Electronic Supplementary Information (ESI)

CO catalytic oxidation on Al-doped graphene-like ZnO monolayer sheets: a first-principles study

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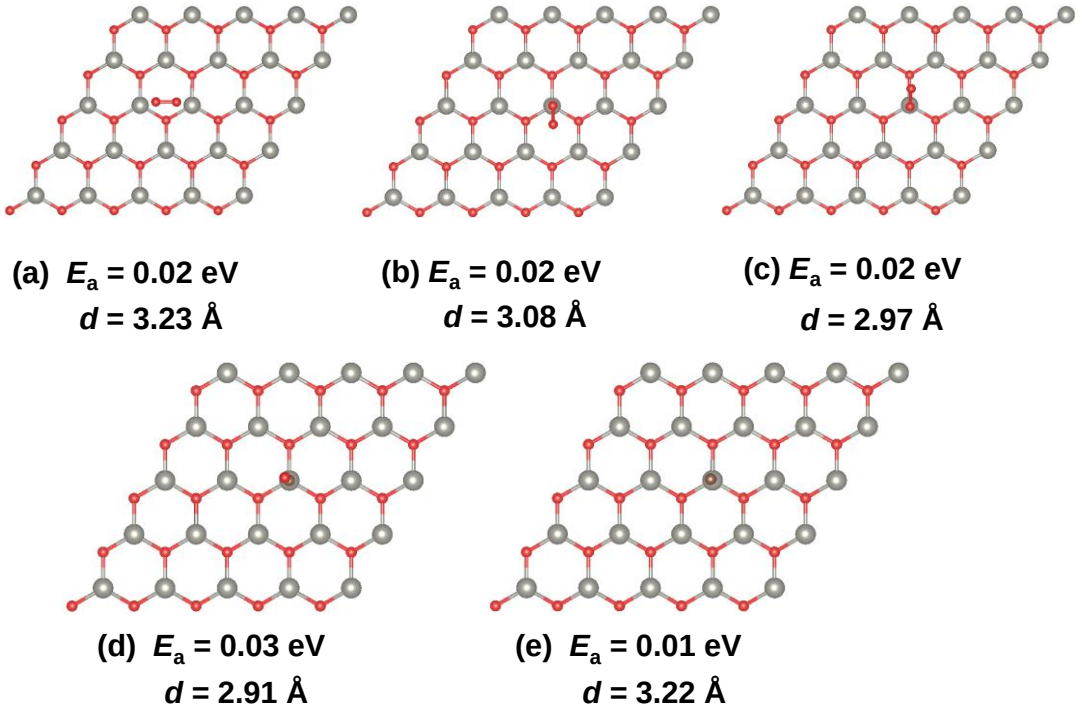

Fig. S1. Several atomic configurations for the O_2 ((a), (b), and (c)) and CO ((d) and (e)) adsorption on the pristine g-ZnO monolayer sheet. The nearest distance between the adsorbed molecules and the sheet, and the adsorption energies are given.

