two oxygen facing the surface.

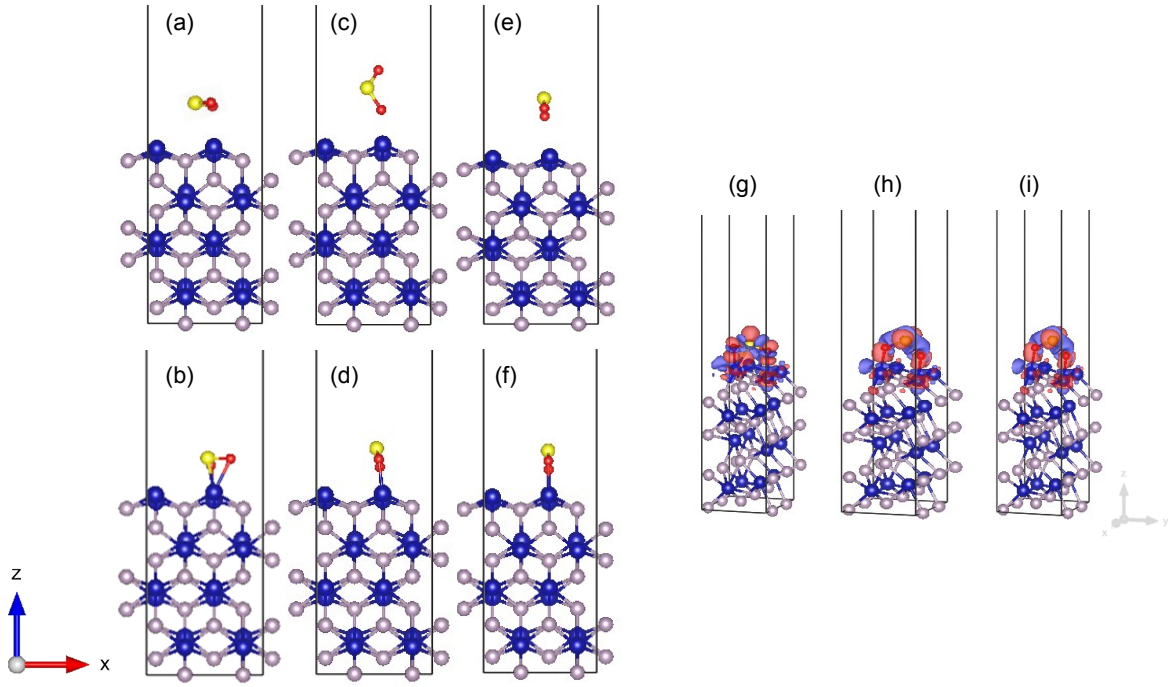

Figure S2. Initial and relaxed structures for SO_2 adsorbed on (001)-Co (cobalt terminated) surface with (a,b) parallel molecular configuration, (c,d) perpendicular molecular configuration, (e,f) and perpendicular molecule with two oxygen atoms facing the surface. Charge density difference for relaxed structures starting with SO_2 (g) parallel, (h), perpendicular, and (h) perpendicular with two oxygen facing the surface.

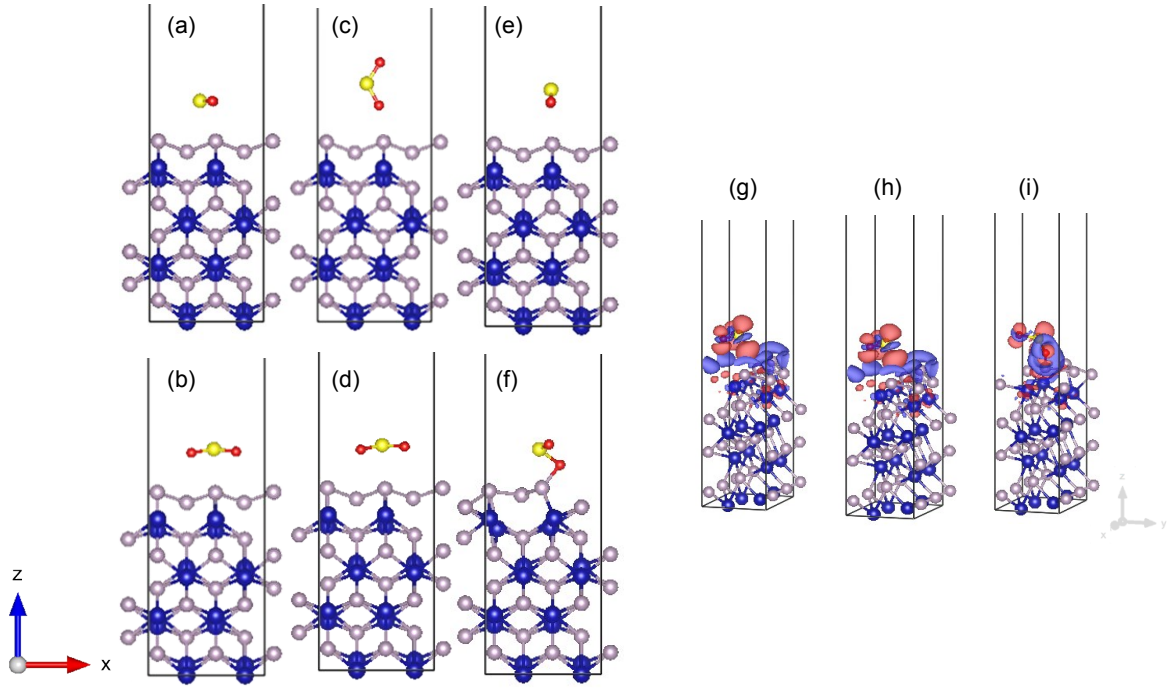

Figure S3. Initial and relaxed structures for SO_2 adsorbed on (001)-P (phosphorous terminated) surface with (a,b) parallel molecular configuration, (c,d) perpendicular molecular configuration, (e,f) and perpendicular molecule with two oxygen atoms facing the surface. Charge density difference for relaxed structures starting with SO_2 (g) parallel, (h), perpendicular, and (h) perpendicular with two oxygen facing the surface.

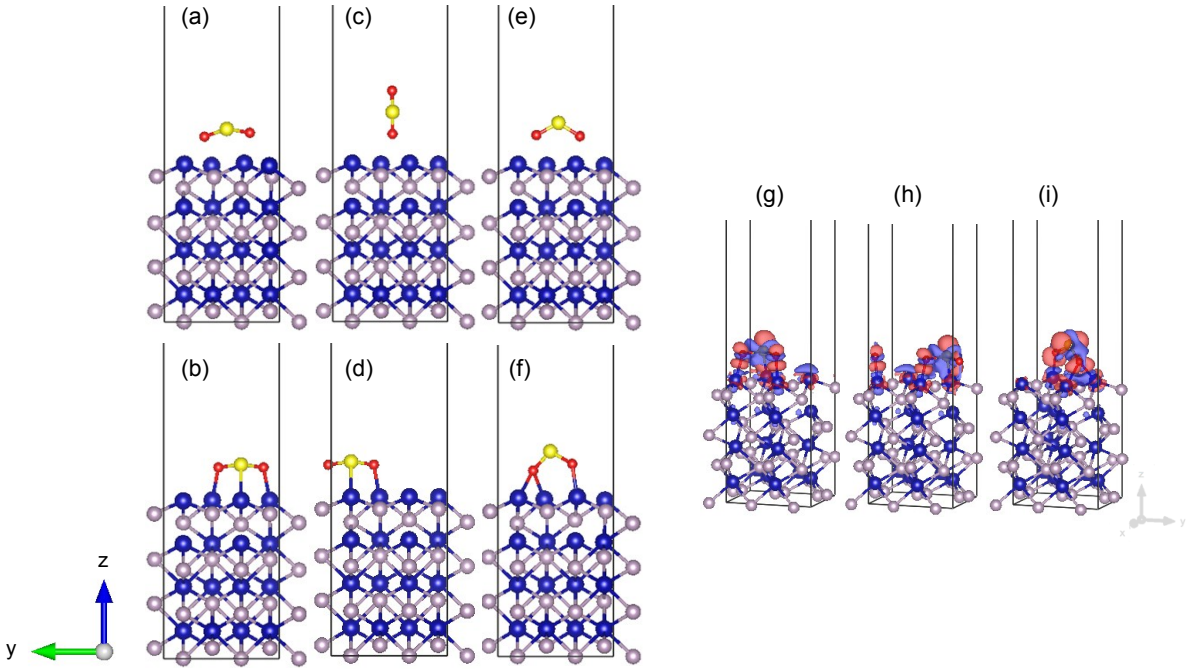

Figure S4. Initial and relaxed structures for SO_2 adsorbed on (010)-Co (cobalt terminated) surface with (a,b) parallel molecular configuration, (c,d) perpendicular molecular configuration, (e,f) and perpendicular molecule with two oxygen atoms facing the surface. Charge density difference for relaxed structures starting with SO_2 (g) parallel, (h), perpendicular, and (h) perpendicular with two oxygen facing the surface.

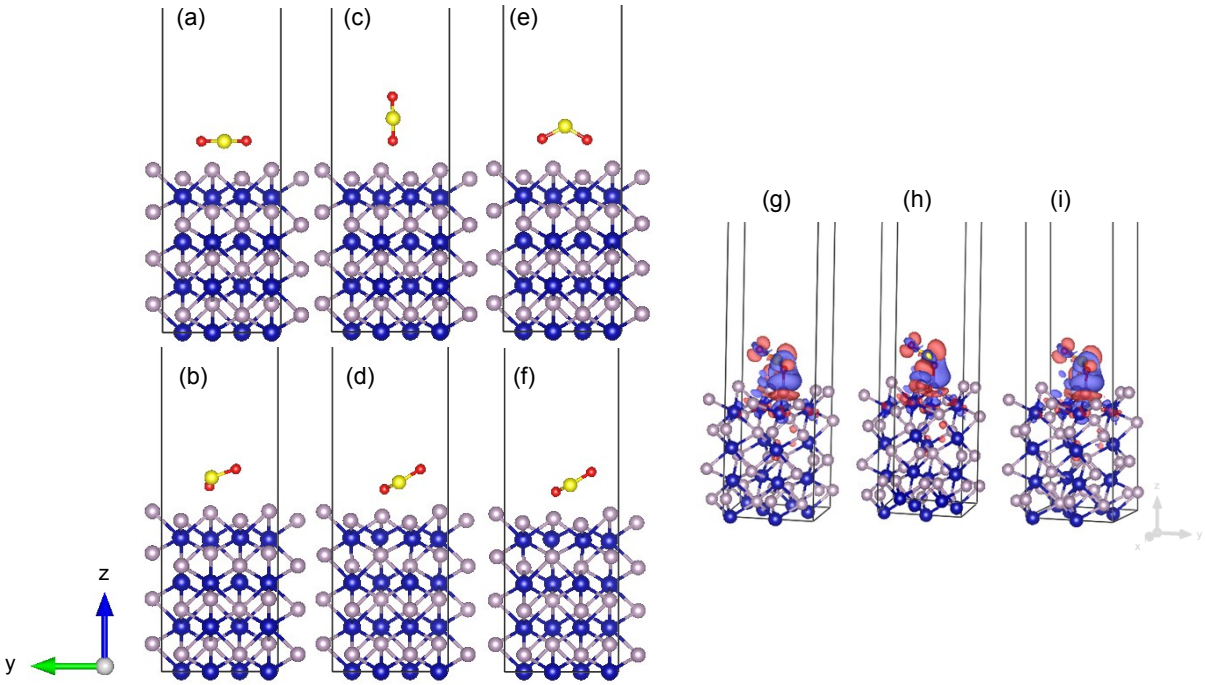

Figure S5. Initial and relaxed structures for SO_2 adsorbed on (010)-P (phosphorous terminated) surface with (a,b) parallel molecular configuration, (c,d) perpendicular molecular configuration, (e,f) and perpendicular molecule with two oxygen atoms facing the surface. Charge density difference for relaxed structures starting with SO_2 (g) parallel, (h), perpendicular, and (h) perpendicular with two oxygen facing the surface.

