Ab Initio Investigation of Tunable CO_2 Reduction Reactions on the Two Dimensional Ferroelectric Y_2CO_2

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Supplementary Information

CO_2	Isolated	Poled up	Poled down
C	2.040	0.990	0.943
O1	-1.009	-1.177	-1.205
O2	-1.004	-1.164	-1.220
Total	0.027	-1.350	-1.483

Table S1. Charge transfer (eV) to CO_2 adsorbed on an O_V on poled up and poled down Y_2CO_2.

CO	Isolated	Poled up	Poled down
C	1.141	-0.072	-0.090
O	-1.115	-1.180	-1.189
Total	0.026	-1.251	-1.279

Table S2. Charge transfer (eV) to CO adsorbed on an O_V on poled up and poled down Y_2CO_2.

CH_3OH	Isolated	Poled up	Poled down
C	0.4569	0.3872	0.2679
O	-1.1125	-1.1719	-1.1944
H	0.0251	0.0482	0.0707
H	0.0298	0.0583	0.0805
H	0.0579	0.0679	0.1381
H	0.5759	0.6178	0.5787
Total	0.0332	0.0074	-0.0586

Table S3. Charge transfer (eV) to CH_3OH adsorbed on an O_V on poled up and poled down Y_2CO_2.

CH_4	Isolated	Poled up	Poled down
C	-0.135	-0.170	-0.181
H	0.029	0.046	0.074
H	0.036	0.044	0.074
H	0.040	0.052	-0.091
H	0.060	-0.007	0.082
Total	0.029	-0.036	-0.043

Table S4. Charge transfer (eV) to CH_4 adsorbed on an O_V on poled up and poled down Y_2CO_2.

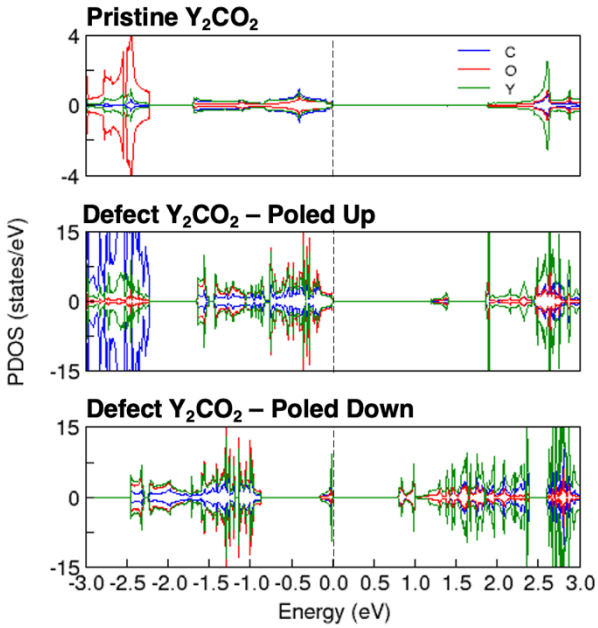

Figure S1. Projected density of states (PDOS) for pristine Y_2CO_2, poled up O-defect Y_2CO_2 and poled down O-defect Y_2CO_2.

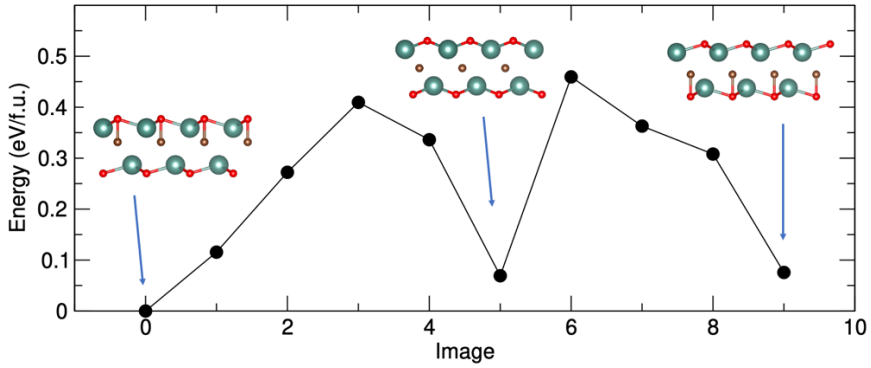

Figure S2. Nudged elastic band calculation of switching barrier between poled up and poled down O_V defected Y_2CO_2 surface.