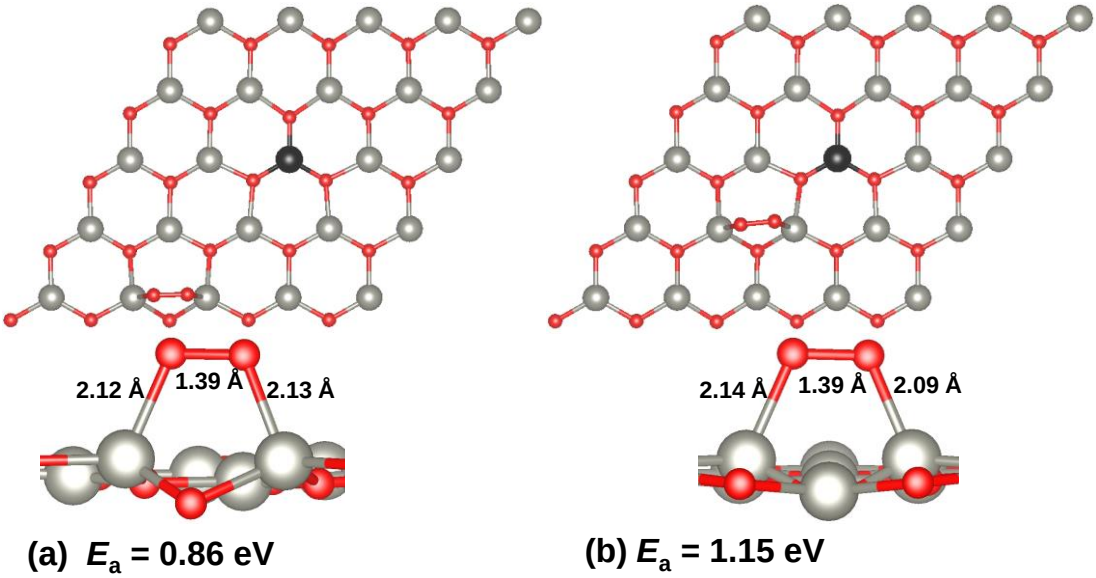

Fig. S2. Atomic configurations of two typical states for the O_2 adsorption at the sites away from the doped Al atom on the Al-g-ZnO monolayer sheet. The adsorption energies are given.

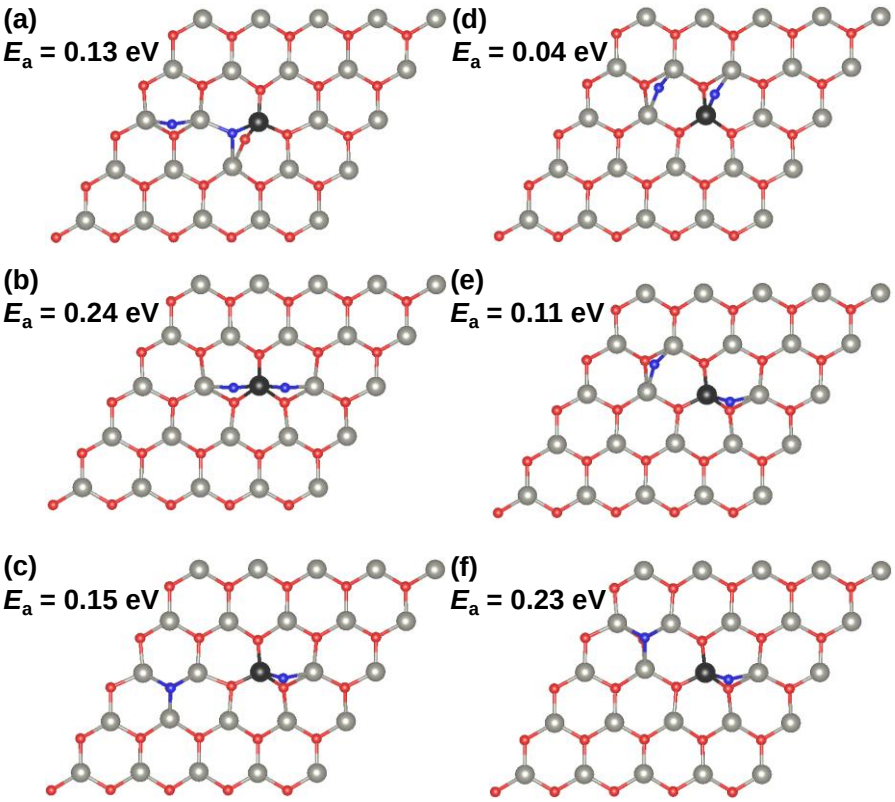

Fig. S3. The atomic configurations and adsorption energies for the states of O_2 dissociative adsorption on the Al-g-ZnO monolayer sheet. The O atoms from the dissociated O_2 are denoted as blue spheres. The adsorption energies were calculated with respect to the free O_2 molecule and the bare Al-g-ZnO sheet.