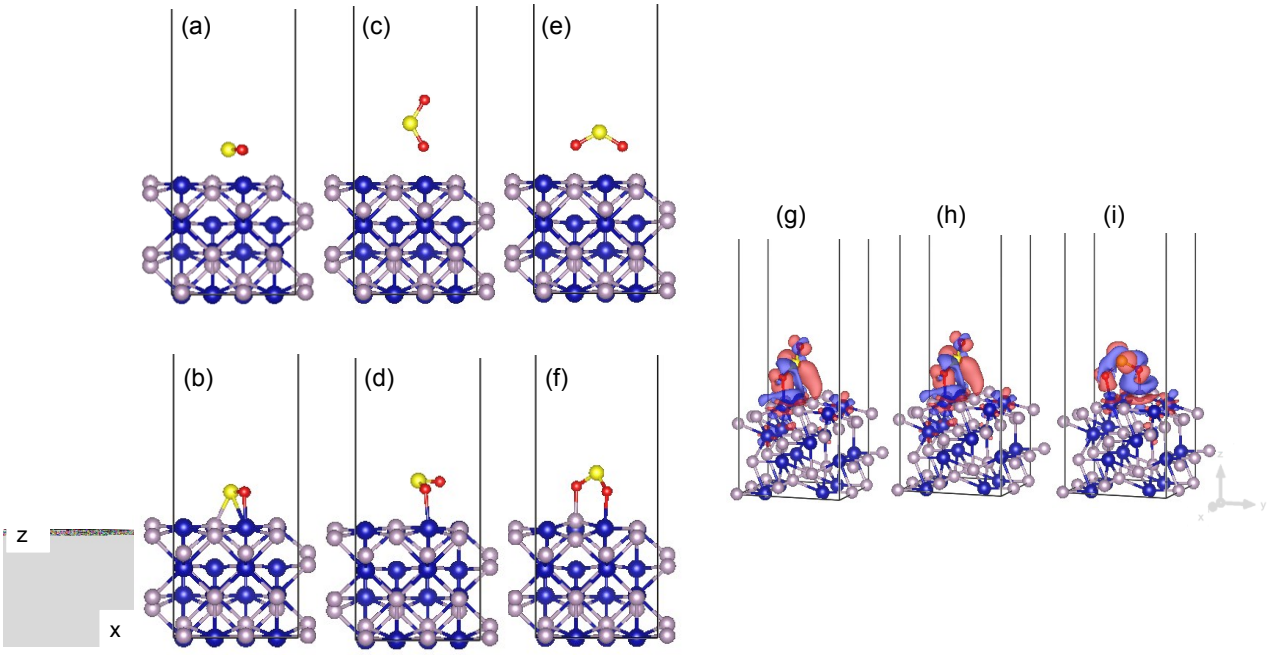

Figure S6. Initial and relaxed structures for SO_2 adsorbed on (011)-Co (cobalt terminated) surface with (a,b) parallel molecular configuration, (c,d) perpendicular molecular configuration, (e,f) and perpendicular molecule with two oxygen atoms facing the surface. Charge density difference for relaxed structures starting with SO_2 (g) parallel, (h), perpendicular, and (h) perpendicular with two oxygen facing the surface.

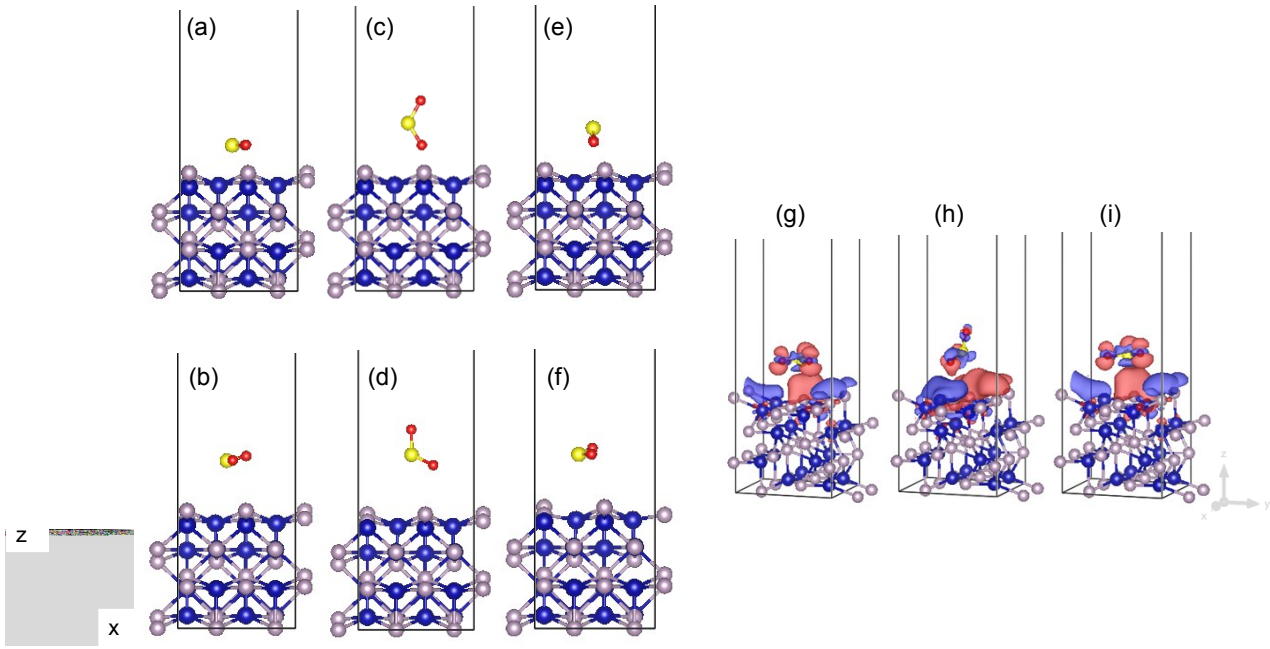

Figure S7. Initial and relaxed structures for SO_2 adsorbed on (011)-P (phosphorous terminated) surface with (a,b) parallel molecular configuration, (c,d) perpendicular molecular configuration, (e,f) and perpendicular molecule with two oxygen atoms facing the surface. Charge density difference for relaxed structures starting with SO_2 (g) parallel, (h), perpendicular, and (h) perpendicular with two oxygen facing the surface.

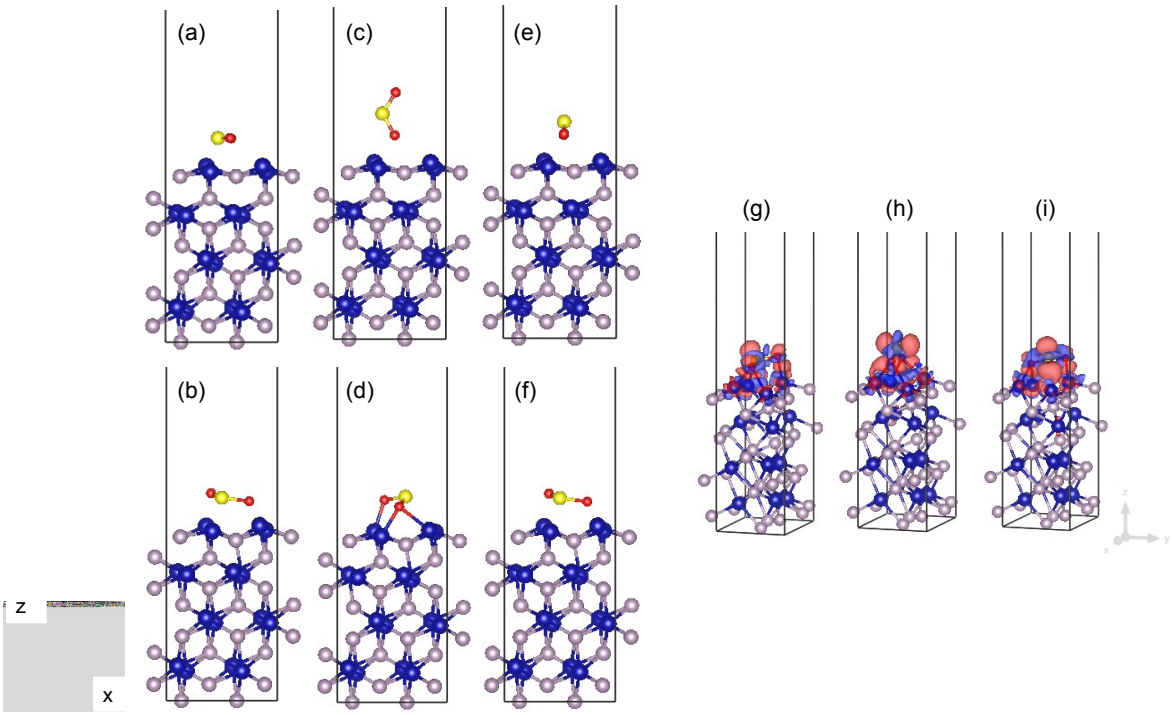

Figure S8. Initial and relaxed structures for SO_2 adsorbed on (101)-Co (cobalt terminated) surface with (a,b) parallel molecular configuration, (c,d) perpendicular molecular configuration, (e,f) and perpendicular molecule with two oxygen atoms facing the surface. Charge density difference for relaxed structures starting with SO_2 (g) parallel, (h), perpendicular, and (h) perpendicular with two oxygen facing the surface.

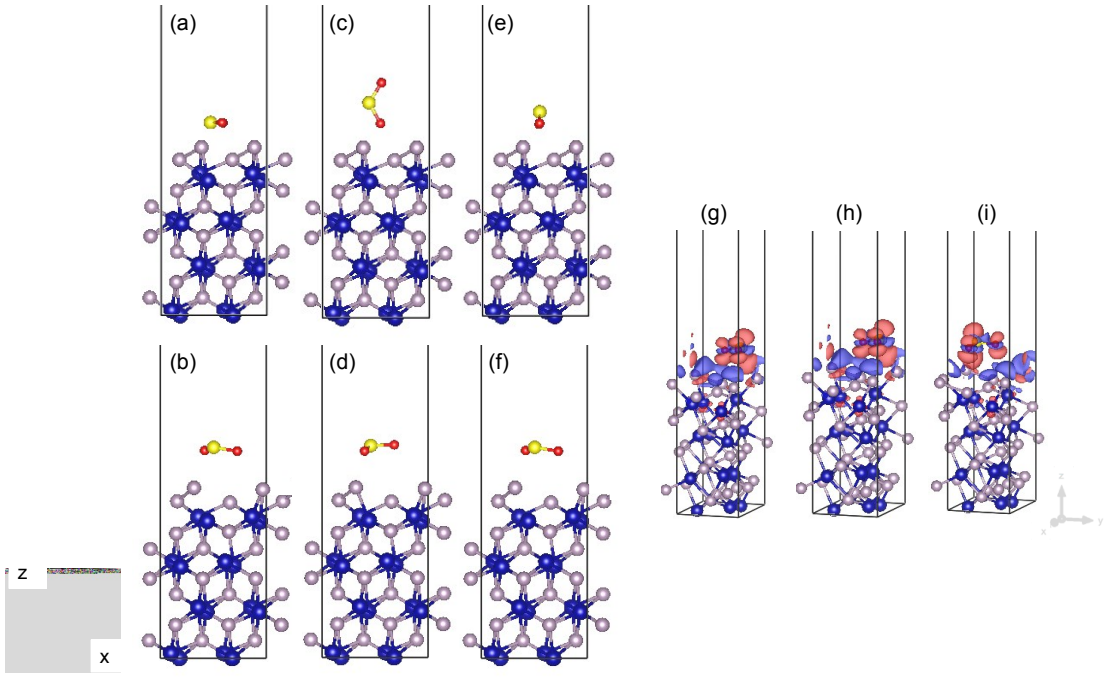

Figure S9. Initial and relaxed structures for SO_2 adsorbed on (101)-P (phosphorous terminated) surface with (a,b) parallel molecular configuration, (c,d) perpendicular molecular configuration, (e,f) and perpendicular molecule with two oxygen atoms facing the surface. Charge density difference for relaxed structures starting with SO_2 (g) parallel, (h), perpendicular, and (h) perpendicular with two oxygen facing the surface.

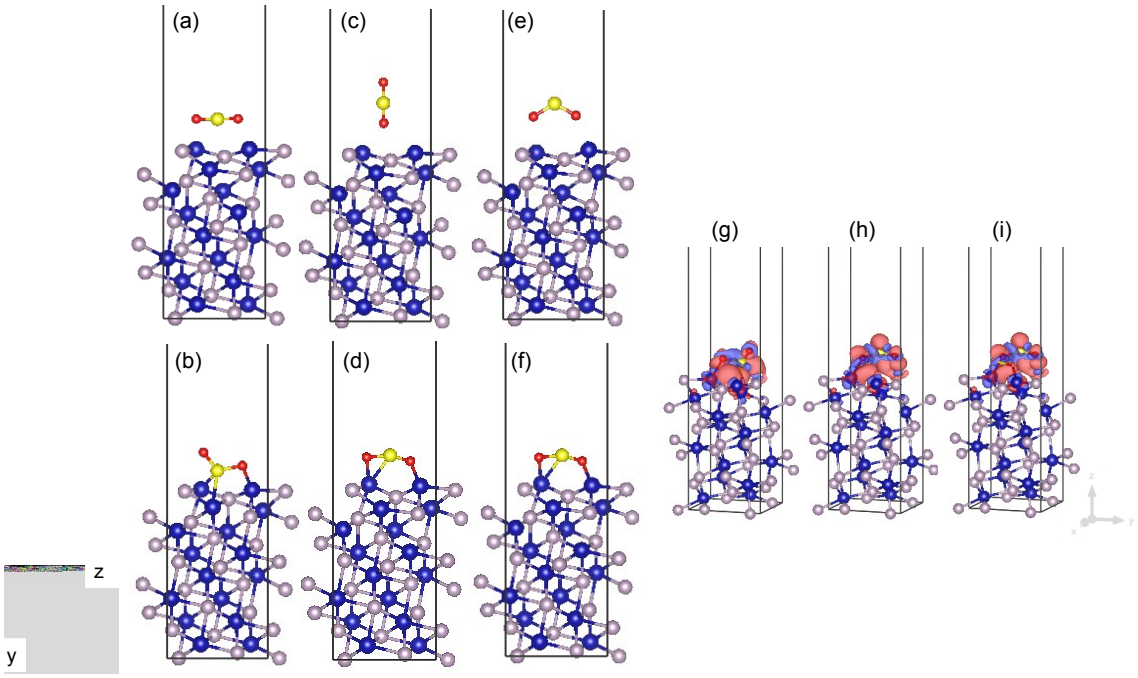

Figure S10. Initial and relaxed structures for SO_2 adsorbed on (110)-Co (cobalt terminated) surface with (a,b) parallel molecular configuration, (c,d) perpendicular molecular configuration, (e,f) and perpendicular molecule with two oxygen atoms facing the surface. Charge density difference for relaxed structures starting with SO_2 (g) parallel, (h), perpendicular, and (h) perpendicular with two oxygen facing the surface.

