Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Novel joint catalytic properties of Fe and N co-doped graphene for CO oxidation

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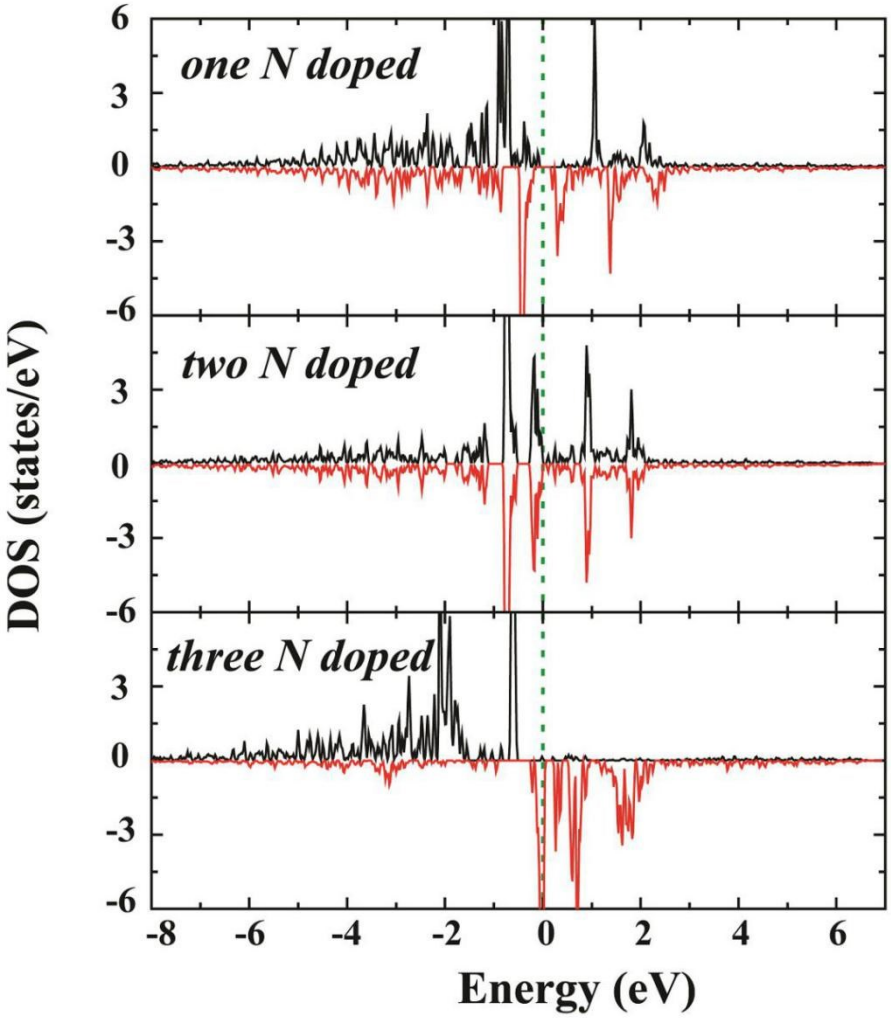

Fig. S1 *d* orbitals of Fe atom for one, two and three N doping at the situations without O_2 molecule adsorbed, respectively.

