Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supporting Information for

"Elucidating the Role of Oxygen Coverage in CO_2 Reduction on Mo_2C"

Mudit Dixit[1,‡], Xi Peng[1,‡], Marc D. Porosoff[2], Heather D. Willauer[3] and Giannis Mpourmpakis[1,*]

[1]Department of Chemical Engineering, University of Pittsburgh, Pittsburgh, PA 15261, USA
[2]Department of Chemical Engineering, University of Rochester, Rochester, NY 14627, USA
[3]Materials Science and Technology Division, Naval Research Laboratory, Washington DC, USA

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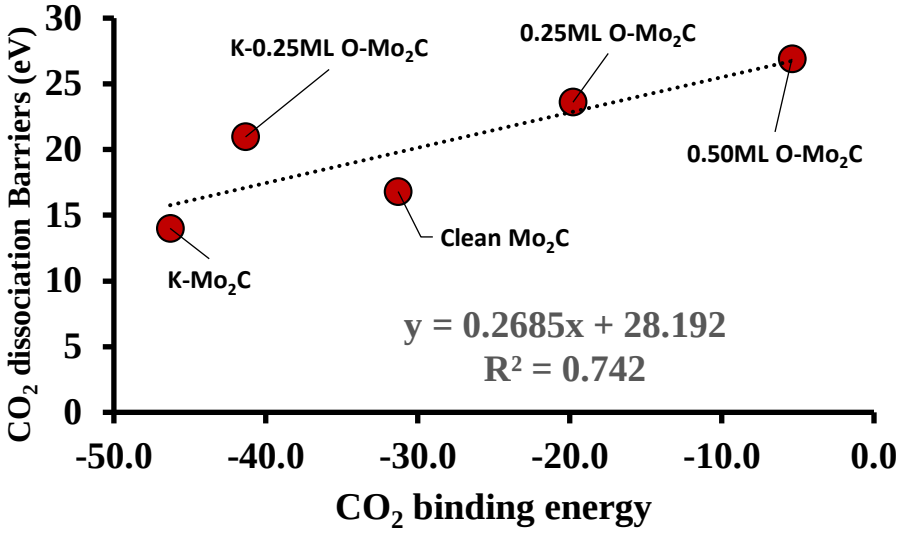

Figure S1. CO_2 dissociation barriers vs. CO_2 binding energy on clean, oxygen covered and K-promoted Mo_2C surfaces.