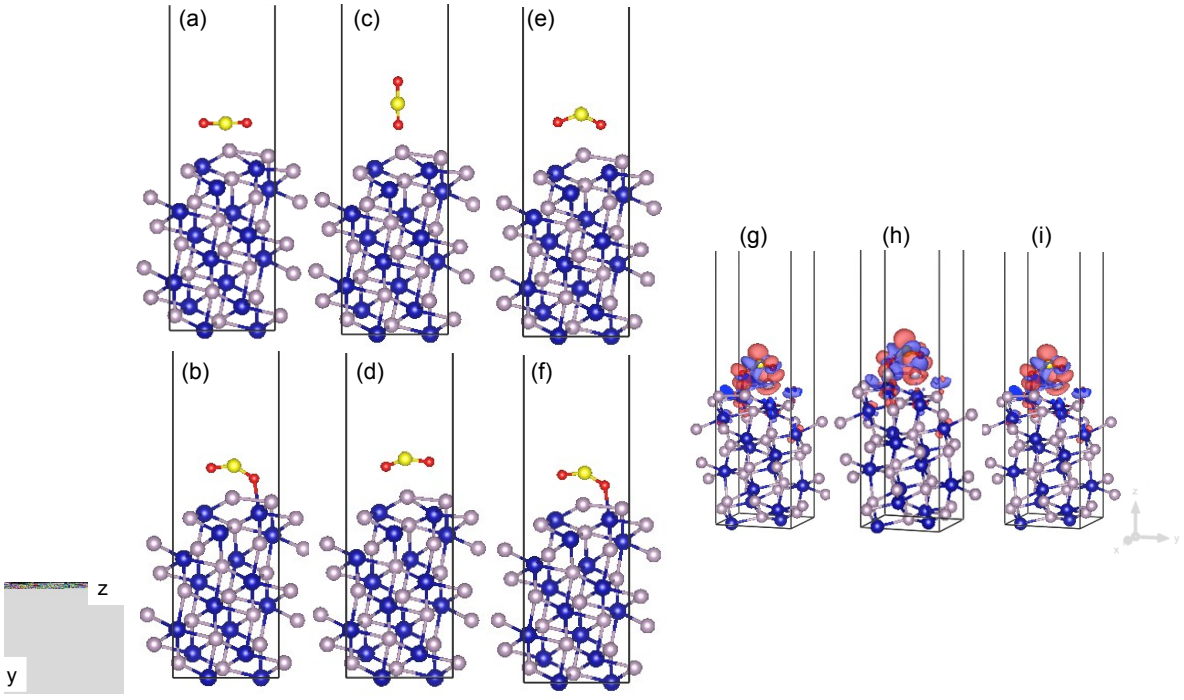

Figure S11. Initial and relaxed structures for SO_2 adsorbed on (110)-P (phosphorous terminated) surface with (a,b) parallel molecular configuration, (c,d) perpendicular molecular configuration, (e,f) and perpendicular molecule with two oxygen atoms facing the surface. Charge density difference for relaxed structures starting with SO_2 (g) parallel, (h), perpendicular, and (h) perpendicular with two oxygen facing the surface.

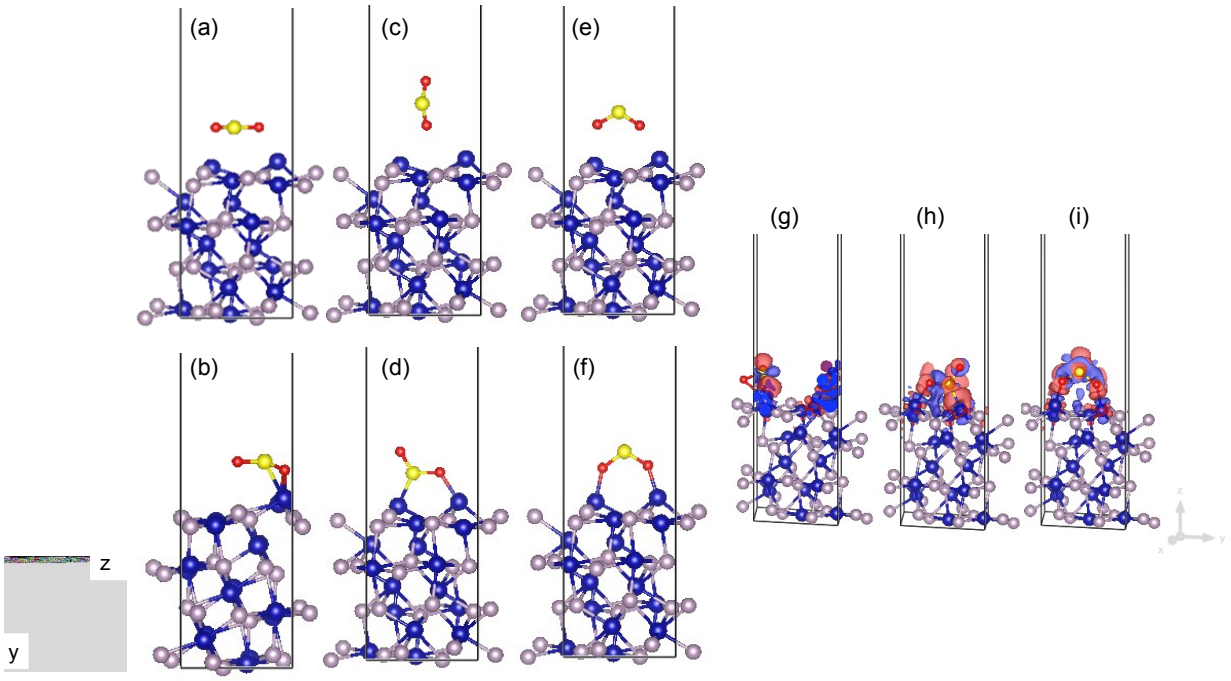

Figure S12. Initial and relaxed structures for SO_2 adsorbed on (111)-Co (cobalt terminated) surface with (a,b) parallel molecular configuration, (c,d) perpendicular molecular configuration, (e,f) and perpendicular molecule with two oxygen atoms facing the surface. Charge density difference for relaxed structures starting with SO_2 (g) parallel, (h), perpendicular, and (h) perpendicular with two oxygen facing the surface.

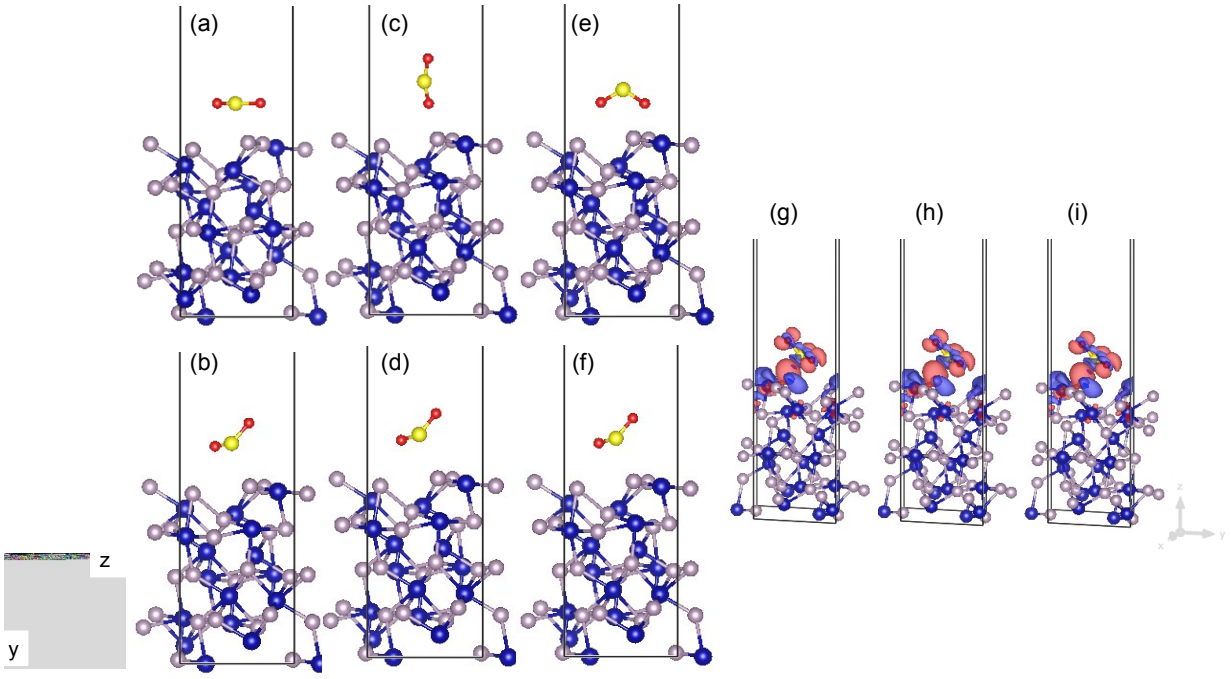

Figure S13. Initial and relaxed structures for SO_2 adsorbed on (111)-P (phosphorous terminated) surface with (a,b) parallel molecular configuration, (c,d) perpendicular molecular configuration, (e,f) and perpendicular molecule with two oxygen atoms facing the surface. Charge density difference for relaxed structures starting with SO_2 (g) parallel, (h), perpendicular, and (h) perpendicular with two oxygen facing the surface.

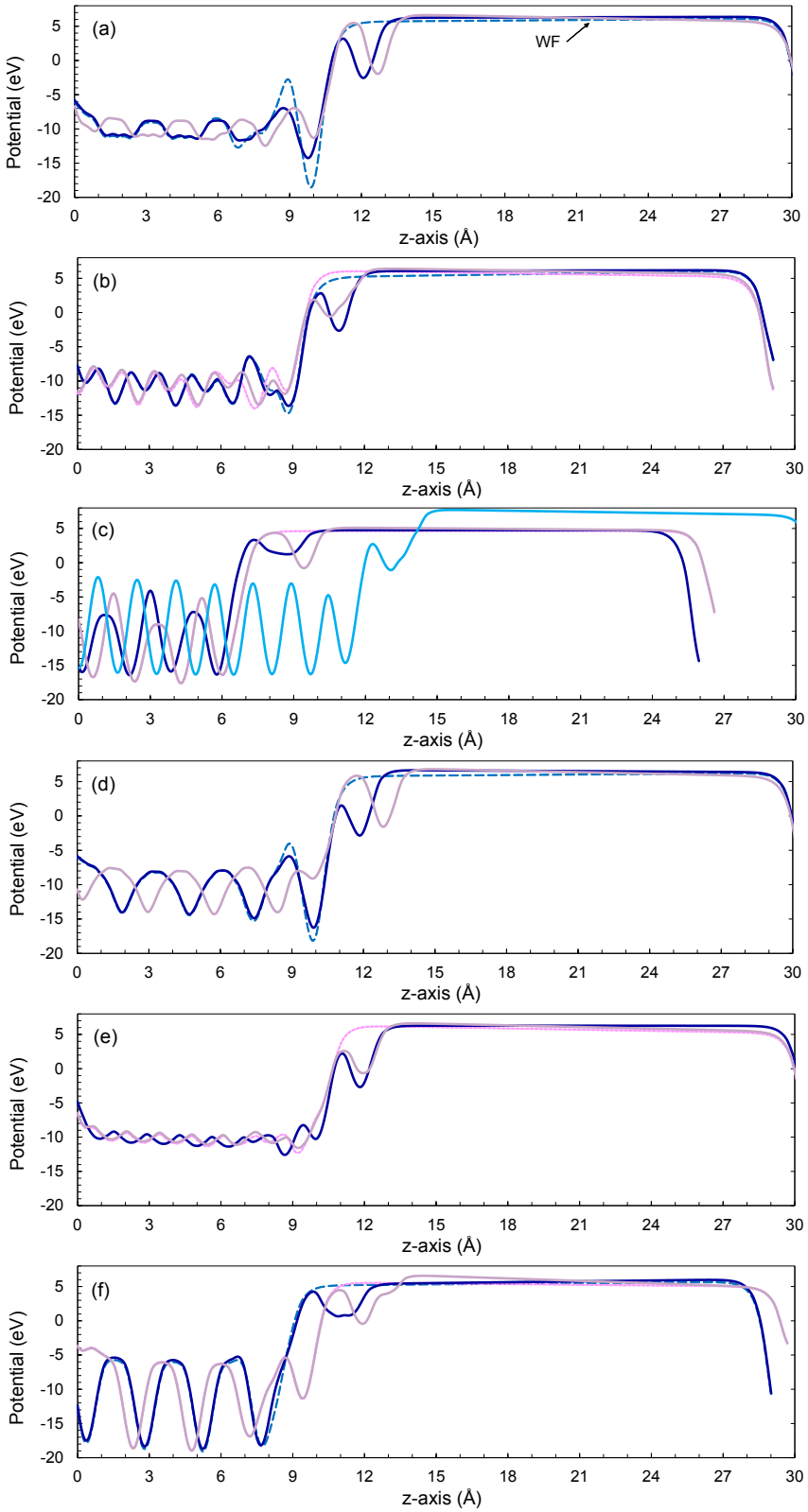

Figure S14. Planar average potential energy profiles in the z-direction and work functions (WF) for (a) (001), (b) (010), (c) (011), (100), (d) (101), (e) (110), (f) and (111) surfaces. Cobalt terminated surfaces as blue lines, and phosphorous terminated surfaces as pink lines ((100) surface in light blue). Dashed lines for relaxed systems after adsorbing SO_2.

