Supporting Information

Al atom on MoO_3(010) surface: adsorption and penetration using density functional theory

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The optimized structure parameters of Al atom at H site on MoO_3(010)

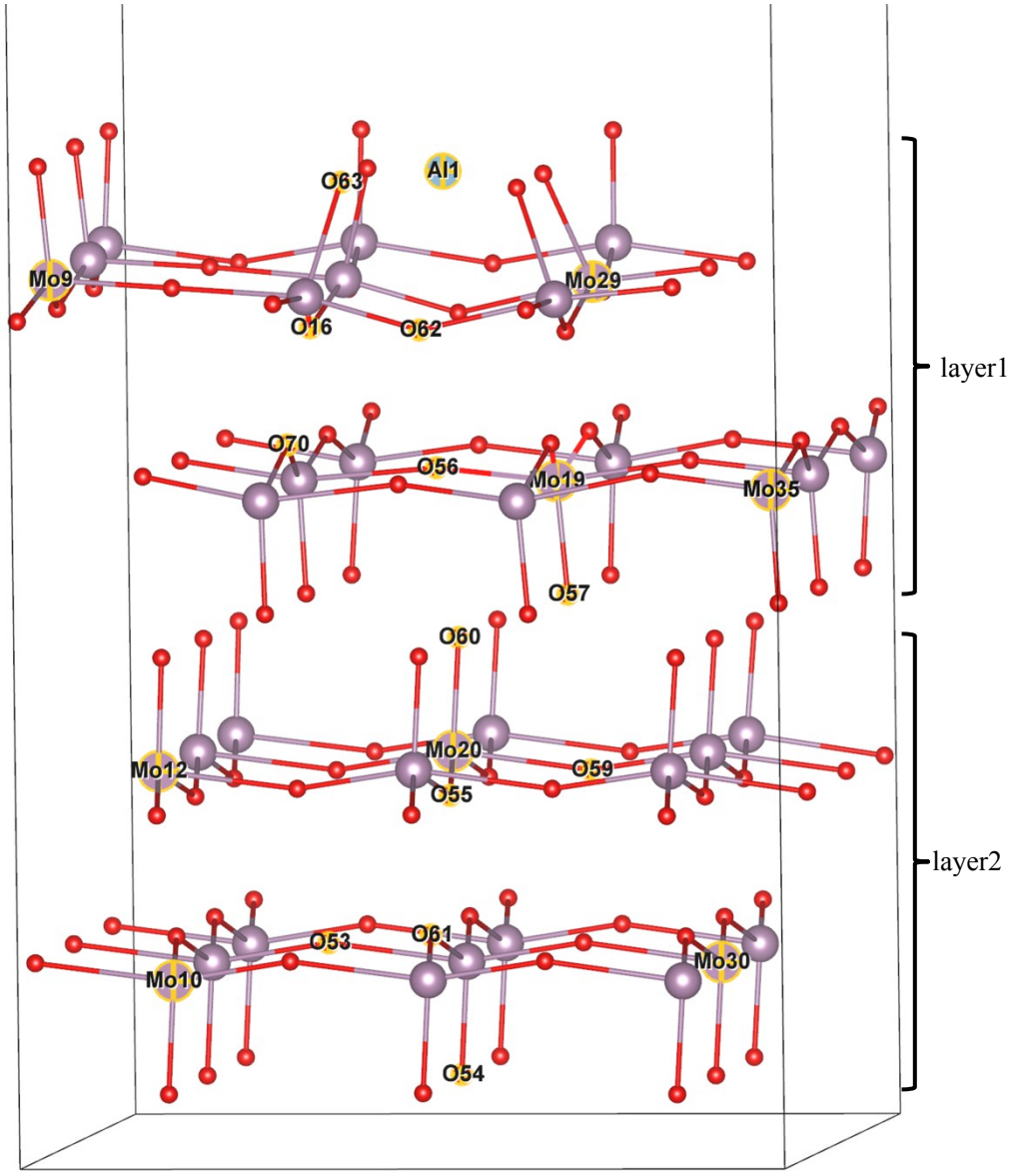
Lattice parameters of Al atom at H site on MoO_3(010)