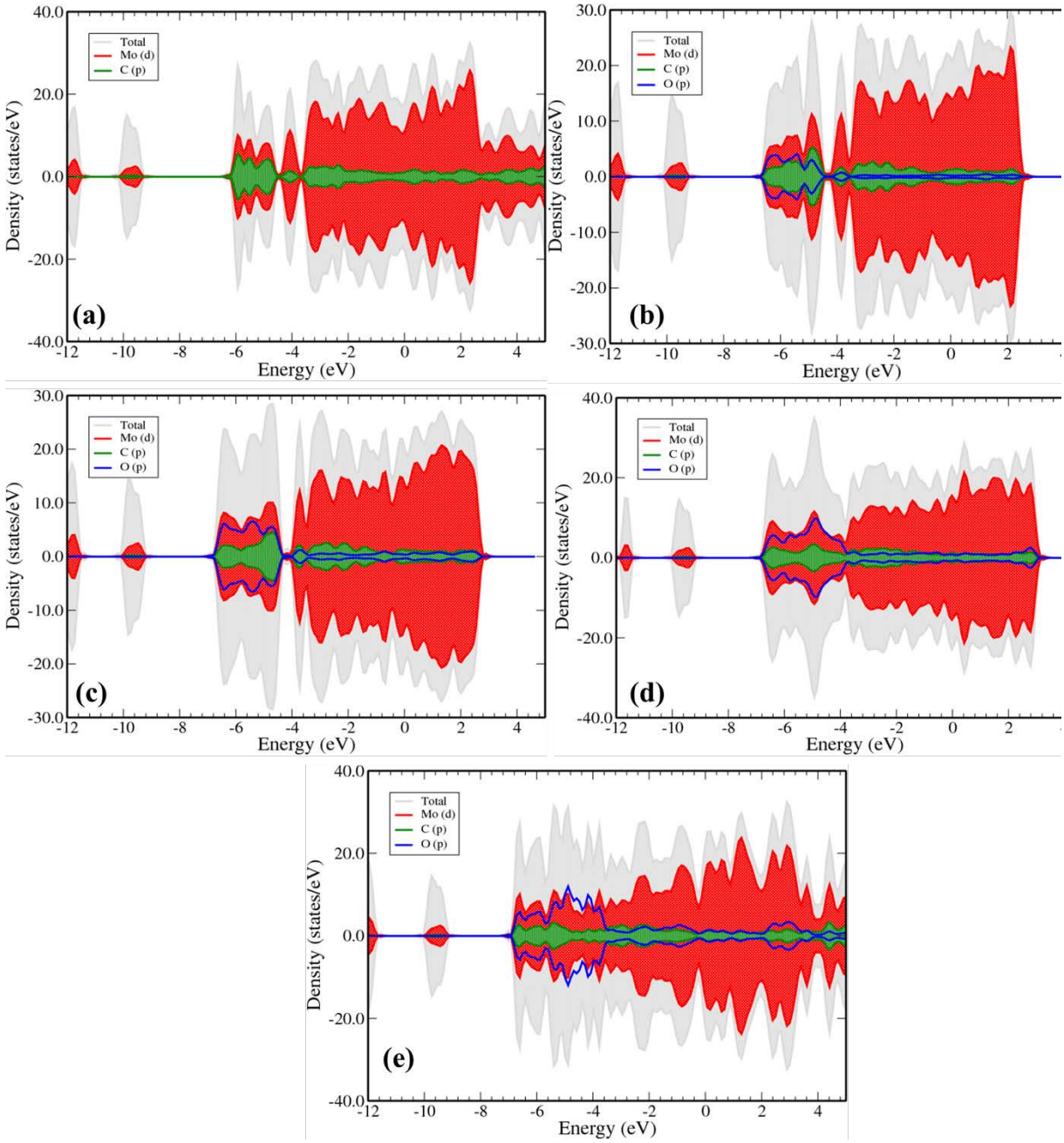

Figure S2. Density of States (DOS) of (a) Clean Mo_2C, Mo_2C with the oxygen coverage of (b) 0.25 ML, (c) 0.50 ML, (d) 0.75 ML, (e) 1.0 ML.

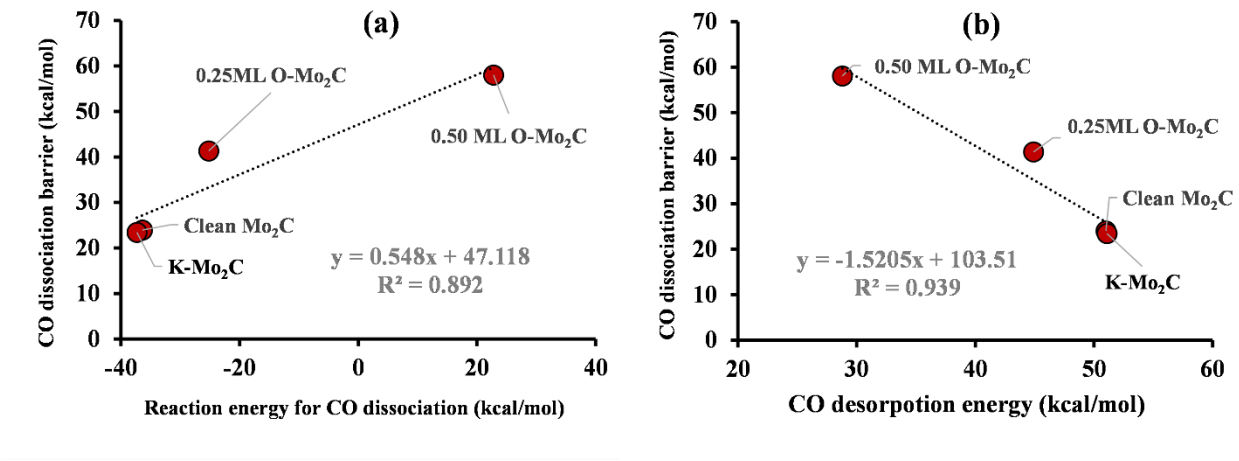

Figure S3. CO dissociation barriers vs. (a) CO dissociation reaction energies and (b) CO desorption energies

