Electronic Supplementary Information (ESI)

Electrocatalytic performance of different cobalt molybdate structures for the water oxidation in alkaline media

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Crystallographic data for the α-$CoMoO_4$

Space group: C12/m1 or C2/m (#12)

Table S1. Lattice parameters for α-$CoMoO_4$.

Lattice	***a*/Å**	***b*/Å**	***c*/Å**	***α*/º**	***β*/º**	***γ*/º**
parameters	9.666(8)	8.854(8)	7.755(8)	90	113.82(20)	90

Table S2. Atomic positions for Co, Mo, and O in the α-$CoMoO_4$ structure.

Site label	**x**	**y**	**z**	**Occupancy**
Co_1	0.3108	0	0.1555	1
Co_2	0	0.3094	0.5000	1
Mo_1	0.2844	0	0.6391	1
Mo_2	0	0.2852	0	1
O_1	0.5035	0.1515	0.2395	1
O_2	0.1528	0.1656	0.0772	1
O_3	0.1642	0.1534	0.5815	1
O_4	0.3476	0	0.4376	1
O_5	0.3487	0	0.9156	1

Crystallographic data for the β-$CoMoO_4$

Space group: C12/m1 ou C2/m (#12)

Table S3. Lattice parameters for β-$CoMoO_4$.

Lattice	***a*/Å**	***b*/Å**	***c*/Å**	***α*/º**	***β*/º**	***γ*/º**
parameters	10.251(1)	9.294(1)	7.0452(9)	90	106.962(8)	90

Table S4. Atomic positions for Co, Mo, and O in the β-$CoMoO_4$ structure.

Site_label	**x**	**y**	**z**	**Occupancy**
Co_1	0.30066	0	0.14516	0.5
Co_2	0	0.32042	0.5	0.5
Mo_1	0.22885	0	0.5958	0.5
Mo_2	0	0.24749	0	0.5
O_1	0.45942	0.1576	0.20923	1
O_2	0.14132	0.13771	0.1122	1
O_3	0.13407	0.15539	0.53103	1
O_4	0.35476	0	0.45854	0.5
O_5	0.29853	0	0.85499	0.5

Crystallographic data for the H-$CoMoO_4$

Space group: P-1 (#2)

Table S5. Lattice parameters for H-$CoMoO_4$.

Lattice	***a*/Å**	***b*/Å**	***c*/Å**	***α*/º**	***β*/º**	***γ*/º**
parameters	6.844	6.933	9.339	76.617	84.188	74.51

Table S6. Atomic positions for Co, Mo, and O in the H-$CoMoO_4$ structure.

Site label	**x**	**y**	**z**	**Occupancy**
Co_1	0.1542	0.6464	0.6992	1
Co_2	0.1961	0.8287	0.9728	1
Mo_1	0.0059	0.1935	0.6845	1
Mo_2	0.2482	0.2943	0.0522	1
O_1	0.1446	0.9280	0.7475	1
O_2	0.1573	0.3643	0.6741	1
O_3	0.9176	0.2209	0.5124	1
O_4	0.7895	0.2633	0.8022	1
O_5	0.2056	0.5466	0.9299	1
O_6	0.1285	0.1367	0.9836	1
O_7	0.1590	0.3092	0.2306	1
O_8	0.5049	0.1893	0.0581	1
O_9	0.4686	0.5953	0.6313	1
O_{10}	0.5430	0.9860	0.5430	0.5

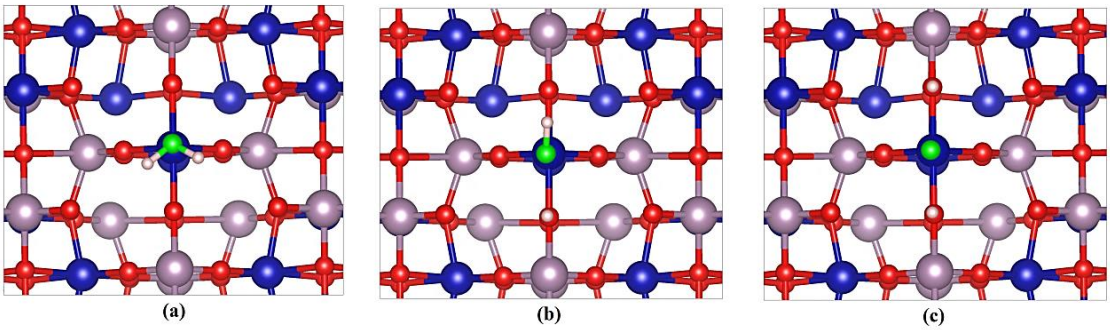

Figure S1. Representation of the water dissociation mechanism at the Co site on the (110) surface of the α-$CoMoO_4$ catalyst. (a) intermediate I_1, (b) I_2, and (c) I_3. Atoms: red = surface oxygens, blue = cobalt, gray = molybdenum, green = oxygen of the water molecule, and white = hydrogen.

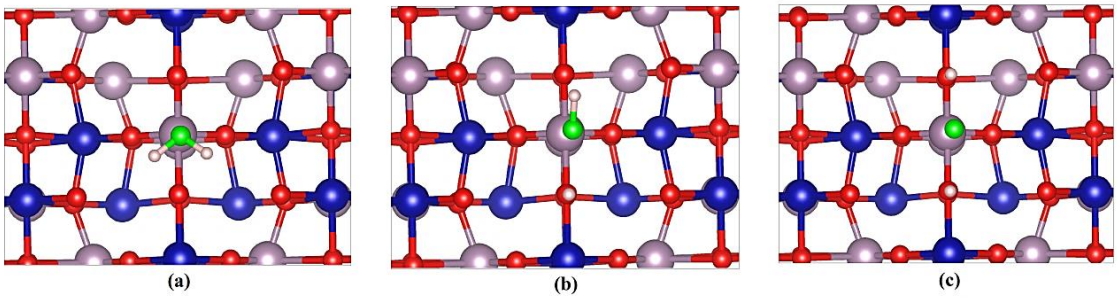

Figure S2. Representation of the water dissociation mechanism at the Mo site on the (110) surface of the α-$CoMoO_4$ catalyst. (a) intermediate I_1, (b) I_2, and (c) I_3. Atoms: red = surface oxygens, blue = cobalt, gray = molybdenum, green = oxygen of the water molecule, and white = hydrogen.

Table S7. Adsorption energy (E_{ads}) and energy changes involved in the steps of water dissociation (ΔE_1 and ΔE_2) on $CoMoO_4$.

Site	E_{ads} (eV)	ΔE_1 (eV)	ΔE_2 (eV)
Co-site	–0.69	+0.22	+0.25
Mo-site	–0.63	+0.24	+0.28