

Supplementary Material

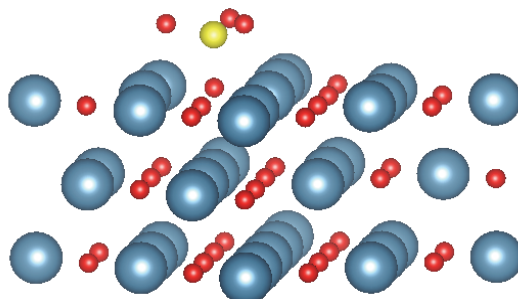


Figure S1. Side view of bonding geometry on CaO surface in electrostatic field of 0.5 eV/Å; S in light yellow, O in red, Ca in blue.

Table S1 Effect of positive electric field on adsorption energies and structural parameters for SO₃ adsorption on CaO surface

Electrostatic field V/Å	E_{ads} kJ/mol	$d_{\text{S-O}_{\text{CaO}}}$ /Å	$d_{\text{S-O}_{\text{SO}_3}}$ /Å	bond angles of O _{SO₃} -S-O _{SO₃} /°	bond angles of O _{CaO} -S-O _{SO₃} /°
0	-321.9	1.60	1.47	113.65	104.32
0.005	-318.4	1.60	1.47	113.75	104.20
0.01	-318.8	1.60	1.47	113.75	104.20
0.02	-319.5	1.60	1.47	113.71	104.24
0.03	-320.3	1.60	1.47	113.71	104.24
0.04	-321.0	1.60	1.47	113.71	104.24
0.05	-321.7	1.60	1.47	113.71	104.24
0.06	-322.5	1.60	1.47	113.68	104.28
0.08	-323.9	1.60	1.47	113.68	104.28
0.10	-325.5	1.60	1.47	113.65	104.31
0.15	-329.3	1.60	1.47	113.62	104.35
0.20	-333.1	1.60	1.47	113.54	104.42
0.25	-337.1	1.60	1.47	113.46	104.47
0.30	-341.0	1.60	1.47	113.41	104.52
0.35	-345.1	1.60	1.47	113.54	104.56
0.40	-349.2	1.59	1.47	113.51	104.62
0.45	-353.3	1.59	1.47	113.46	104.67
0.50	-357.6	1.59	1.47	113.59	104.71

Table S2 Effect of negative electric field on adsorption energies and structural parameters for SO₃ adsorption on CaO surface

Electrostatic field V/Å	E_{ads} kJ/mol	$d\text{S-O}_{\text{CaO}}$ /Å	$d\text{S-O}_{\text{SO}_3}$ /Å	bond angles of $\text{O}_{\text{SO}_3}\text{-S-O}_{\text{SO}_3}$ /°	bond angles of $\text{O}_{\text{CaO}}\text{-S-O}_{\text{SO}_3}$ /°
-0.005	-321.9	1.60	1.47	113.74	104.21
-0.01	-317.6	1.60	1.47	113.74	104.21
-0.02	-317.3	1.60	1.47	113.76	104.19
-0.03	-316.6	1.60	1.47	113.76	104.19
-0.04	-315.8	1.60	1.47	113.77	104.18
-0.05	-315.1	1.60	1.47	113.79	104.15
-0.06	-314.4	1.60	1.47	113.79	104.15
-0.08	-313.6	1.61	1.47	113.80	104.13
-0.10	-312.2	1.61	1.47	113.83	104.11
-0.15	-310.8	1.61	1.47	113.87	104.06
-0.20	-307.2	1.61	1.47	113.95	104.00
-0.25	-303.7	1.61	1.47	113.99	103.96
-0.30	-300.3	1.61	1.47	114.03	103.93
-0.35	-296.9	1.61	1.47	114.13	103.85
-0.40	-293.6	1.61	1.47	114.16	103.82
-0.45	-290.3	1.61	1.47	114.22	103.76
-0.50	-287.0	1.61	1.47	114.25	103.73

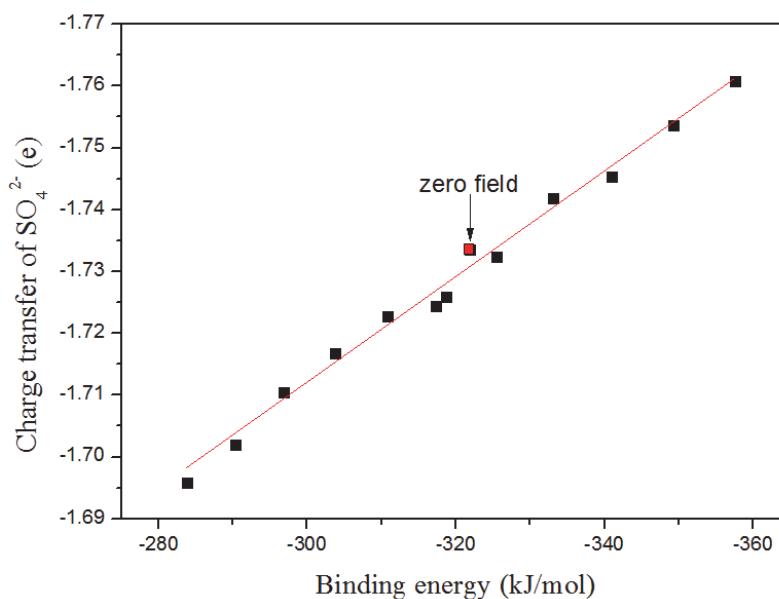


Fig. S2. The variation of charge transfer with respect to the binding energy.