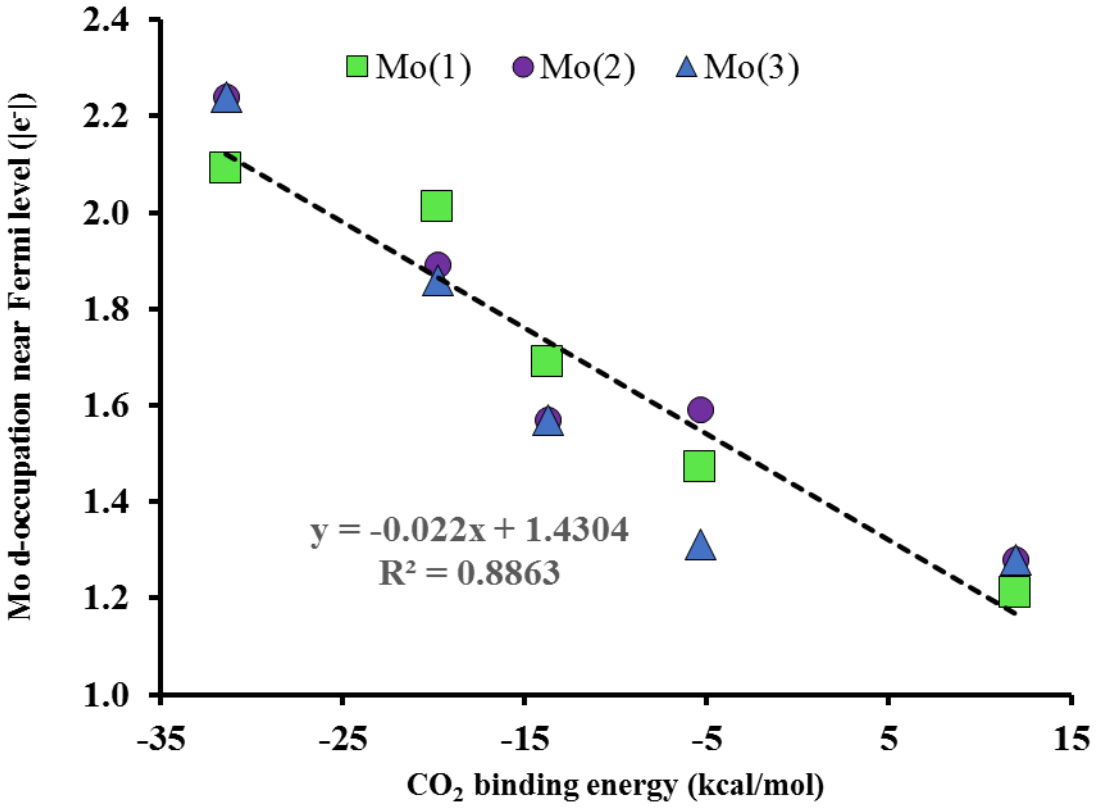

Figure S4. d-occupation of Mo atoms of CO_2 binding site near Fermi level vs. CO_2 binding energy at different oxygen coverage.