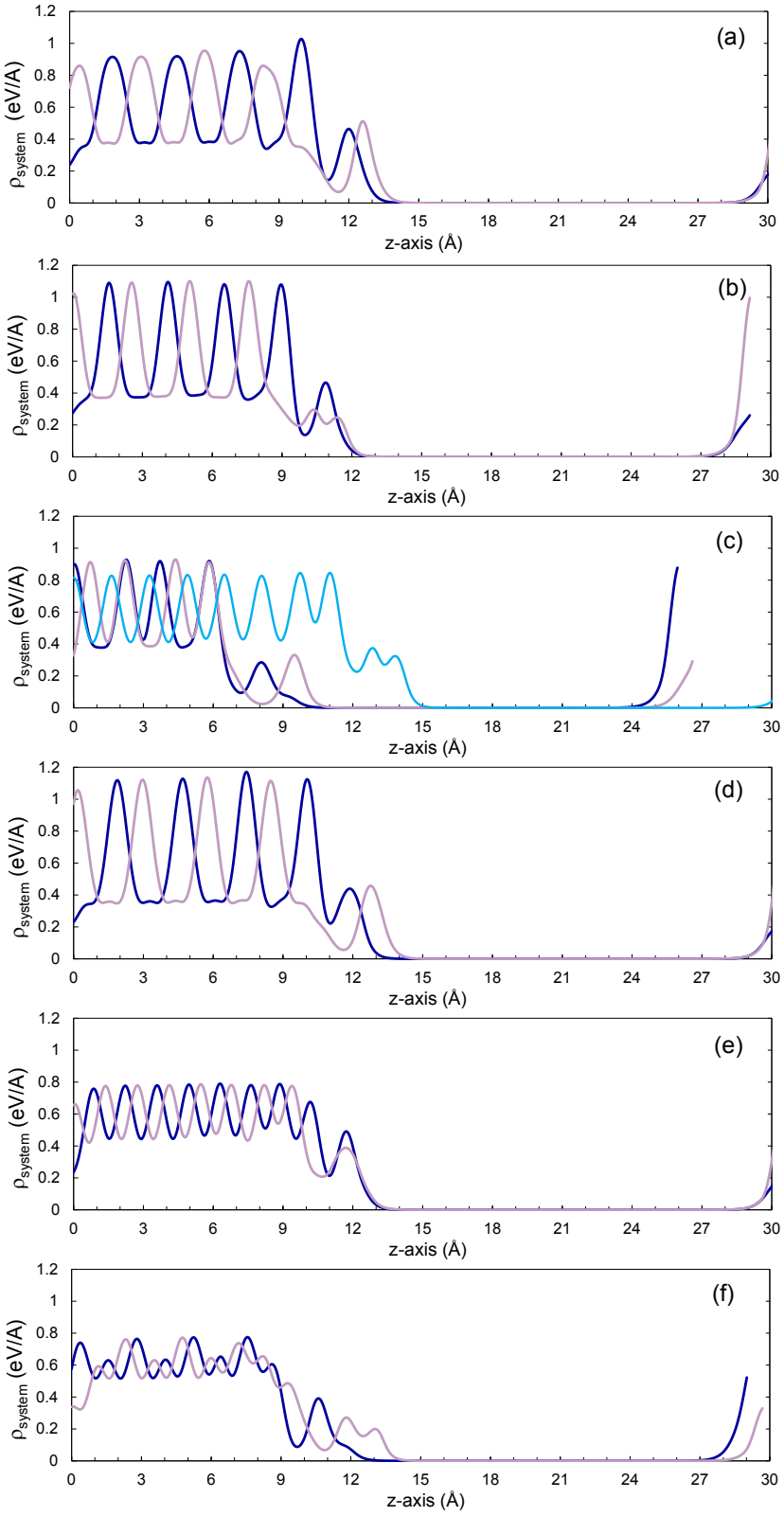

Figure S15. Planar average charge density profiles in the z-direction for the relaxed systems after adsorption in (a) (001), (b) (010), (c) (011), (100), (d) (101), (e) (110), (f) and (111) surfaces. Cobalt terminated surfaces as blue lines, and phosphorous terminated surfaces as pink lines ((100) surface in light blue).

Table S1. Energies, bonds lengths and angles after SO_2 adsorption on the different studied surfaces.

Facet	E_{vaccum} (eV)	E_f (eV)	WF (eV)	$E_{ads\ max}$ (eV)	O-S-O (°)	d_{S-O1} (Å)	d_{S-O2} (Å)	d_{O1-M} (Å)	d_{O2-CoP} (Å)	d_{S-CoP} (Å)
(001)-Co	6.07	1.05	5.01	1.29	114.902	1.5326	1.5432	2.1133	1.9910	2.2003
(001)-P	6.05	1.26	4.79	0.55	116.857	1.4614	1.4608	3.4844	3.4879	2.9214
(010-Co	6.00	0.70	5.30	2.96	107.741	1.5799	1.5800	1.8918	1.8915	2.1757
(010)-P	6.03	0.85	5.18	0.31	107.391	1.4623	1.7438	3.8467	1.6527	2.9925
(011)-Co	4.60	0.03	4.57	0.59	113.267	1.5239	1.4844	2.0611	2.8866	2.7201
(011)-P	4.63	-0.62	5.25	0.31	118.315	1.4528	1.4523	3.4758	3.4535	3.4539
(100)	6.93	1.79	5.14	1.24	107.546	1.4688	1.7844	3.0463	1.6501	2.2355
(101)-Co	6.18	1.14	5.04	2.82	107.419	1.6186	1.5456	1.9068	1.9558	2.1916
(101)-P	6.19	1.30	4.89	0.85	117.256	1.4616	1.4551	3.4581	3.2769	2.9093
(110)-Co	6.09	1.03	5.06	2.26	115.049	1.5317	1.5324	1.9449	3.2577	3.5398
(110)-P	6.18	1.21	4.97	0.77	113.789	1.5247	1.4731	2.0943	3.1246	3.0510
(111)-Co	5.64	0.68	4.95	1.93	114.226	1.5834	1.4704	2.2318	3.2344	2.2335
(111)-P	5.54	0.60	4.94	0.40	118.43	1.4514	1.4578	3.6409	3.3743	3.8658

E_{vacuum}: vacuum potential energy, which is a product of the electron charge and the electrostatic potential in the vacuum near the surface.
E_f: Fermi level (electrochemical potential of electrons) inside the surface.
WF: Work function (defined as the minimum energy needed to remove an electron from the surface to a point outside the solid).

Table S2. Coordinates and Bader charges for non-polar CoP (100) surface.

#	Atom	x	y	z	Bader charge (e^-)	#	Atom	x	y	z	Bader charge (e^-)
1	P	4.4674	0.6342	1.6313	-0.1476	19	Co	3.5077	2.764	8.0343	0.1676
2	P	4.4674	0.6342	4.8938	-0.1648	20	Co	3.5708	2.713	11.0093	0.1364
3	P	4.4656	0.6358	8.0931	-0.15	21	Co	3.4954	4.9473	0	0.2124
4	P	4.4378	0.7205	11.4235	-0.1559	22	Co	3.4954	4.9473	3.2625	0.1703
5	P	2.5322	1.5421	0	-0.2203	23	Co	3.4949	4.9472	6.4724	0.1541
6	P	2.5322	1.5421	3.2625	-0.1672	24	Co	3.4848	4.9658	9.6908	0.1327
7	P	2.5332	1.5202	6.4838	-0.1552	25	Co	0.972	2.1763	1.6313	0.161
8	P	2.5784	1.4612	9.6821	-0.1219	26	Co	0.972	2.1763	4.8938	0.1611
9	P	1.9352	4.313	1.6313	-0.1469	27	Co	0.9774	2.1703	8.1348	0.1695
10	P	1.9352	4.313	4.8938	-0.1614	28	Co	1.0139	2.1907	11.0856	0.1373
11	P	1.935	4.3051	8.0986	-0.1707	29	Co	0.9632	0	0	0.2137
12	P	1.9716	4.1852	11.2198	0.6738	30	Co	0.9632	0	3.2625	0.1706
13	P	0	3.4052	0	-0.2227	31	Co	0.9609	5.5405	6.4901	0.1541
14	P	0	3.4052	3.2625	-0.1689	32	Co	0.956	5.5183	9.748	0.1312
15	P	0.0163	3.4096	6.4991	-0.1617	33	S	1.031	2.8485	13.2221	1.4088
16	P	5.0617	3.4646	9.6787	-0.1131	34	O	2.0942	2.1263	13.9332	-1.1183
17	Co	3.5042	2.771	1.6313	0.1617	35	O	1.6599	4.4681	12.8154	-1.1362
18	Co	3.5042	2.771	4.8938	0.1668						

Table S3. Coordinates and Bader charges of cobalt and phosphorous terminated (001) surfaces.

(001)-Co						(001)-P					
#	Atom	x	y	z	Bader charge (e^-)	#	Atom	x	y	z	Bader charge (e^-)
1	P	2.1482	0.1252	0.0000	-0.0321	1	P	2.1482	0.1252	3.9999	-0.1611
2	P	2.1528	0.1311	5.5263	-0.1589	2	P	2.1563	5.0183	9.7421	-0.1414
3	P	0.5169	3.2544	0.9080	-0.1229	3	P	0.5169	3.2544	4.9076	-0.1560
4	P	0.5154	3.2591	6.4534	-0.1541	4	P	0.5047	3.5433	10.3440	-0.0080
5	P	2.1482	2.6574	3.6789	-0.1865	5	P	2.1482	2.6574	2.1366	-0.1800
6	P	2.1402	2.7895	9.3193	-0.1788	6	P	2.1491	2.6818	7.6811	-0.1108
7	P	0.5169	0.7222	2.7709	-0.1554	7	P	0.5169	0.7222	1.2289	-0.2783
8	P	0.5158	0.7237	8.2921	-0.1277	8	P	0.5154	0.7496	6.7770	-0.1721
9	P	5.4108	0.1252	0.0000	-0.0322	9	P	5.4108	0.1252	3.9999	-0.1620
10	P	5.4063	0.1328	5.5247	-0.1518	10	P	5.3742	5.0158	9.7518	-0.1415
11	P	3.7795	3.2544	0.9080	-0.1220	11	P	3.7795	3.2544	4.9076	-0.1551
12	P	3.7845	3.2289	6.4283	-0.1420	12	P	3.7668	3.5041	10.3130	-0.0567
13	P	5.4108	2.6574	3.6789	-0.1873	13	P	5.4108	2.6574	2.1366	-0.1798
14	P	5.4183	2.8584	9.3559	-0.1640	14	P	5.4070	2.6785	7.6830	-0.1122
15	P	3.7795	0.7222	2.7709	-0.1564	15	P	3.7795	0.7222	1.2289	-0.2783
16	P	3.7779	0.7836	8.3414	-0.1895	16	P	3.7782	0.7469	6.7640	-0.1571
17	Co	2.1482	4.2264	2.1366	0.1636	17	Co	2.1482	4.2264	0.5947	0.1517
18	Co	2.2177	4.2374	7.5988	0.1704	18	Co	2.1436	4.2218	6.0808	0.1594
19	Co	0.5169	4.2176	4.3132	0.1678	19	Co	0.5169	4.2176	2.7709	0.1720
20	Co	0.5447	4.2485	9.7647	0.1696	20	Co	0.5121	4.1902	8.1744	0.1576
21	Co	2.1482	1.6942	1.5420	0.1587	21	Co	2.1482	1.6942	0.0000	0.1398
22	Co	2.1371	1.6963	7.0572	0.1740	22	Co	2.1466	1.6907	5.5353	0.1573
23	Co	0.5169	1.6854	4.9076	0.1669	23	Co	0.5169	1.6854	3.3656	0.1647
24	Co	0.5018	1.7084	10.1468	0.1094	24	Co	0.5219	1.7232	8.8200	0.2177
25	Co	5.4108	4.2264	2.1366	0.1636	25	Co	5.4108	4.2264	0.5947	0.1516
26	Co	5.3507	4.2369	7.5997	0.1665	26	Co	5.4136	4.2213	6.0814	0.1588
27	Co	3.7795	4.2176	4.3132	0.1599	27	Co	3.7795	4.2176	2.7709	0.1726
28	Co	3.7757	4.2683	9.8333	0.3403	28	Co	3.7773	4.1838	8.1452	0.1471
29	Co	5.4108	1.6942	1.5420	0.1587	29	Co	5.4108	1.6942	0.0000	0.1397
30	Co	5.4168	1.6920	7.0501	0.1748	30	Co	5.4105	1.6903	5.5357	0.1563
31	Co	3.7795	1.6854	4.9076	0.1620	31	Co	3.7795	1.6854	3.3656	0.1649
32	Co	3.7805	1.7363	10.2838	0.2551	32	Co	3.7756	1.6867	8.8247	0.2194
33	S	3.4308	2.7439	12.2084	1.6393	33	S	3.6799	1.9293	12.7721	2.1704
34	O	4.7133	1.9055	12.1726	-1.0963	34	O	2.4270	1.2063	12.5637	-1.1742
35	O	3.6119	4.2257	11.8171	-1.1427	35	O	4.9155	1.1632	12.6296	-1.1765

Table S4. Coordinates and Bader charges of cobalt and phosphorous terminated (010) surfaces.