a	b	c	alpha	beta	gamma
11.17288	11.52252	33.06249	90.0000	90.0000	90.0000

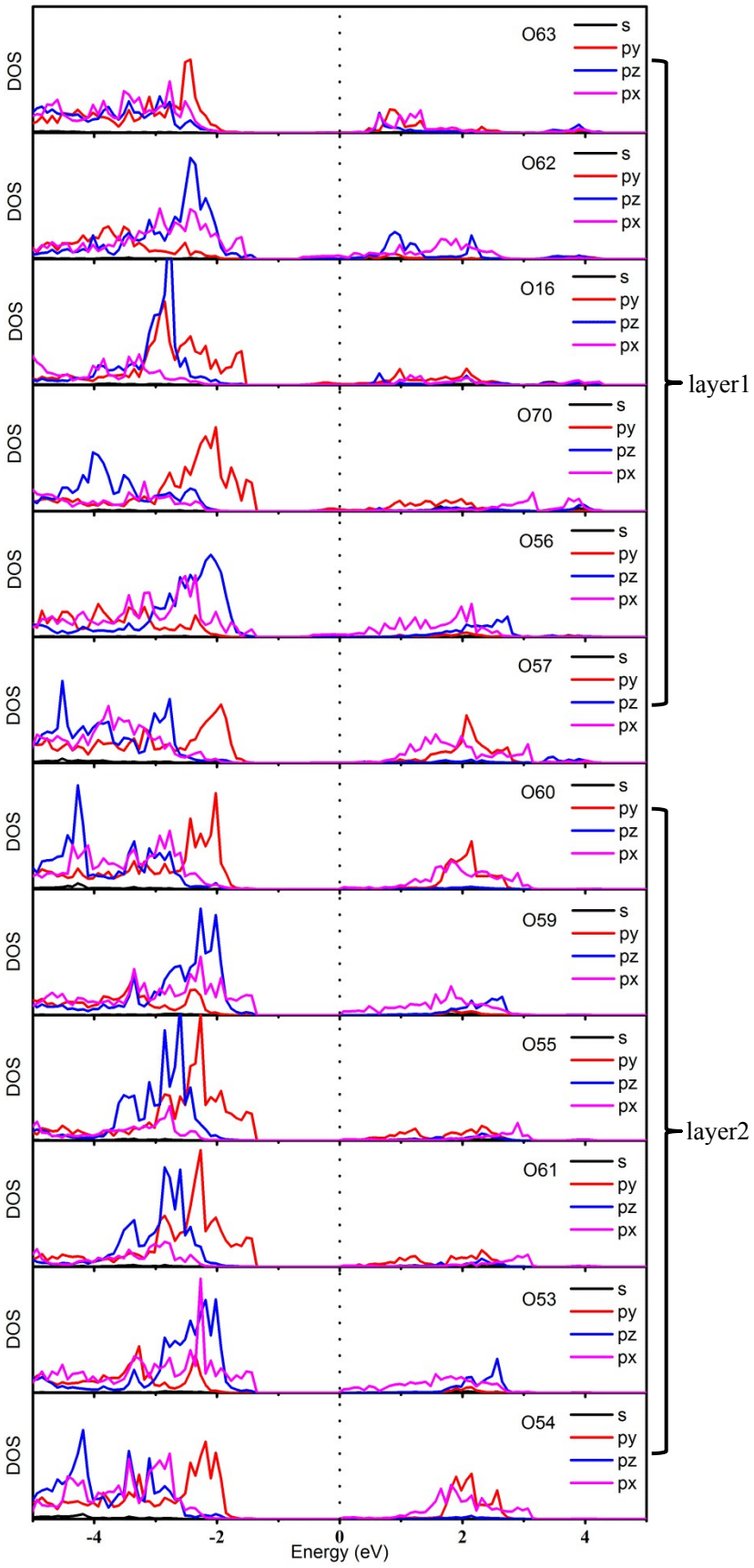
	x	y	z
O1	0.08333	0.17050	0.09890
O2	0.08369	0.16119	0.38683
O3	0.08531	0.99322	0.44611
O4	0.25456	0.33022	0.37909
O5	0.25001	0.01061	0.09127
O6	0.25086	0.18311	0.03194
O7	0.25000	0.17197	0.15785
O8	0.24594	0.16530	0.31133
O9	0.24582	0.32836	0.24976
O10	0.08122	0.99406	0.32142
O11	0.08336	0.33094	0.16585
O12	0.08325	0.15503	0.22475
O13	0.41667	0.17000	0.09939
O14	0.41940	0.17419	0.39316
O15	0.41716	0.99944	0.44730
O16	0.58145	0.32907	0.36966
O17	0.58328	0.01053	0.09134
O18	0.58260	0.18303	0.03193
O19	0.58328	0.17183	0.15802
O20	0.58521	0.15778	0.30981
O21	0.58813	0.32059	0.24984
O22	0.41661	0.99565	0.32085
O23	0.41663	0.33159	0.16575
O24	0.41607	0.15943	0.22510
O25	0.74983	0.17016	0.09900