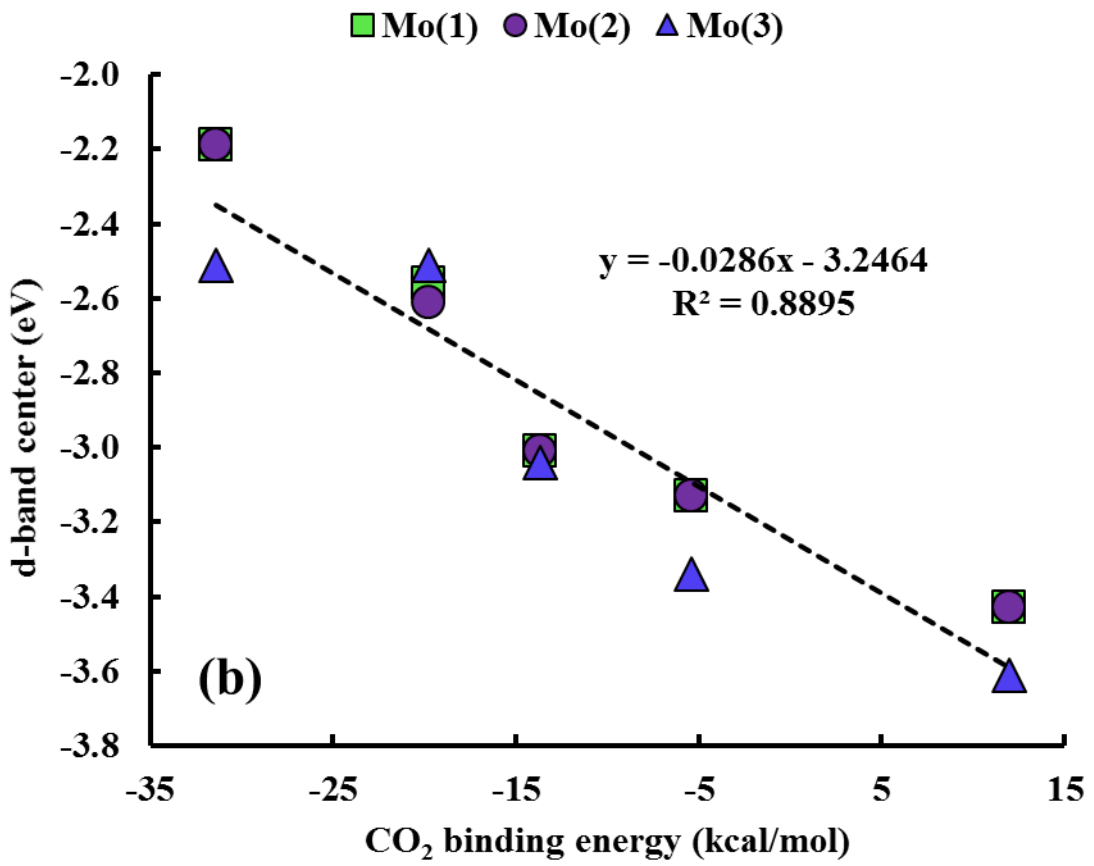

Figure S5. d-band center of Mo atoms of CO_2 binding site near Fermi level vs. CO_2 binding energy at different oxygen coverage.

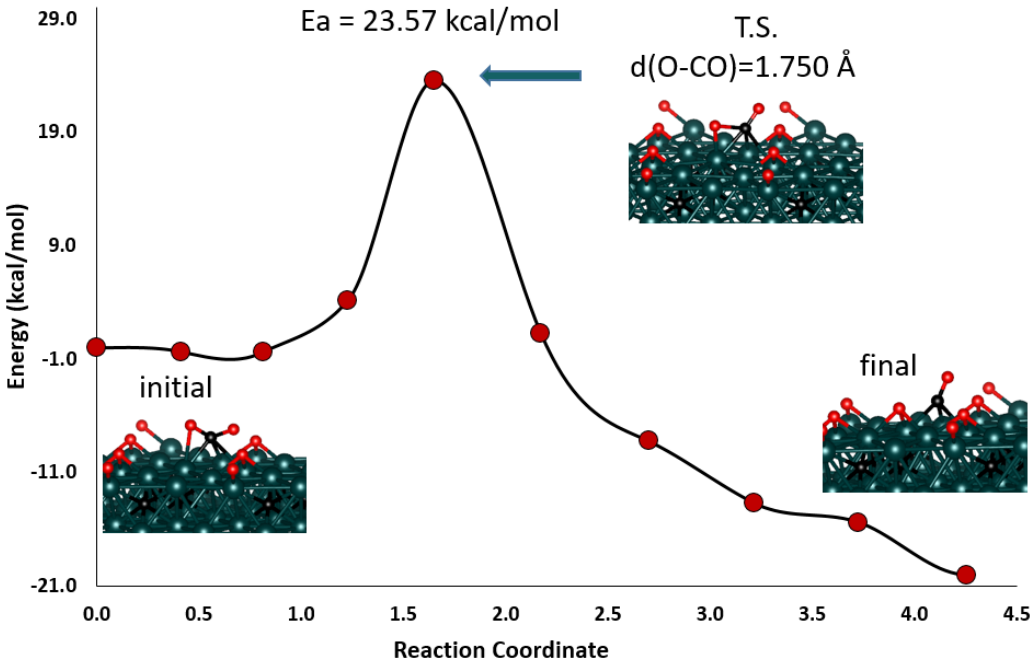

Figure S6. CO_2 dissociation profile on hollow site at 0.25 ML O-Mo_2C surface.