(010)-Co					
#	Atom	x	y	z	Bader charge (e^-)
1	P	0.6342	2.1482	0.0000	-0.0499
2	P	0.6245	2.1499	5.0466	-0.1432
3	P	1.5421	0.5169	3.1292	-0.1582
4	P	1.4544	0.5256	8.2300	-0.2272
5	P	4.3130	2.1482	2.5322	-0.1768
6	P	4.3272	2.1541	7.6363	-0.1353
7	P	3.4052	0.5169	0.5970	0.0016
8	P	3.4009	0.5137	5.6432	-0.1380
9	P	0.6342	5.4108	0.0000	-0.0500
10	P	0.6240	5.4124	5.0379	-0.1433
11	P	1.5421	3.7795	3.1292	-0.1577
12	P	1.4545	3.7845	8.2306	-0.2279
13	P	4.3130	5.4108	2.5322	-0.1759
14	P	4.3170	5.4171	7.7256	-0.1549
15	P	3.4052	3.7795	0.5970	0.0016
16	P	3.4012	3.7873	5.6434	-0.1377
17	Co	2.7710	2.1482	4.1013	0.1561
18	Co	2.6254	2.1547	8.9923	0.1789
19	Co	4.9473	0.5169	4.0925	0.1552
20	Co	4.9893	0.5336	9.0143	0.3548
21	Co	2.1763	2.1482	1.5691	0.1019
22	Co	2.2040	2.1512	6.5546	0.1714
23	Co	0.0000	0.5169	1.5604	0.1131
24	Co	5.5179	0.5157	6.5257	0.1681
25	Co	2.7710	5.4108	4.1013	0.1565
26	Co	2.5723	5.4183	8.9717	0.1967
27	Co	4.9473	3.7795	4.0925	0.1558
28	Co	4.9893	3.7776	9.0138	0.3544
29	Co	2.1763	5.4108	1.5691	0.1019
30	Co	2.1973	5.4134	6.5321	0.1780
31	Co	0.0000	3.7795	1.5604	0.1128
32	Co	5.5183	3.7884	6.5258	0.1693
33	S	3.4687	2.1577	11.0356	1.4662
34	O	4.3758	0.8871	10.8726	-1.1078
35	O	4.3694	3.4326	10.8722	-1.1106

(010)-P					
#	Atom	x	y	z	Bader charge (e^-)
1	P	0.6342	2.1482	3.5043	-0.1612
2	P	0.6785	2.1713	8.4539	0.0361
3	P	1.5421	0.5169	1.5691	-0.1829
4	P	1.4926	0.4368	6.6068	-0.1718
5	P	4.3130	2.1482	0.9721	-0.3578
6	P	4.3119	2.1507	5.9822	-0.1701
7	P	3.4052	0.5169	4.1013	-0.1554
8	P	3.4234	0.4800	9.0662	-0.0366
9	P	0.6342	5.4108	3.5043	-0.1541
10	P	0.6947	5.4970	8.5641	-0.0188
11	P	1.5421	3.7795	1.5691	-0.1815
12	P	1.5443	3.7987	6.6053	-0.1586
13	P	4.3130	5.4108	0.9721	-0.3590
14	P	4.3280	5.4205	5.9777	-0.1705
15	P	3.4052	3.7795	4.1013	-0.1564
16	P	3.2436	3.7170	8.7992	0.7105
17	Co	2.7710	2.1482	2.5409	0.1609
18	Co	2.7380	2.0299	7.5531	0.0817
19	Co	4.9473	0.5169	2.5322	0.1753
20	Co	4.9481	0.5435	7.5152	0.1252
21	Co	2.1763	2.1482	0.0088	0.2258
22	Co	2.1939	2.1552	5.0506	0.1600
23	Co	0.0000	0.5169	0.0000	0.1535
24	Co	5.5386	0.5205	5.0096	0.1410
25	Co	2.7710	5.4108	2.5409	0.1582
26	Co	2.8223	5.4604	7.5838	0.0839
27	Co	4.9473	3.7795	2.5322	0.1779
28	Co	5.0390	3.8442	7.6186	0.1537
29	Co	2.1763	5.4108	0.0088	0.2257
30	Co	2.1894	5.4059	5.0410	0.1460
31	Co	0.0000	3.7795	0.0000	0.1542
32	Co	5.5373	3.7682	5.0355	0.1528
33	S	1.1639	2.7682	10.7303	1.5025
34	O	1.5161	1.5598	11.4749	-1.1304
35	O	2.6508	3.5898	10.3368	-1.1599

Table S5. Coordinates and Bader charges of cobalt and phosphorous terminated (011) surfaces.

(011)-Co						(011)-P					
#	Atom	x	y	z	Bader charge (e^-)	#	Atom	x	y	z	Bader charge (e^-)
1	P	2.1482	5.0758	1.5466	-0.1539	1	P	2	1.6594	0.0000	-0.2148
2	P	2.1285	0.8819	5.2925	-0.2169	2	P	2	5.0565	3.717156	-0.0906
3	P	0.5169	3.1002	0.7305	-0.2546	3	P	1	3.1001	2.922579	-0.1073
4	P	0.5259	6.4984	4.4647	-0.1041	4	P	1	6.5244	6.564898	-0.2006
5	P	2.1482	0.6519	2.1590	-0.1210	5	P	2	4.7429	0.612403	-0.2372
6	P	2.1290	4.0788	6.3059	0.3232	6	P	2	0.6606	4.413382	-0.1213
7	P	0.5169	0.0167	0.1179	-0.1690	7	P	1	0.0166	2.309909	-0.1530
8	P	0.5411	3.4271	3.8544	-0.1032	8	P	1	3.3318	6.114887	-0.2490
9	P	5.4108	5.0758	1.5466	-0.1594	9	P	5	1.6594	0.0000	-0.2152
10	P	5.4250	0.9527	5.4114	-0.2081	10	P	5	5.0584	3.715237	-0.0856
11	P	3.7795	3.1002	0.7305	-0.2616	11	P	4	3.1001	2.922579	-0.1016
12	P	3.7754	6.4888	4.4857	-0.1247	12	P	4	6.4583	6.563378	-0.1820
13	P	5.4108	0.6519	2.1590	-0.1321	13	P	5	4.7429	0.612403	-0.2373
14	P	5.4393	4.0175	5.8917	-0.1394	14	P	5	0.6583	4.406797	-0.1142
15	P	3.7795	0.0167	0.1179	-0.1673	15	P	4	0.0166	2.309909	-0.1547
16	P	3.7530	3.4183	3.9172	-0.1359	16	P	4	3.4012	6.108115	-0.2719
17	Co	2.1482	2.8488	2.2769	0.1593	17	Co	2	6.9397	0.730511	0.25306
18	Co	2.1327	6.2353	5.8417	0.1364	18	Co	2	2.8813	4.417461	0.15594
19	Co	0.5169	5.3273	0.0000	0.1863	19	Co	1	5.3272	2.192067	0.14629
20	Co	0.4867	1.1950	3.6995	0.1643	20	Co	1	1.1564	5.768907	0.20327
21	Co	2.1482	1.5795	0.0065	0.2264	21	Co	2	1.5794	2.198466	0.14811
22	Co	2.1553	4.9630	3.6588	0.1560	22	Co	2	4.9662	5.8643	0.16271
23	Co	0.5169	6.5965	2.2704	0.1465	23	Co	1	3.1800	0.723846	0.17074
24	Co	0.6113	2.5380	5.7999	0.1767	24	Co	1	6.5772	4.351928	0.15311
25	Co	5.4108	2.8488	2.2769	0.1587	25	Co	5	6.9397	0.730511	0.25320
26	Co	5.4291	6.2599	5.8225	0.1350	26	Co	5	2.8807	4.411196	0.14854
27	Co	3.7795	5.3273	0.0000	0.1861	27	Co	4	5.3272	2.192067	0.14819
28	Co	3.8081	1.1951	3.7391	0.1725	28	Co	4	1.1681	5.775492	0.23981
29	Co	5.4108	1.5795	0.0065	0.2274	29	Co	5	1.5794	2.198466	0.14808
30	Co	5.4078	4.9207	3.7103	0.1391	30	Co	5	4.9655	5.856888	0.17224
31	Co	3.7795	6.5965	2.2704	0.1553	31	Co	4	3.1800	0.723846	0.17099
32	Co	3.6902	2.5020	5.9019	0.3260	32	Co	4	6.5655	4.366432	0.15133
33	S	3.2584	3.1080	8.8846	1.5657	33	S	3	3.8892	9.358491	2.22960
34	O	2.1810	4.0293	8.1539	-1.1719	34	O	3	2.4718	9.373927	-1.1573
35	O	3.8120	2.1014	7.8769	-1.1180	35	O	4	4.8383	9.61337	-1.1607

Table S6. Coordinates and Bader charges of cobalt and phosphorous terminated (101) surfaces.

(101)-Co						(101)-P					
#	Atom	x	y	Z	Bader charge (e^-)	#	Atom	x	y	z	Bader charge (e^-)
1	P	5.6946	4.4673	0.9453	-0.1207	1	P	0.9188	4.4674	2.0292	-0.1790
2	P	0.9188	4.4673	3.7568	-0.1891	2	P	2.5740	4.4674	4.8407	-0.1693
3	P	2.4983	4.4625	6.5489	-0.1601	3	P	4.1595	4.4329	7.7049	-0.1745
4	P	4.0239	4.5290	9.3705	-0.1512	4	P	6.2376	4.6195	10.2708	0.0766
5	P	4.0846	2.5322	0.0000	-0.0207	5	P	5.7398	2.5322	1.0839	-0.2626
6	P	5.7398	2.5322	2.8115	-0.1566	6	P	0.9641	2.5322	3.8957	-0.1604
7	P	0.9493	2.5143	5.5982	-0.1492	7	P	2.6121	2.5192	6.6750	-0.1616
8	P	2.5322	2.5585	8.3372	-0.1752	8	P	4.2171	2.5535	9.4968	-0.1128
9	P	0.8692	1.9351	0.0000	-0.0245	9	P	2.5244	1.9352	1.0839	-0.2632
10	P	2.5243	1.9351	2.8115	-0.1627	10	P	4.1795	1.9352	3.8957	-0.1644
11	P	4.1719	1.9409	5.5829	-0.1614	11	P	5.8228	1.9247	6.6545	-0.1886
12	P	5.7589	1.9366	8.3862	-0.1307	12	P	1.0171	1.9240	9.5793	-0.0911
13	P	2.4791	0.0000	0.9453	-0.1109	13	P	4.1343	0.0000	2.0292	-0.1729
14	P	4.1342	0.0001	3.7568	-0.1794	14	P	5.7895	0.0000	4.8407	-0.1620
15	P	5.7323	0.0187	6.5552	-0.1764	15	P	0.9599	0.0478	7.5893	-0.1381
16	P	0.8053	5.0280	9.5739	-0.2362	16	P	2.0493	0.0344	10.3596	-0.0371
17	Co	3.8532	3.5042	2.0292	0.1545	17	Co	3.8533	3.5042	0.3016	0.1016
18	Co	5.5084	3.5042	4.8407	0.1732	18	Co	5.5085	3.5042	3.1131	0.1783
19	Co	0.6579	3.5061	7.5273	0.1739	19	Co	0.7376	3.5096	5.8954	0.1663
20	Co	2.3013	3.5275	10.2016	0.3168	20	Co	2.2911	3.5102	8.6263	0.1630
21	Co	1.1502	3.4953	1.7276	0.1619	21	Co	1.1502	3.4954	0.0000	0.1642
22	Co	2.8054	3.4953	4.5391	0.1717	22	Co	2.8054	3.4954	2.8115	0.1737
23	Co	4.3817	3.4934	7.2935	0.1790	23	Co	4.4589	3.5009	5.6332	0.1722
24	Co	5.7596	3.4532	9.9601	0.2745	24	Co	6.0584	3.5158	8.3021	0.1496
25	Co	4.3656	0.9720	1.7276	0.1582	25	Co	4.3657	0.9720	0.0000	0.1658
26	Co	6.0208	0.9720	4.5391	0.1648	26	Co	6.0209	0.9720	2.8115	0.1752
27	Co	1.1776	0.9680	7.3713	0.1802	27	Co	1.2330	0.9807	5.5715	0.1526
28	Co	2.6509	1.0518	9.8989	0.1741	28	Co	2.8468	0.9817	8.3481	0.1727
29	Co	0.6378	0.9631	2.0291	0.1545	29	Co	0.6378	0.9632	0.3016	0.1076
30	Co	2.2930	0.9631	4.8406	0.1701	30	Co	2.2930	0.9632	3.1131	0.1726
31	Co	3.8847	0.9594	7.5344	0.1613	31	Co	3.9360	0.9600	5.8806	0.1695
32	Co	5.4097	0.9611	10.2302	0.3054	32	Co	5.5723	0.9778	8.6518	0.1364
33	S	3.2155	1.8615	11.8557	1.4064	33	S	2.9655	4.0380	12.9090	2.2051
34	O	4.8055	2.0828	11.6491	-1.0644	34	O	2.5991	2.6659	12.5635	-1.1911
35	O	2.5853	3.2486	12.1165	-1.1109	35	O	4.3845	4.3560	12.9607	-1.1742

Table S7. Coordinates and Bader charges of cobalt and phosphorous terminated (110) surfaces.