O26	0.74525	0.17357	0.39181
O27	0.74372	1.00000	0.44655
O28	0.91361	0.33110	0.38869
O29	0.91667	0.01058	0.09107
O30	0.91623	0.18311	0.03177
O31	0.91660	0.17163	0.15777
O32	0.91726	0.15891	0.31089
O33	0.91858	0.31671	0.24874
O34	0.74964	0.99473	0.32281
O35	0.75009	0.33046	0.16565
O36	0.75059	0.15492	0.22485
O37	0.08351	0.50328	0.09963
O38	0.08489	0.49339	0.38633
O39	0.09975	0.32560	0.44728
O40	0.25446	0.66237	0.37777
O41	0.25023	0.34406	0.09191
O42	0.25041	0.51584	0.03229
O43	0.25005	0.50538	0.15857
O44	0.24962	0.49734	0.30848
O45	0.24677	0.66701	0.24959
O46	0.07928	0.33145	0.31942
O47	0.08310	0.66467	0.16576
O48	0.08196	0.49323	0.22533
O49	0.41672	0.50345	0.09970
O50	0.41649	0.49791	0.37234
O51	0.46417	0.38856	0.43884
O52	0.58167	0.66314	0.36801
O53	0.58310	0.34395	0.09189
O54	0.58312	0.51584	0.03228
O55	0.58362	0.50504	0.15843
O56	0.58622	0.49278	0.30652
O57	0.58562	0.66238	0.24933
O58	0.41537	0.32480	0.31739
O59	0.41668	0.66456	0.16576
O60	0.41726	0.49310	0.22563
O61	0.75000	0.50309	0.09953
O62	0.75361	0.49823	0.37296
O63	0.69377	0.38837	0.43821
O64	0.91426	0.66220	0.38601
O65	0.91663	0.34390	0.09178
O66	0.91698	0.51569	0.03226
O67	0.91675	0.50489	0.15801
O68	0.91143	0.49195	0.30718
O69	0.91733	0.66041	0.24866
O70	0.75399	0.32359	0.32111
O71	0.75029	0.66399	0.16558
O72	0.75162	0.49187	0.22536
O73	0.08335	0.83625	0.09884
O74	0.08439	0.82534	0.38727
O75	0.09873	0.65484	0.44683
O76	0.25417	0.99702	0.37946
O77	0.25013	0.67728	0.09201
O78	0.25108	0.84801	0.03186
O79	0.25002	0.83868	0.15772
O80	0.24621	0.82905	0.31084
O81	0.24933	0.99767	0.25295
O82	0.07976	0.65856	0.31871
O83	0.08326	0.99772	0.16380
O84	0.08250	0.83000	0.22452
O85	0.41666	0.83657	0.09933
O86	0.42058	0.82720	0.39272
O87	0.46348	0.61838	0.43627
O88	0.58084	0.99833	0.37828
O89	0.58331	0.67722	0.09201
O90	0.58217	0.84810	0.03185
O91	0.58326	0.83837	0.15792
O92	0.58499	0.82466	0.30991