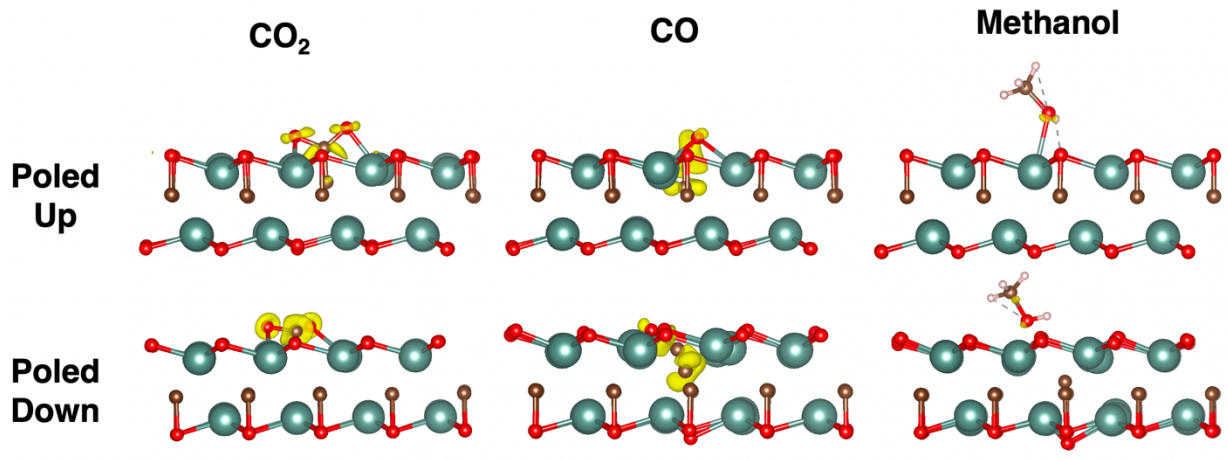

Figure S3. Charge densities for adsorbed CO_2, CO, and methanol.

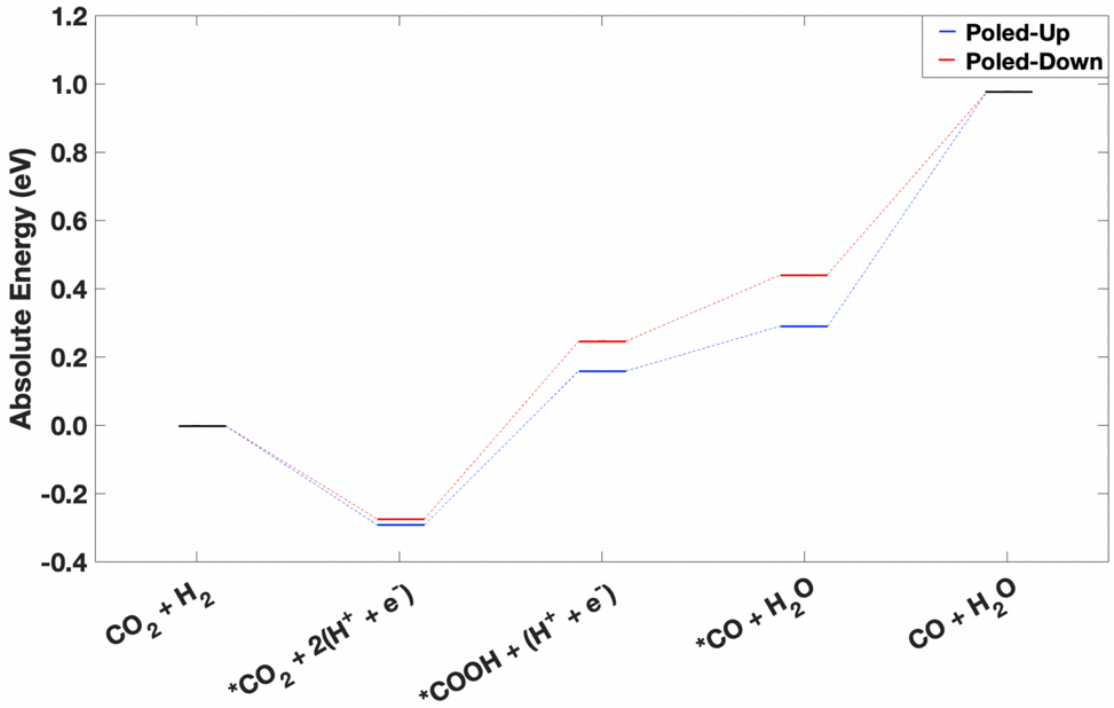

Figure S4. Reaction-energy diagram for CO_2 to CO reaction on a pristine Y_2CO_2 surface.

