Computational Screening for High-Activity MoS_2 Nanosheets-Based Catalysts for the Oxygen Reduction Reaction via Substitutional Doping with Transition Metal

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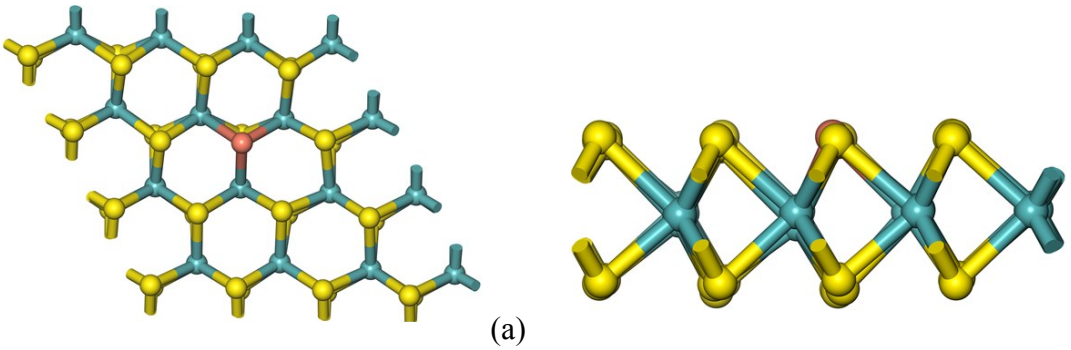
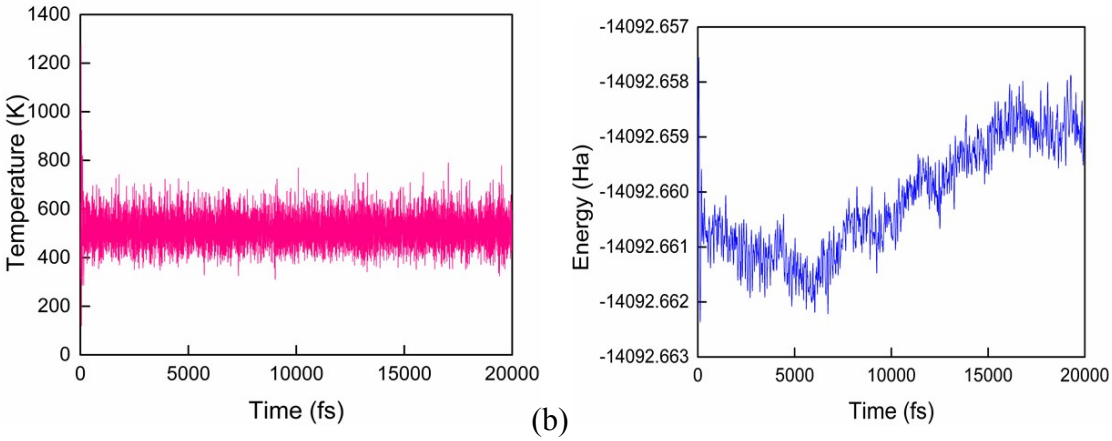
Table S1. The computed adsorption energies of OOH, O, and OH species on various TM-embedded MoS_2 monolayer.

	OOH	O	OH
V	-3.17	-6.59	-4.57
Cr	-2.03	-4.80	-3.47
Mn	-1.86	-4.36	-3.37
Fe	-2.19	-4.52	-3.62
Co	-2.11	-4.16	-3.46
Ni	-1.67	-3.31	-2.77
Cu	-1.67	-2.99	-3.02
Nb	-3.25	-4.40	-4.69
Ru	-1.71	-4.80	-2.99
Rh	-1.67	-3.60	-2.60
Pd	-0.87	-2.16	-1.86
Ag	-1.11	-2.05	-2.34
Ta	-3.45	-6.93	-5.00
W	-3.43	-6.45	-4.24
Re	-2.57	-5.92	-4.14
Os	-2.11	-5.44	-3.51
Ir	-1.88	-4.48	-3.03
Pt	-1.06	-2.99	-2.24
Au	-1.26	-2.68	-2.65



(a)



(b)

Fig. S1. (a) Geometry snapshot and (b) Temperature and energy fluctuations of Cu-embedded MoS_2 monolayer with respect to time in MD simulations at 20 ps at 500K. The temperature was controlled by using the Nosé-Hoover method.