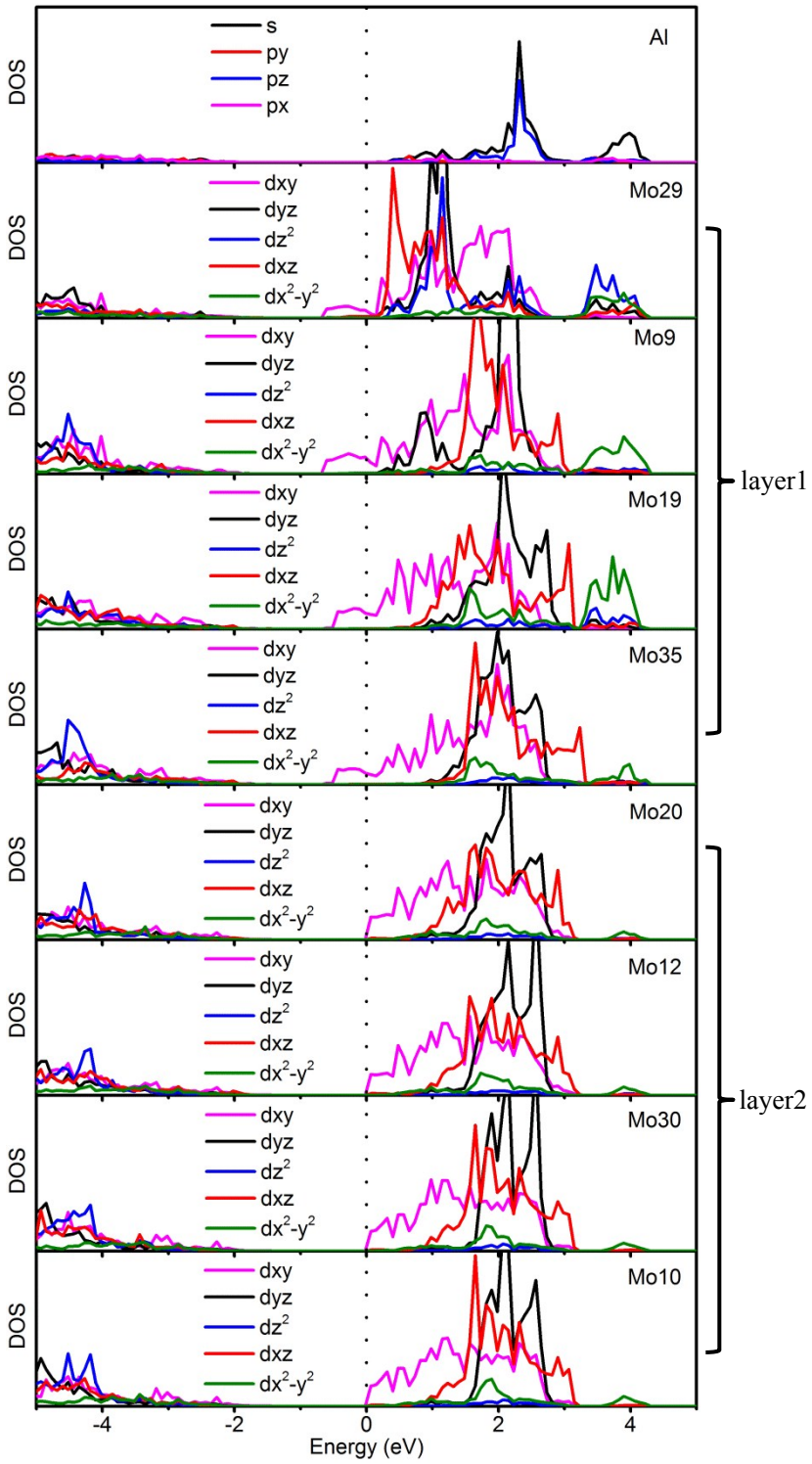
O93	0.58328	0.99062	0.25243
O94	0.41579	0.66727	0.31889
O95	0.41667	0.99803	0.16527
O96	0.41580	0.82787	0.22501
O97	0.74984	0.83628	0.09882
O98	0.74396	0.82756	0.39194
O99	0.69530	0.61882	0.43574
O100	0.91253	0.99603	0.38080
O101	0.91662	0.67722	0.09184
O102	0.91656	0.84796	0.03168
O103	0.91648	0.83867	0.15739
O104	0.91640	0.82240	0.31203
O105	0.91464	0.98807	0.25346
O106	0.75342	0.66797	0.32168
O107	0.74989	0.99713	0.16418
O108	0.75097	0.82747	0.22471
Al1	0.58028	0.50507	0.44038
Mo1	0.08300	0.98573	0.39495
Mo2	0.25015	0.19097	0.08316
Mo3	0.24659	0.33810	0.30075
Mo4	0.08326	0.14983	0.17349
Mo5	0.41645	0.01536	0.39631
Mo6	0.58312	0.19087	0.08316
Mo7	0.58379	0.31249	0.30108
Mo8	0.41659	0.15071	0.17387
Mo9	0.74766	0.01480	0.39550
Mo10	0.91650	0.19088	0.08300
Mo11	0.91907	0.31310	0.29988
Mo12	0.75000	0.14933	0.17360
Mo13	0.08739	0.31937	0.39624
Mo14	0.25022	0.52413	0.08351
Mo15	0.24567	0.67221	0.30067
Mo16	0.08334	0.48382	0.17409
Mo17	0.42003	0.34846	0.38758
Mo18	0.58336	0.52408	0.08350
Mo19	0.58329	0.64908	0.30048
Mo20	0.41696	0.48427	0.17435
Mo21	0.74929	0.34842	0.38782
Mo22	0.91679	0.52406	0.08348
Mo23	0.91912	0.64849	0.29961
Mo24	0.75035	0.48317	0.17410
Mo25	0.08740	0.65216	0.39577
Mo26	0.25020	0.85733	0.08306
Mo27	0.24885	0.00621	0.30400
Mo28	0.08308	0.81784	0.17338
Mo29	0.42017	0.67461	0.38644
Mo30	0.58310	0.85727	0.08305
Mo31	0.58247	0.98102	0.30358
Mo32	0.41651	0.81763	0.17382
Mo33	0.74935	0.67426	0.38671
Mo34	0.91656	0.85727	0.08288
Mo35	0.91568	0.97975	0.30455
Mo36	0.75001	0.81697	0.17354