(110)-Co						(110)-P					
#	Atom	x	y	z	Bader charge (e^-)	#	Atom	x	y	z	Bader charge (e^-)
1	P	0.4710	5.3329	0.0000	-0.1392	1	P	0.4710	1.0754	1.8979	-0.2425
2	P	0.4710	1.0754	2.7426	-0.1338	2	P	0.4710	2.8423	4.6405	-0.1680
3	P	0.4834	2.8491	5.4571	-0.1577	3	P	0.4494	4.6197	7.3620	-0.1257
4	P	0.4628	4.5670	8.2604	-0.2001	4	P	0.5489	0.4157	10.0327	-0.0605
5	P	1.3789	1.8188	0.3234	-0.1510	5	P	1.3789	3.5857	2.2210	-0.1762
6	P	1.3789	3.5857	3.0659	-0.1459	6	P	1.3789	5.3526	4.9638	-0.1646
7	P	1.3674	5.3456	5.7968	-0.1500	7	P	1.3557	1.0840	7.6550	-0.1275
8	P	1.2748	1.0459	8.5357	-0.1729	8	P	0.9122	2.6357	10.2694	-0.0530
9	P	4.1498	3.2042	1.3714	-0.2196	9	P	4.1498	3.2042	0.5265	-0.3395
10	P	4.1498	4.9711	4.1140	-0.1658	10	P	4.1498	4.9711	3.2690	-0.1506
11	P	4.1295	0.6987	6.8100	-0.1289	11	P	4.1340	0.7122	5.9690	-0.1550
12	P	4.0502	2.3437	9.5046	-0.0985	12	P	4.1219	2.5215	8.6527	-0.0739
13	P	3.2419	5.7144	1.6948	-0.1424	13	P	3.2419	5.7144	0.8498	-0.2216
14	P	3.2419	1.4570	4.4374	-0.1617	14	P	3.2419	1.4570	3.5924	-0.1540
15	P	3.2920	3.2133	7.1109	-0.1111	15	P	3.2365	3.2293	6.3495	-0.1744
16	P	3.3180	4.8939	9.9253	-0.1773	16	P	3.2214	5.0462	9.0934	-0.1073
17	Co	2.6077	1.8852	2.2210	0.1440	17	Co	2.6077	1.8852	1.3760	0.1750
18	Co	2.6077	3.6521	4.9638	0.1563	18	Co	2.6077	3.6521	4.1189	0.1702
19	Co	2.5539	5.4242	7.6387	0.1795	19	Co	2.6058	5.4064	6.7971	0.1668
20	Co	2.6015	0.9223	10.1656	0.3852	20	Co	2.6044	1.1160	9.4025	0.2980
21	Co	4.7840	1.0091	0.8450	0.2264	21	Co	4.7840	1.0091	0.0000	0.2586
22	Co	4.7840	2.7760	3.5875	0.1678	22	Co	4.7840	2.7760	2.7426	0.1776
23	Co	4.8022	4.5542	6.2785	0.1603	23	Co	4.7921	4.5470	5.4577	0.1600
24	Co	4.7503	0.2684	8.8642	0.1426	24	Co	4.7884	0.3567	8.1271	0.1447
25	Co	2.0130	4.0139	0.8498	0.2346	25	Co	2.0130	4.0139	0.0049	0.2570
26	Co	2.0130	5.7808	3.5924	0.1678	26	Co	2.0130	5.7808	2.7474	0.1664
27	Co	2.0215	1.5284	6.3072	0.1756	27	Co	2.0231	1.5233	5.4732	0.1568
28	Co	2.0779	3.2148	8.8311	0.1317	28	Co	1.9943	3.3577	8.2562	0.1724
29	Co	5.3787	4.9048	2.2164	0.1652	29	Co	5.3787	4.9048	1.3714	0.1024
30	Co	5.3787	0.6473	4.9590	0.1653	30	Co	5.3787	0.6473	4.1140	0.1726
31	Co	5.3714	2.4205	7.5820	0.1584	31	Co	5.3733	2.4119	6.7464	0.1644
32	Co	5.2470	3.9140	10.2576	0.2854	32	Co	5.2592	4.2293	9.3785	0.1848
33	S	0.5119	2.6737	11.9592	1.6727	33	S	2.5770	2.5452	12.0978	1.9358
34	O	1.4286	1.4984	11.6062	-1.1535	34	O	3.2640	1.3946	11.3705	-1.1834
35	O	1.1573	4.0585	11.8401	-1.1095	35	O	3.2817	3.8327	11.9722	-1.1856

Table S8. Coordinates and Bader charges of cobalt and phosphorous terminated (111) surfaces.

(111)-Co						(111)-P					
#	Atom	x	y	z	Bader charge (e^-)	#	Atom	x	y	z	Bader charge (e^-)
1	P	2.8423	1.9683	0.0000	-0.1671	1	P	2.8423	1.9683	1.9778	-0.2402
2	P	4.6092	3.1848	2.4581	-0.1385	2	P	4.6092	3.1848	4.4362	-0.1464
3	P	6.3933	4.3660	4.8941	-0.1608	3	P	6.3834	4.3388	6.8733	-0.1829
4	P	2.0607	5.5344	7.4487	-0.2350	4	P	2.1126	5.4838	9.2343	-0.0900
5	P	5.3526	1.2980	0.6924	-0.1267	5	P	3.5857	0.0814	0.2122	-0.2341
6	P	1.0951	2.5145	3.1508	-0.1483	6	P	5.3526	1.2980	2.6705	-0.1604
7	P	2.8846	3.7177	5.5449	-0.0937	7	P	1.1351	2.5159	5.1314	-0.1634
8	P	4.5246	4.9031	8.0602	-0.2155	8	P	2.8545	3.8129	7.8360	-0.1860
9	P	6.7380	4.2463	0.4028	-0.1951	9	P	6.7380	4.2463	2.3807	-0.2400
10	P	2.4805	5.4629	2.8608	-0.1688	10	P	2.4805	5.4629	4.8388	-0.1655
11	P	2.4637	0.4753	5.2862	-0.1337	11	P	2.4382	0.4668	7.3172	-0.1510
12	P	4.1734	1.6053	7.8151	-0.1423	12	P	4.1702	1.6191	9.6024	-0.1692
13	P	3.2239	5.2034	0.2899	-0.1668	13	P	3.2239	5.2034	2.2676	-0.2031
14	P	3.2239	0.2365	2.7480	-0.1533	14	P	3.2239	0.2365	4.7257	-0.1564
15	P	4.9772	1.4174	5.2256	-0.1702	15	P	4.9655	1.3453	7.1411	-0.0571
16	P	0.7901	2.5401	7.6681	-0.1785	16	P	6.3872	2.3927	9.6435	-0.0718
17	Co	5.4189	6.0053	0.4804	0.2063	17	Co	3.6520	4.7887	0.0000	0.2482
18	Co	5.4190	1.0384	2.9385	0.1688	18	Co	5.4189	6.0053	2.4581	0.1630
19	Co	1.1790	2.2631	5.3639	0.1675	19	Co	5.4370	1.0670	4.8786	0.1707
20	Co	2.9051	3.3696	7.6275	0.1298	20	Co	1.2008	2.2933	7.3241	0.1754
21	Co	4.5429	3.4444	0.2123	0.2014	21	Co	4.5429	3.4444	2.1900	0.1179
22	Co	6.3098	4.6609	2.6704	0.1802	22	Co	6.3098	4.6609	4.6483	0.1740
23	Co	2.0654	5.8542	5.1223	0.1797	23	Co	2.0637	5.8766	6.9406	0.1525
24	Co	2.1053	0.7919	7.4320	0.1475	24	Co	1.9264	0.8856	9.3588	0.2202
25	Co	1.5233	0.9631	1.4455	0.1709	25	Co	1.5233	0.9631	3.4233	0.1719
26	Co	3.2902	2.1797	3.9036	0.1684	26	Co	7.5477	5.9300	0.9653	0.1317
27	Co	5.1022	3.3359	6.3485	0.1985	27	Co	3.3239	2.1335	5.8703	0.1776
28	Co	6.5980	4.4222	8.6265	0.3702	28	Co	4.9496	3.2184	8.1093	0.1054
29	Co	2.4141	3.5197	1.7049	0.1755	29	Co	6.6716	2.3032	1.2247	0.2461
30	Co	4.1810	4.7362	4.1633	0.1587	30	Co	2.4141	3.5197	3.6831	0.1668
31	Co	5.9233	5.8907	6.4862	0.1617	31	Co	4.1966	4.7381	6.1121	0.1722
32	Co	5.9573	0.9986	8.8588	0.3409	32	Co	5.9916	5.9115	8.4190	0.1494
33	S	6.3075	2.8292	11.4022	1.7219	33	S	3.4730	3.3903	11.9794	2.1945
34	O	6.0707	1.5263	10.6364	-1.1229	34	O	3.4923	2.4472	13.0824	-1.1429
35	O	6.5010	4.0427	10.4928	-1.1304	35	O	4.6147	4.2803	11.8071	-1.1770

Table S9. Vibrational frequencies for SO_2 adsorbed on the studied CoP surfaces.

	(001)-Co	(001)-P	(010)-Co	(010)-P	(011)-Co	(011)-P	(101)-Co	(101)-P	(110)-Co	(110)-P	(111)-Co	(111)-P	(100)	SO_2 (isolated)
f1 =	28.52	36.20	24.36	34.18	27.39	37.43	26.36	36.48	29.31	32.91	28.83	37.18	33.45	38.27
f2 =	24.38	30.95	21.99	16.61	21.05	31.97	19.99	31.42	25.67	26.34	25.32	31.69	19.40	32.65
f3 =	11.96	14.66	15.96	12.78	14.36	14.81	14.48	14.73	16.07	13.75	14.61	14.82	12.73	14.94
f4 =	10.25	6.86	15.18	11.58	8.99	3.24	12.38	6.65	12.61	10.13	11.02	4.19	10.74	0.65
f5 =	7.75	3.37	12.24	8.60	6.31	2.01	11.21	3.50	10.78	7.08	9.21	2.64	8.53	0.38
f6 =	6.87	2.18	9.10	5.52	4.59	1.65	8.43	2.08	8.06	4.74	7.51	1.56	5.50	0.21
f7 =	3.61	1.60	4.21	4.53	3.47	0.66	7.74	1.99	5.54	3.36	4.98	1.48	4.56	0.02 i
f8 =	3.38	1.46	4.15	3.07	2.92	0.49	4.26	1.38	3.37	2.40	3.59	1.18	3.45	0.15 i
f9 =	1.87	0.68	3.31	1.97	1.07	0.16	4.01	1.10	2.85	2.09	1.32	1.06	1.75	0.45 i

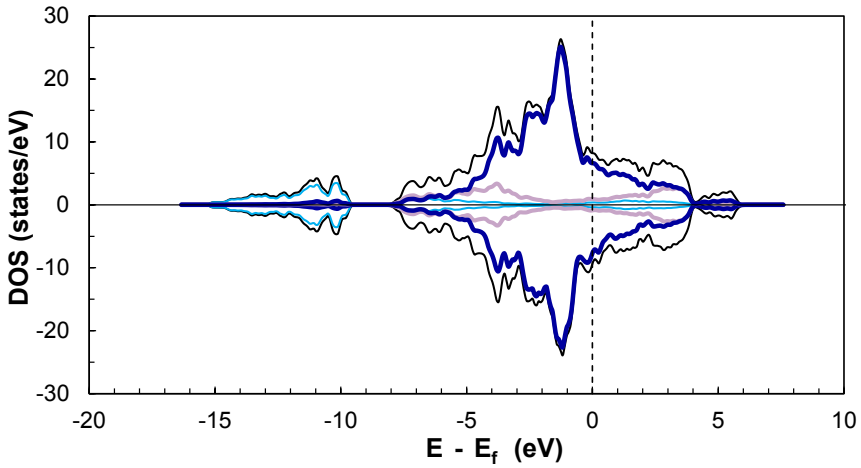

Figure S16. TDOS and PDOS for (100) surface before SO_2 adsorption. Total DOS as black lines, dark blue lines for cobalt d-orbitals, pink for phosphorous p-orbitals, and light blue for global s-orbitals. Fermi level indicated by black dashed line at 0 eV.