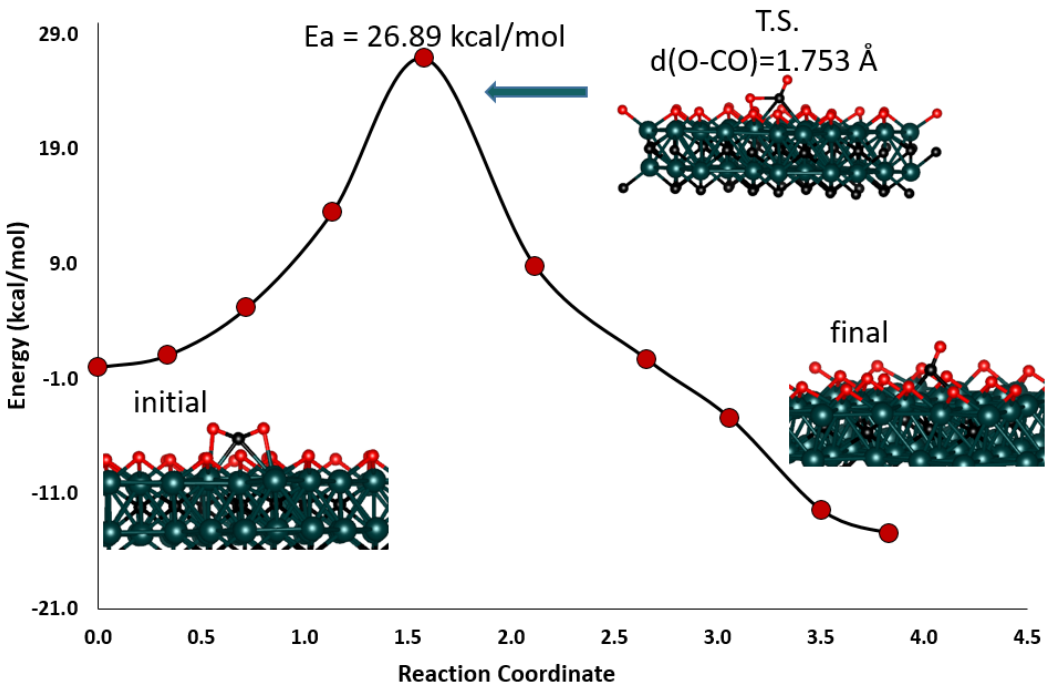

Figure S7. CO_2 dissociation profile on hollow site at 0.5 ML O-Mo_2C surface.

Table S1. Bader charges of different atoms in clean and K-promoted Mo_2C surface.

Atom	Bader charges (e)	
	Clean Mo_2C Surface	**K-promoted Mo_2C Surface**
Mo	0.61	0.75
Mo	0.75	0.77
Mo	0.48	0.76
Mo	0.79	0.76
Mo	0.2	0.76
Mo	0.77	0.77
Mo	0.49	0.77
Mo	0.79	0.76
Mo	0.2	0.79
Mo	0.77	0.79
Mo	0.53	0.78
Mo	0.78	0.78
Mo	0.21	0.78
Mo	0.76	0.76
Mo	0.47	0.78
Mo	0.79	0.78
Mo	0.2	0.57
Mo	0.77	0.2
Mo	0.48	0.17
Mo	0.79	0.2
Mo	0.23	0.19
Mo	0.78	0.09
Mo	0.88	0.18
Mo	0.76	0.46
Mo	0.19	0.42
Mo	0.77	0.48
Mo	0.5	0.51
Mo	0.79	0.83
Mo	0.47	0.42
Mo	0.77	0.46
Mo	0.47	0.5
Mo	0.78	0.44
C	-0.88	-0.89
C	-1.34	-0.88
C	-0.88	-0.89
C	-1.33	-0.89
C	-0.88	-0.89

C	-1.34	-0.88
C	-0.88	-0.88
C	-1.33	-0.89
C	-0.88	-1.34
C	-1.34	-1.33
C	-0.87	-1.34
C	-1.36	-1.33
C	-0.88	-1.34
C	-1.34	-1.36
C	-0.88	-1.34
C	-1.34	-1.35
O	0.77	0.72
K	0	0.88
C	-1	-1.08
O	-0.98	-1.07