Supporting Figure S1. The optimized configuration of Al atom at H site of MoO_3(010) surface.



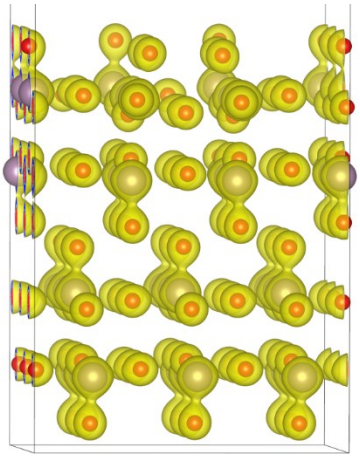
Supporting Figure S2. The PDOS of some oxygen atoms in the configuration of Al atom at H site of MoO_3(010) surface.



Supporting Figure S3. The PDOS of Al atom and some Mo atoms in the configuration of Al atom at H site of MoO_3(010) surface.

The charge density difference is that the charge density of Al/MoO_3 subtracts that of Al atom and MoO_3(010). Al atom has three valence electrons; Mo and O atom both have six valence electrons.

The charge density of Al atom is smaller than that of Mo and O atom. The isovalues of the charge density are represented with 0.25 a.u for pure MoO_3, while the isovalues of the charge density are represented with 0.018 a.u for Al/MoO_3(010).



Supporting Figure S4. Isosurface (isovalues: 0.25 a.u) of the charge density of pure MoO_3.