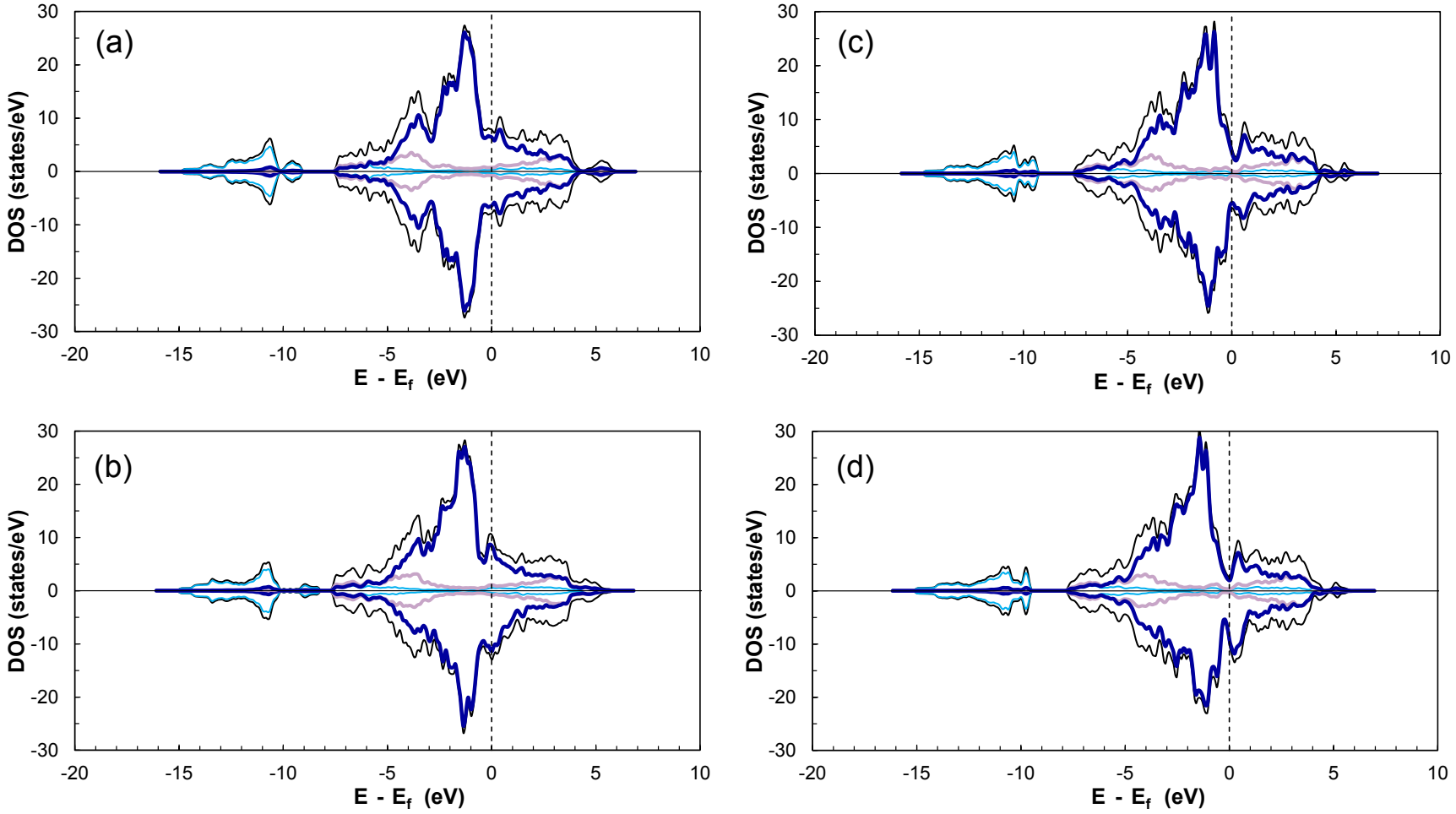

Figure S17. TDOS and PDOS for (a) (001)-Co, (b) (001)-P, (c) (010)-Co, and (d) (010)-P empty cleavages (without adsorbed SO_2). Total DOS as black lines, dark blue lines for cobalt d-orbitals, pink for phosphorous p-orbitals, and light blue for global s-orbitals. Fermi level indicated by black dashed line at 0 eV.

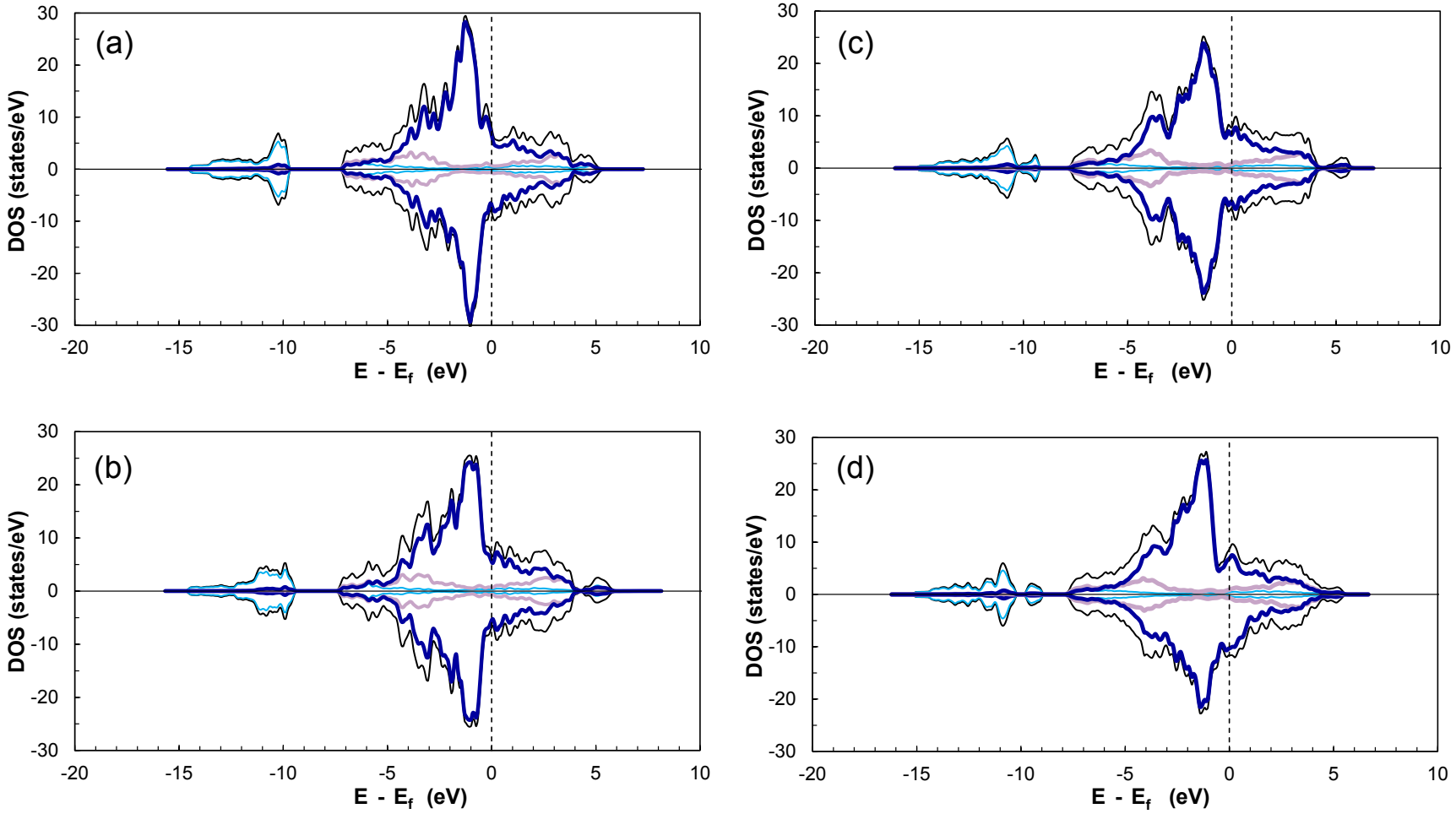

Figure S18. TDOS and PDOS for (a) (011)-Co, (b) (011)-P, (c) (101)-Co, and (d) (101)-P empty cleavages (without adsorbed SO_2). Total DOS as black lines, dark blue lines for cobalt d-orbitals, pink for phosphorous p-orbitals, and light blue for global s-orbitals. Fermi level indicated by black dashed line at 0 eV.

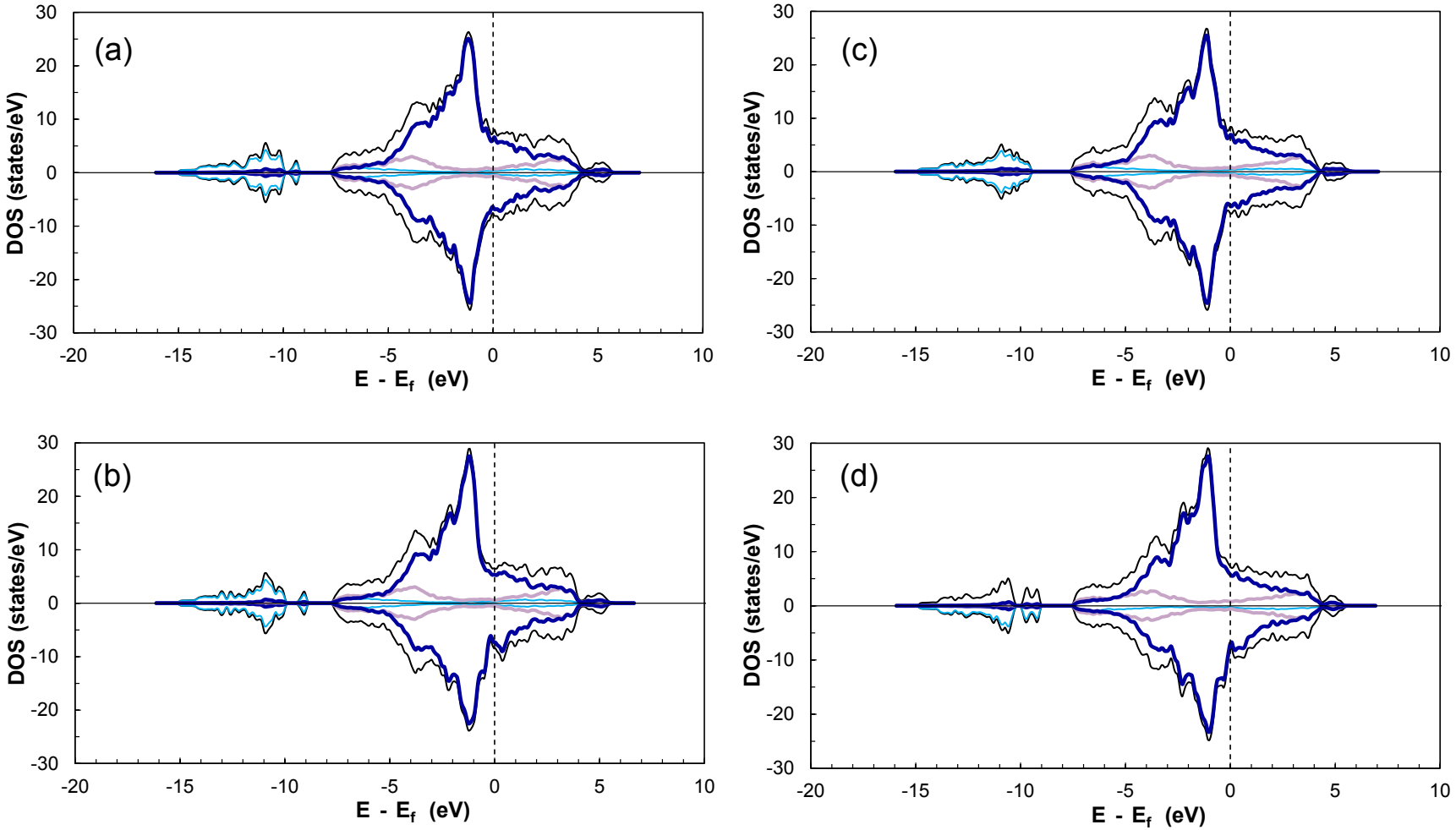

Figure S19. TDOS and PDOS for (a) (110)-Co, (b) (110)-P, (c) (111)-Co, and (d) (111)-P empty cleavages (without adsorbed SO_2). Total DOS as black lines, dark blue lines for cobalt d-orbitals, pink for phosphorous p-orbitals, and light blue for global s-orbitals. Fermi level indicated by black dashed line at 0 eV.