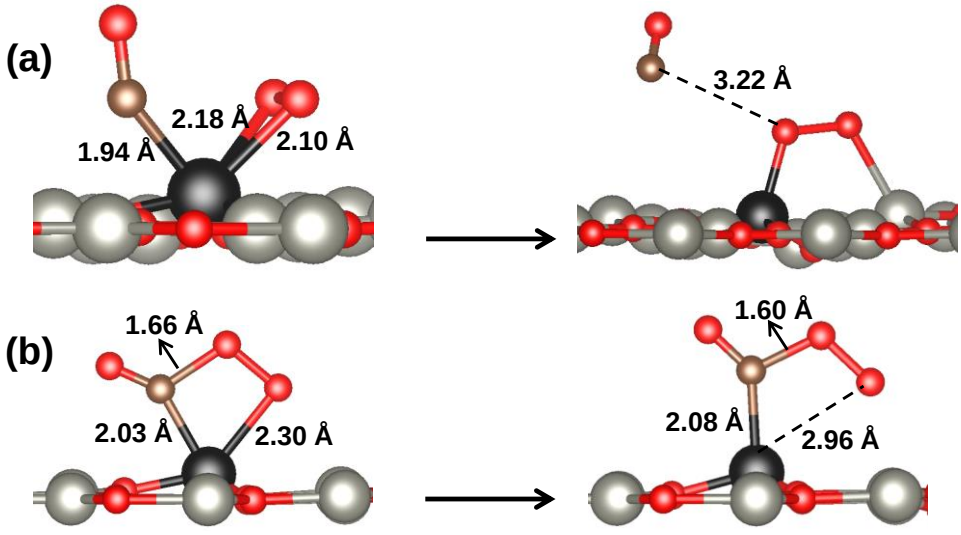

Fig. S4. Atomic configuration of the considered initial (left) and fully optimized (right) states for the coadsorption of O_2 and CO molecules on the Al-g-ZnO monolayer sheet.

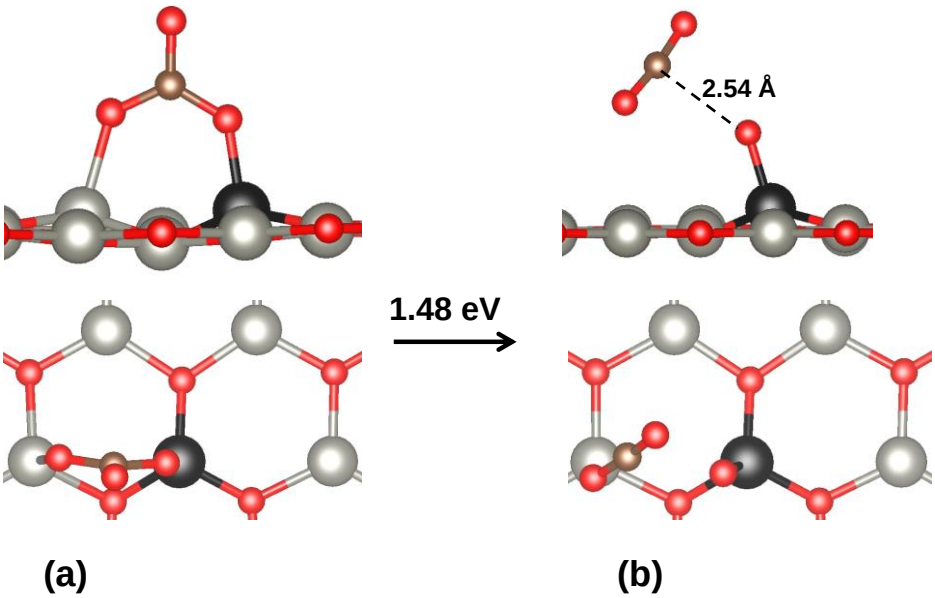

Fig. S5. Atomic configuration of the carbonate-like MS state and the state of CO_2 physisorbed on the atomic O-covered Al-g-ZnO monolayer sheet are shown in (a) and (b), respectively. The former is more stable than the latter by 1.48 eV.