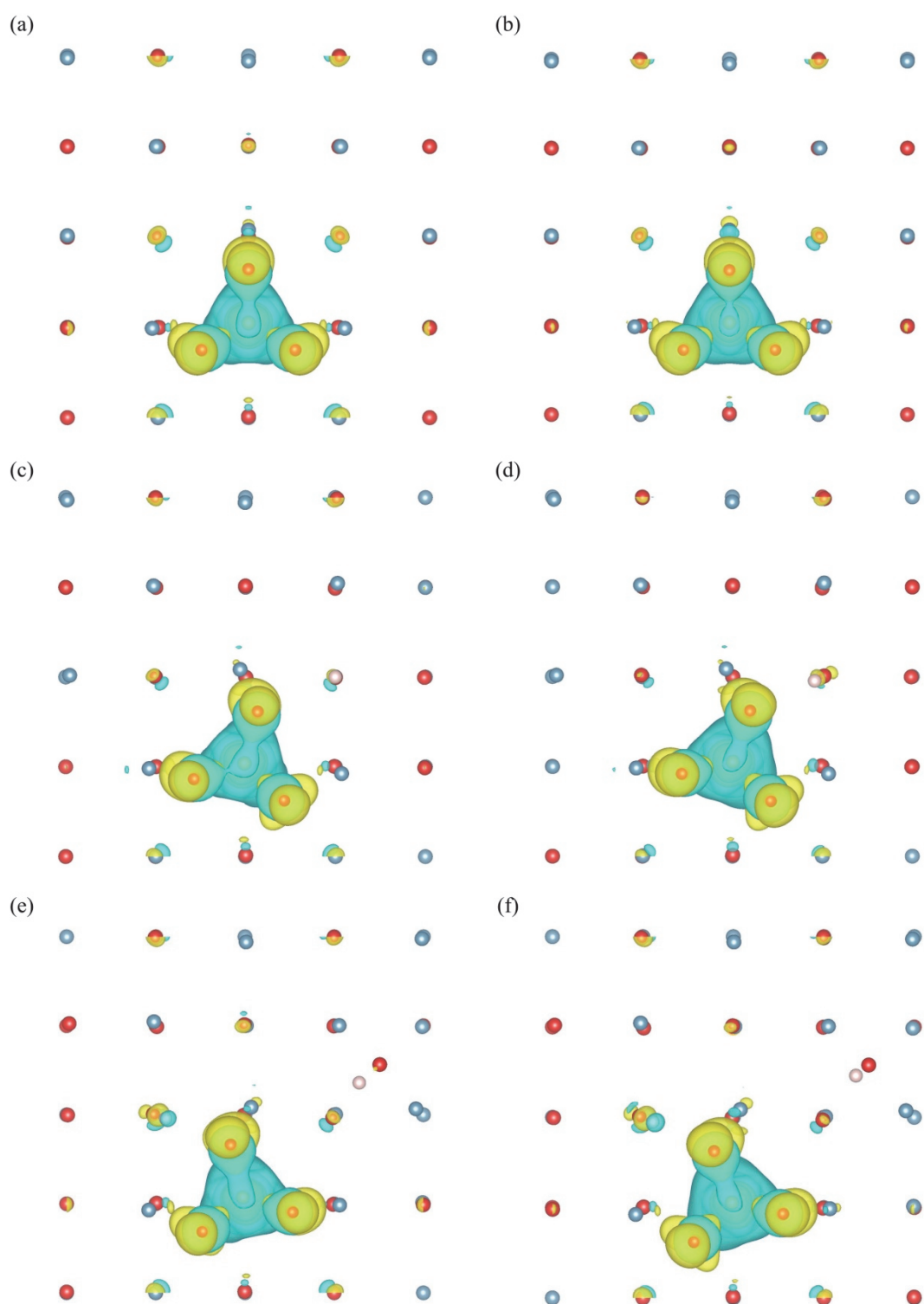


Fig. S3. Top view of the CDD plot at an electric field of 0.5 V/\AA corresponding to Fig.8. (a) and (b) clean CaO, (c) and (d) $-H$, (e) and (f) $-H&OH$; (a), (c) and (e) is in a positive field; (b), (d) and (f) is in a negative field; charge accumulation is in yellow and charge depletion is in blue.

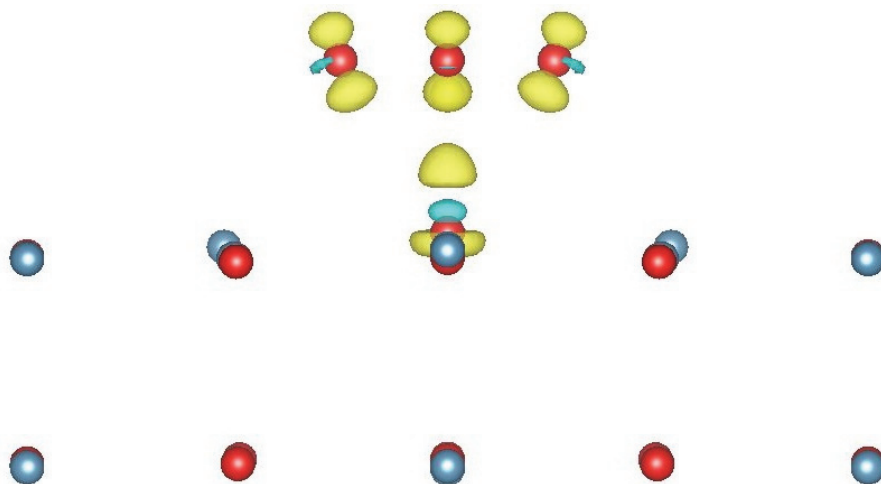


Fig. S4. CDD plot of SO₃ bound on the CaO(100) surface with an electric field of 0.5 V/Å in a positive field; charge accumulation is in yellow and charge depletion is in blue.