Supplementary material for

"**Single Pd atomic catalyst on Mo_2CO_2 monolayer (MXene): unusual activity to CO oxidation by trimolecular Eley-Rideal mechanism**"

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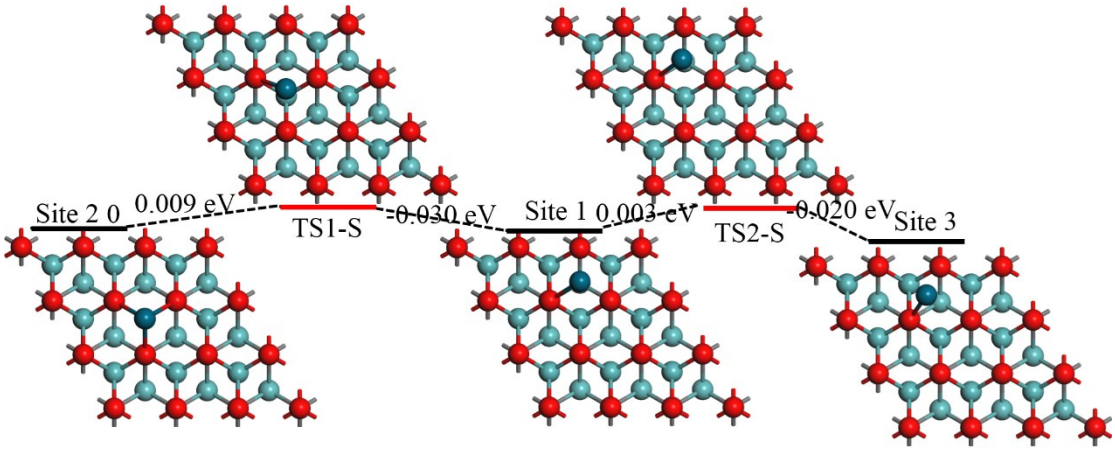

Fig. S1. Diffusion pathways of single Pd atom on the pristine Mo_2CO_2 monolayer.

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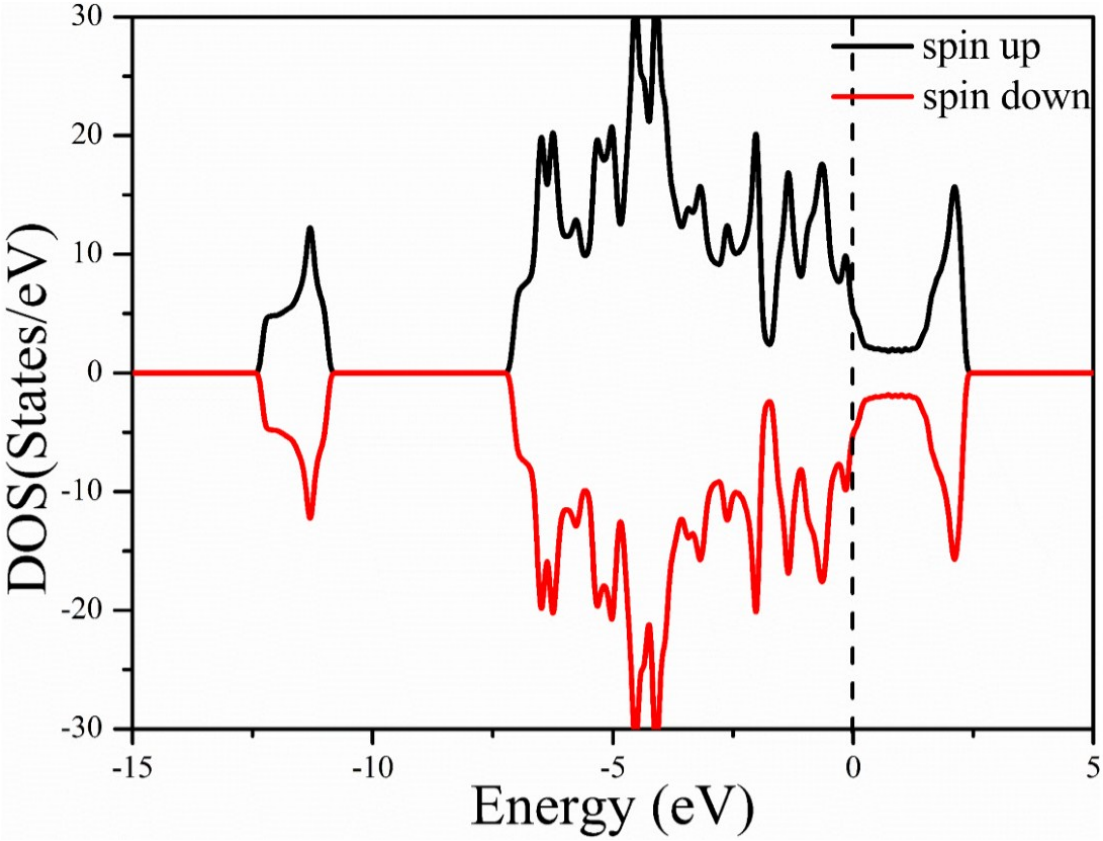

Fig. S2. The density of states of pristine Mo_2CO_2. The dashed line at energy zero represents the Fermi level.

Table S1. The test with various force thresholds for the total energies of the Pd/O_V-Mo_2CO_2 substrate and that with CO adsorbate. The structures were found to have almost no changes for the different values for the force thresholds.

Force threshold (Ha/Å)	Substrate (Ha)	CO adsorbed on substrate (Ha)
0.002	-3505.7177426	-3618.9931082
0.0007 (~ 0.019 eV)	-3505.7177519	-3618.9931137
0.00037 (~ 0.010 eV)	-3505.7177519	-3618.9931137

Table S2. The adsorption energies of CO, O_2, CO_2, 2CO in the 3x3 and 4x4 supercells on Pd/O_V-Mo_2CO_2. All the adsorption energies are for the most favored adsorption configurations. The negative values represent the exothermic adsorption.

Supercell	3x3	4x4
E_{CO}	-1.20 eV	-1.19 eV
E_{O_2}	-0.36 eV	-0.37 eV
E_{CO_2}	-0.30 eV	-0.30 eV
E_{2CO}	-2.10 eV	-2.11 eV

Table S3. The most favored adsorption energies for CO and O_2 on Au(111), Ag(111), Pt(111) and Pd(111); the adsorption energy and dissociation adsorption energies for CO and O on Ru(0001) and Rh(111) and the activation barriers involved in the CO oxidation reaction.

Catalysts	E_{CO} (eV)	E_{O_2} / E_O (eV)	E_a (eV)
Au(111)[2]	-0.30	-0.04	1.97
Ag(111)[2]	-0.29	-0.16	1.03
Pt(111)[3]	-1.58	-0.72	0.46
Pd(111)[4]	-1.47	-2.39	0.61
Ru(0001)[1, 5]	-1.26	-/-3.46	1.68
Rh(111)[1, 5]	-1.35	-/-2.43	1.17

References

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