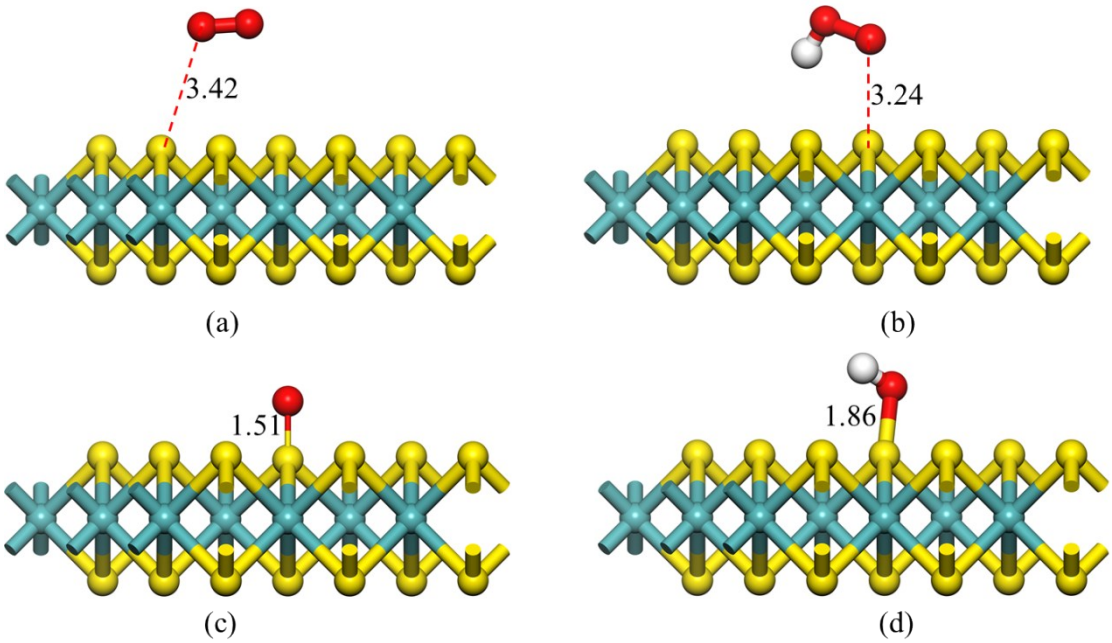


Fig. S2. The optimized adsorption configurations of (a) O_2, (b) OOH, (c) O, and (d) OH species on the pristine MoS_2 monolayer.

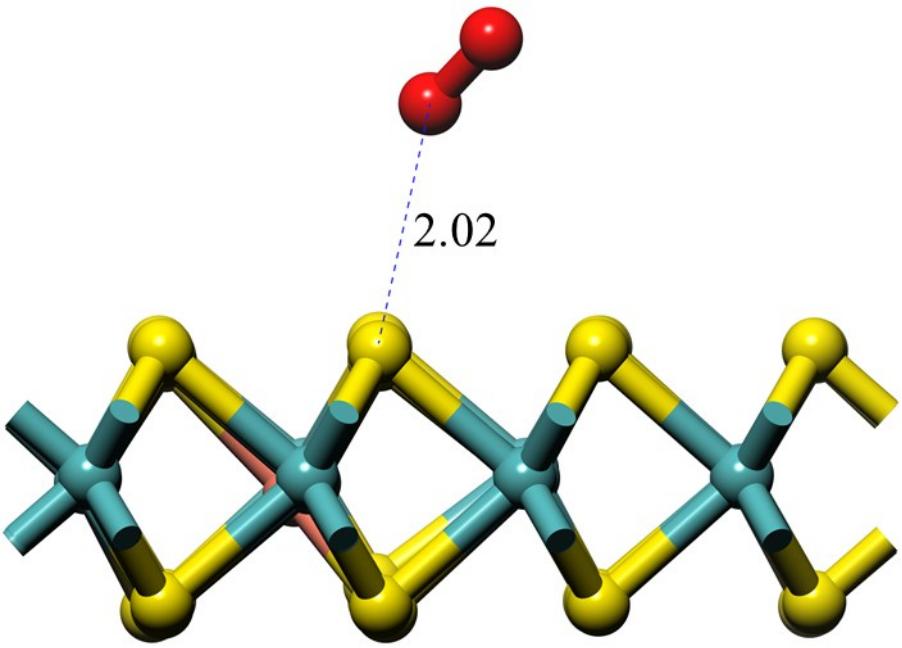


Fig. S3. The optimized structure of O_2 adsorption on the Cu-doped MoS_2 monolayer (one Mo atom in MoS_2 monolayer is substituted by one Cu atom).