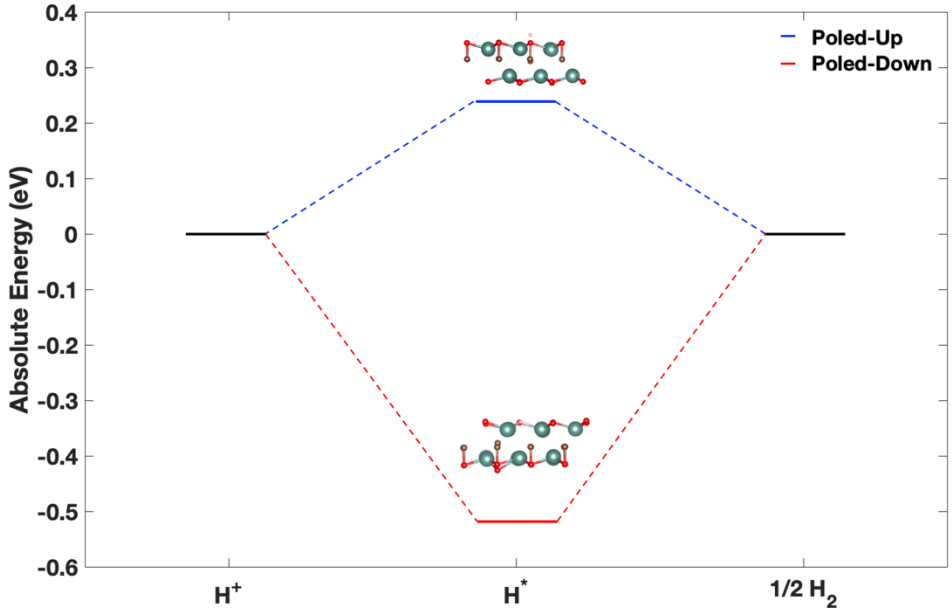

Figure S5. Energy diagram for hydrogen evolution reaction (HER) on a defect Y_2CO_2 surface.

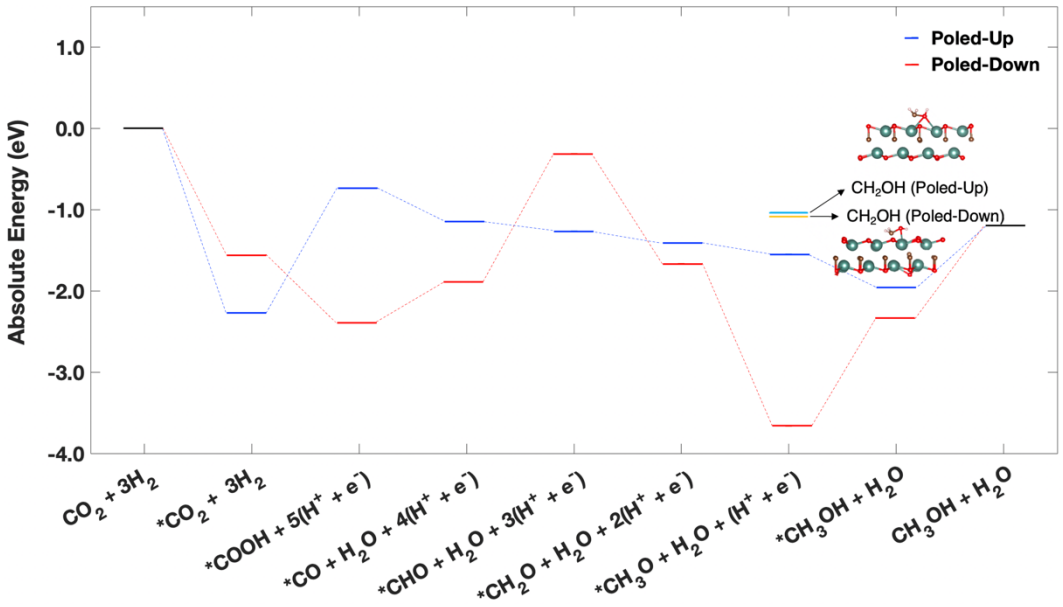

Figure S6. Energy diagram for methanol formation process. The energies of CH_2OH as an alternative to CH_3O on poled up and poled down O-defect Y_2CO_2 are labelled with green and yellow lines.

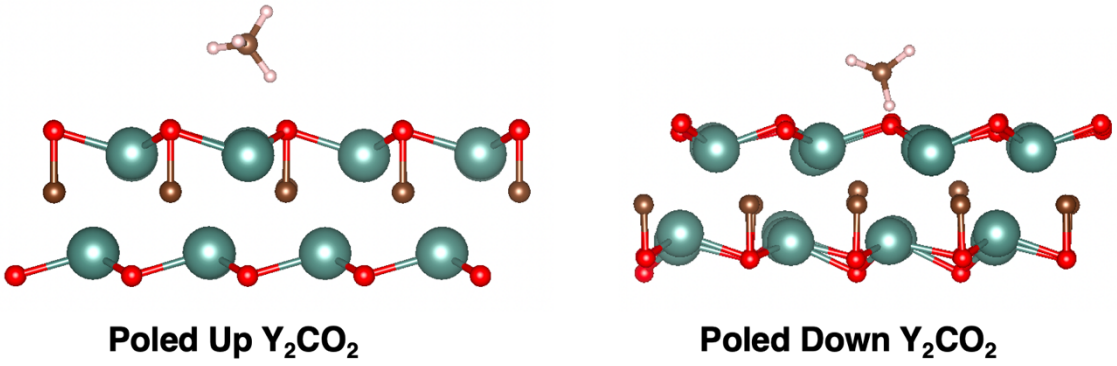

Figure S7. Optimized geometries of CH_4 adsorbed at the poled up and poled down Y_2CO_2 oxygen defect site.