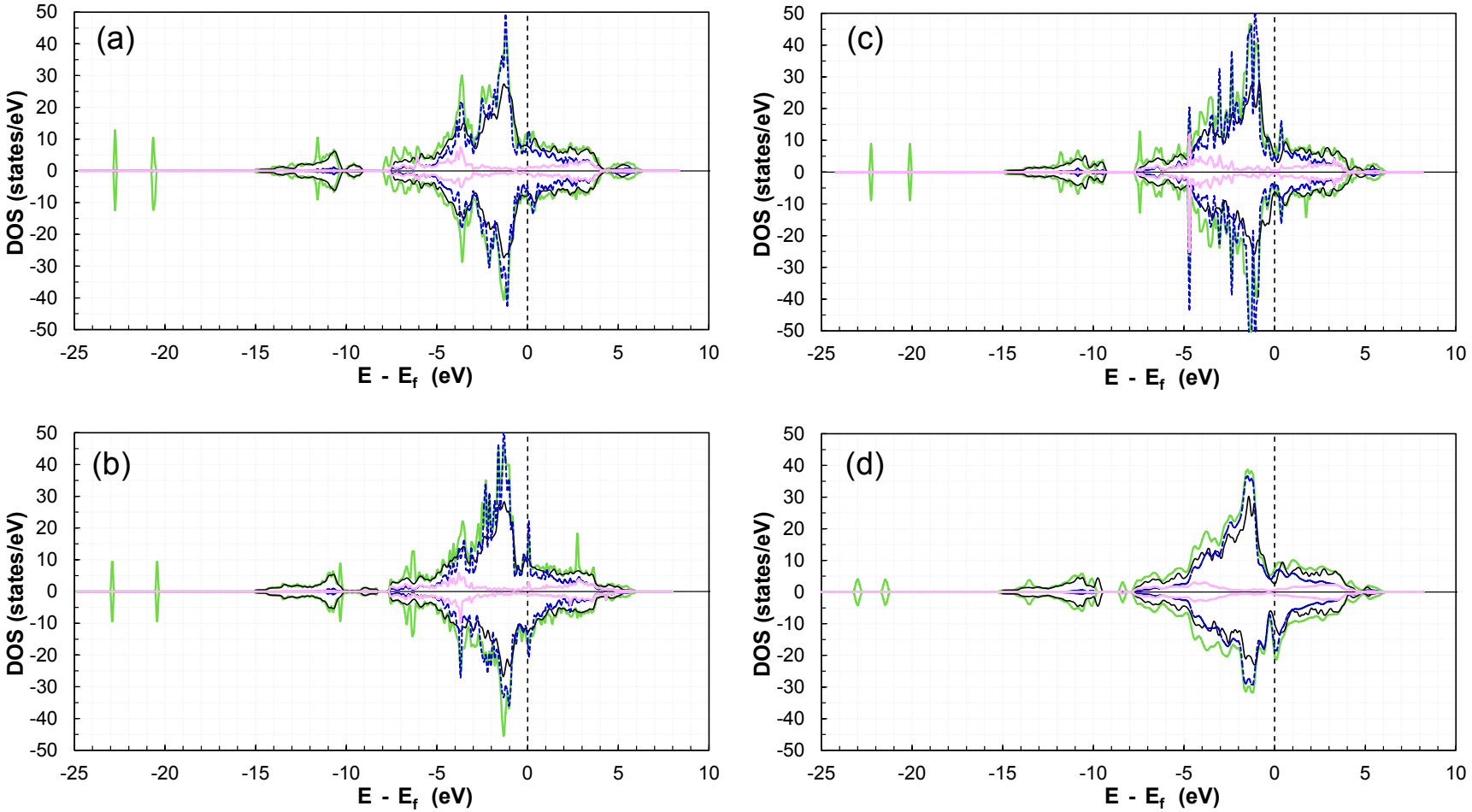

Figure S20. TDOS and PDOS for (a) (001)-Co, (b) (001)-P, (c) (010)-Co, and (d) (010)-P before and after SO_2 adsorption. Total DOS before adsorption as black lines, green lines for TDOS after adsorption, dark blue dashed lines for cobalt d-orbitals, and pink lines for phosphorous p-orbitals (both after adsorption). Fermi level indicated by black dashed line at 0 eV.

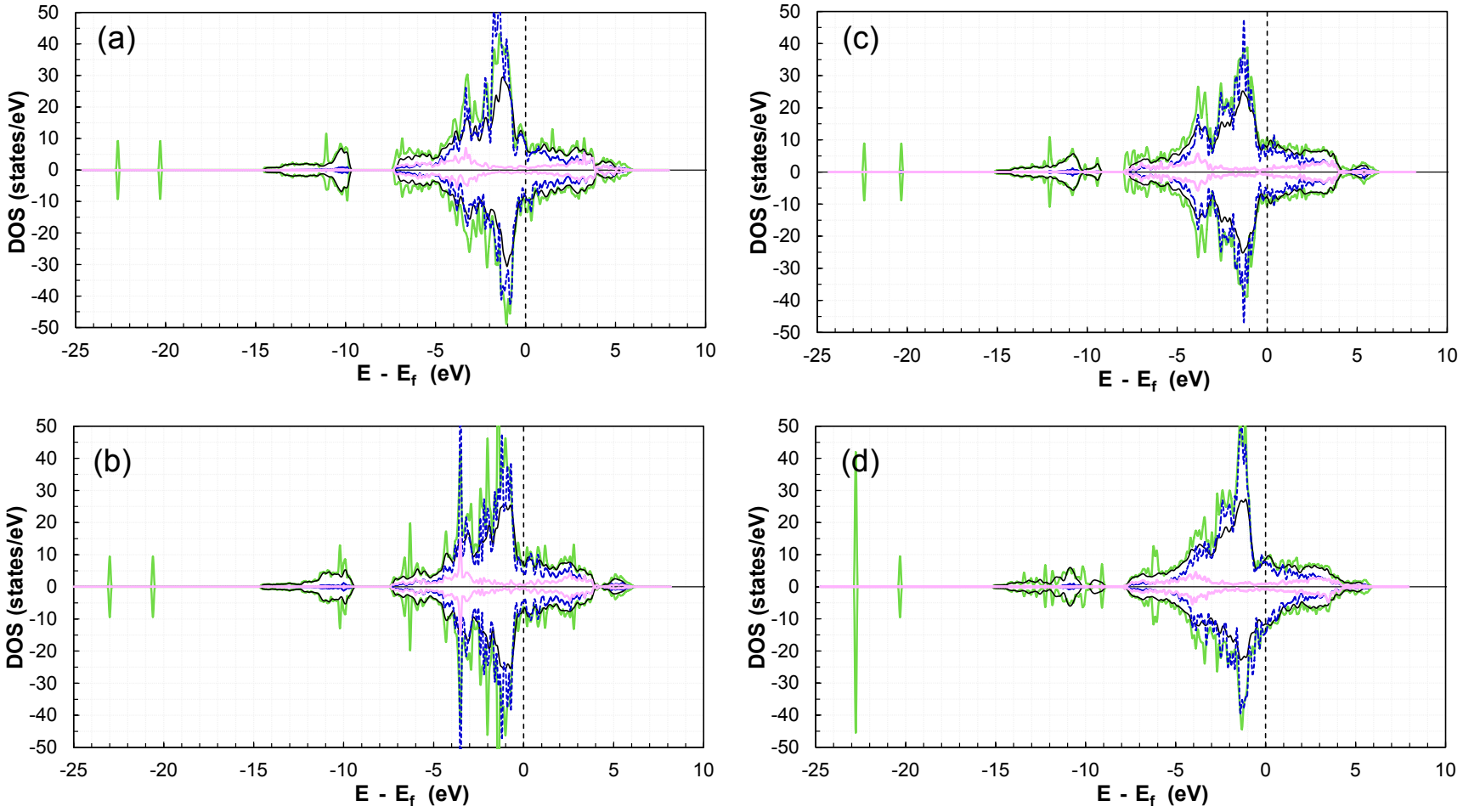

Figure S21. TDOS and PDOS for (a) (011)-Co, (b) (011)-P, (c) (101)-Co, and (d) (101)-P before and after SO_2 adsorption. Total DOS before adsorption as black lines, green lines for TDOS after adsorption, dark blue dashed lines for cobalt d-orbitals, and pink lines for phosphorous p-orbitals (both after adsorption). Fermi level indicated by black dashed line at 0 eV.

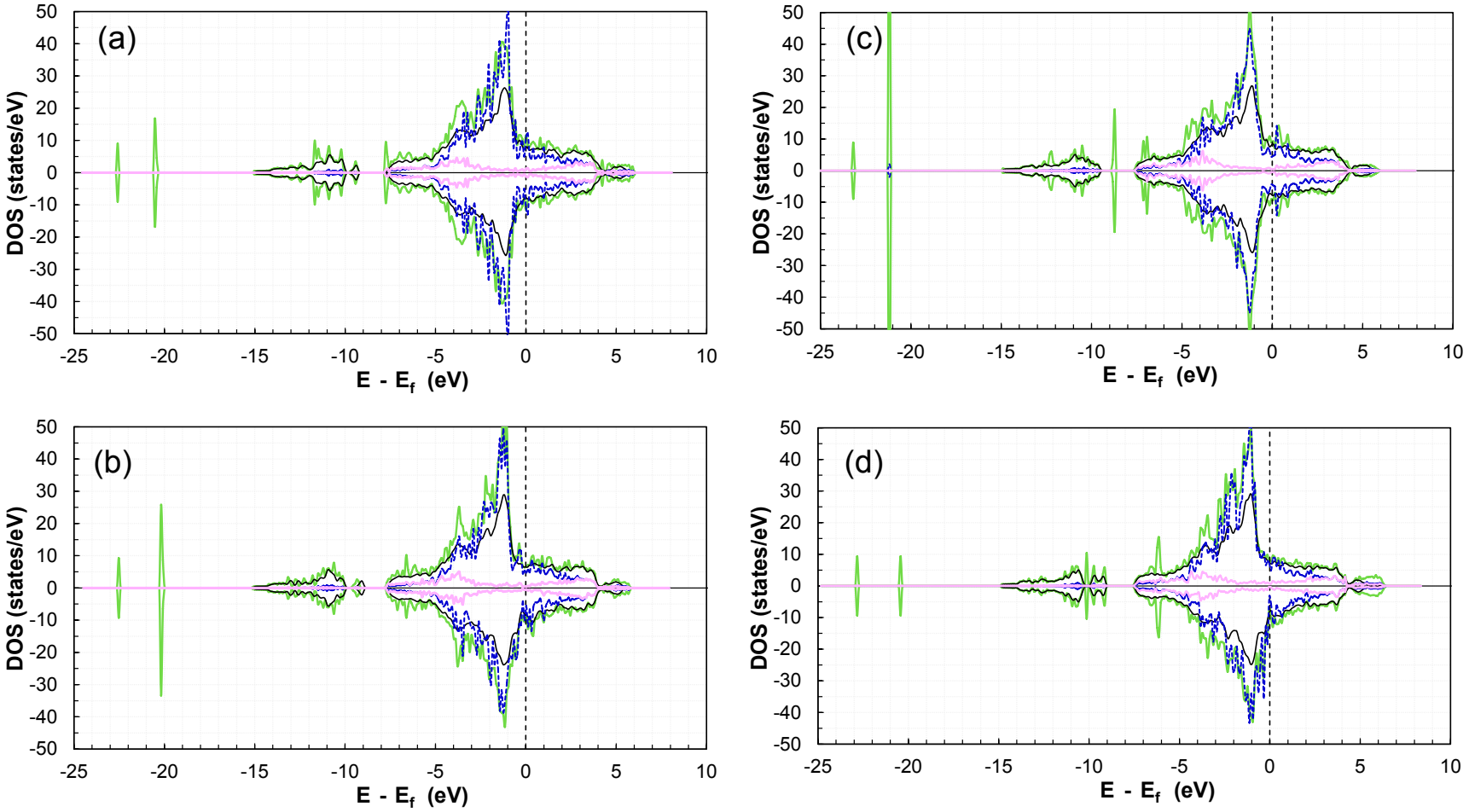

Figure S22. TDOS and PDOS for (a) (110)-Co, (b) (110)-P, (c) (111)-Co, and (d) (111)-P before and after SO_2 adsorption. Total DOS before adsorption as black lines, green lines for TDOS after adsorption, dark blue dashed lines for cobalt d-orbitals, and pink lines for phosphorous p-orbitals (both after adsorption). Fermi level indicated by black dashed line at 0 eV.

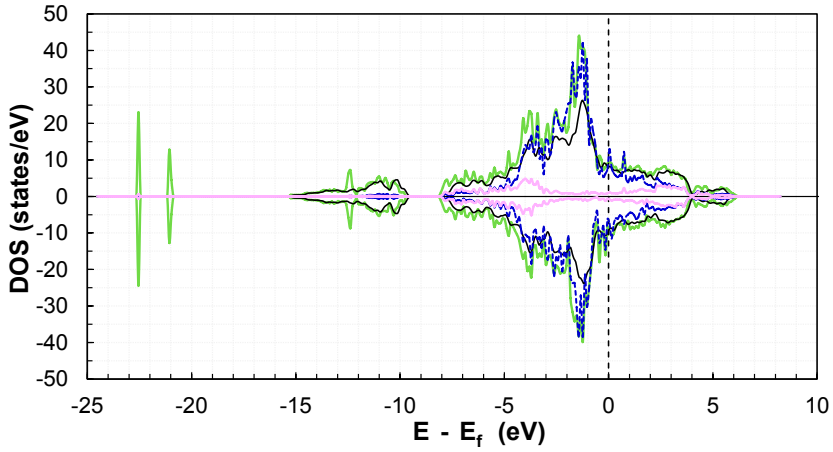

Figure S23. TDOS and PDOS for (100) surface before and after SO_2 adsorption. Total DOS before adsorption as black lines, green lines for TDOS after adsorption, dark blue dashed lines for cobalt d-orbitals, and pink lines for phosphorous p-orbitals (both after adsorption). Fermi level indicated by black dashed line at 0 eV.

Table S10. Calculated values of zero-point energy and thermochemical contributions (enthalpy and Gibbs free energy) obtained at 298 K and 0.03 atm for studied CoP surfaces.

	(001)-Co	**(001)-P**	**(010)-Co**	**(010)-P**	**(011)-Co**	**(011)-P**	**(100)**	**(101)-Co**	**(101)-P**	**(110)-Co**	**(110)-P**	**(111)-Co**	**(111)-P**
E_{ZPE} (kJ/mol)	19.67	19.54	22.05	19.72	17.99	18.41	19.97	21.72	19.81	22.79	20.51	21.23	19.11
Thermal correction to $U_{(T)}$ (kJ/mol) *	30.19	32.30	30.85	30.25	29.32	30.00	30.44	30.39	32.44	32.64	32.20	31.88	33.31
Thermal correction to $G_{(T)}$ (kJ/mol) **	9.31	1.95	14.75	9.55	5.95	1.83	9.77	15.36	2.55	14.10	7.89	10.64	-2.27

* Thermal correction to $U_{(T)} = H(T) = E_{ZPE} + \Delta U_{(0\rightarrow T)}$
** Thermal correction to $G_{(T)} = E_{ZPE} + \Delta U_{(0\rightarrow T)} + TS$