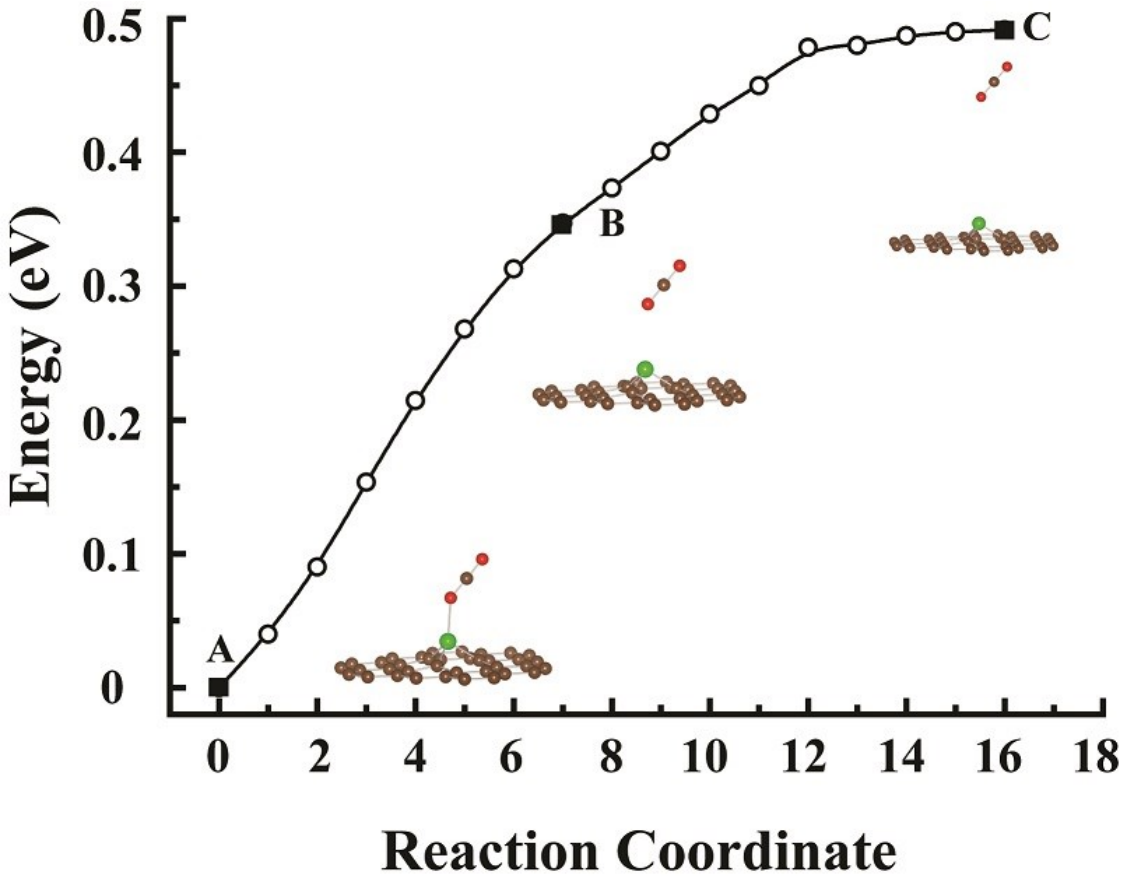

Fig. S2 The energy path of CO_2 molecule leaving from the substrate.

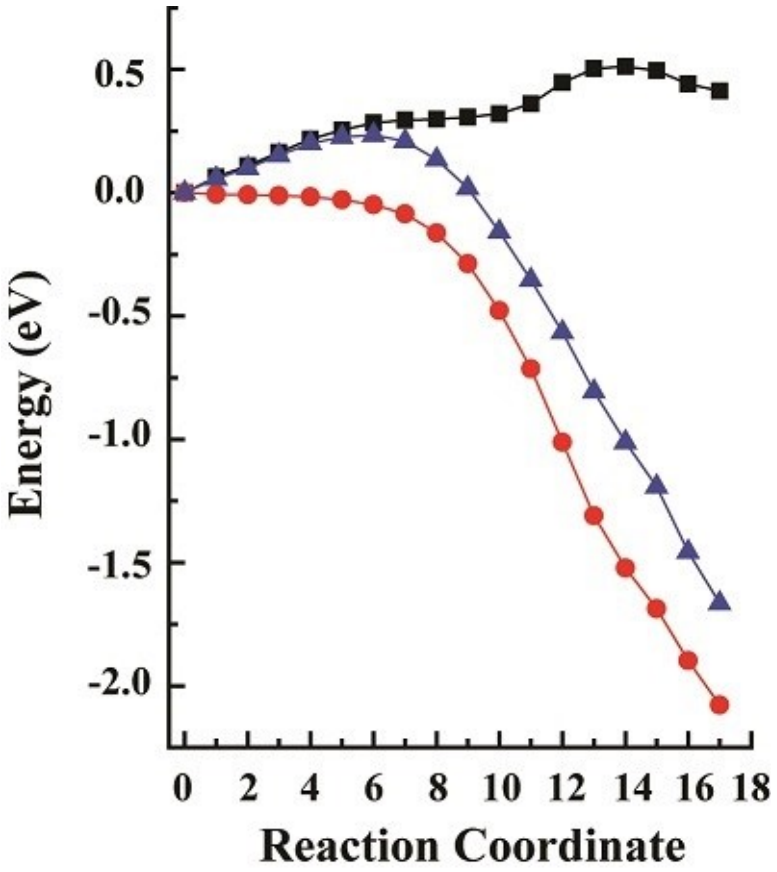

Fig. S3 Then energy curves of CO_2 molecule and O_2 molecule in the Fig. 8 (a) reactive process, respectively. The black line stands for the energy increase (E_{CO2}) in the CO_2 molecule released process, and the red line stands for the energy decrease (E_{O2}) in the O_2 molecule adsorbed process. In the calculations, we used the relative positional configurations of CO_2 and O_2 molecule in Fig. 8(a) reactive process. The blue line is the total energy, which can be defined as $\Delta E=E_{CO2}+E_{O2}$. We can find that the total energy have a same trend with the energy path in Fig. 8(a) reactive process.

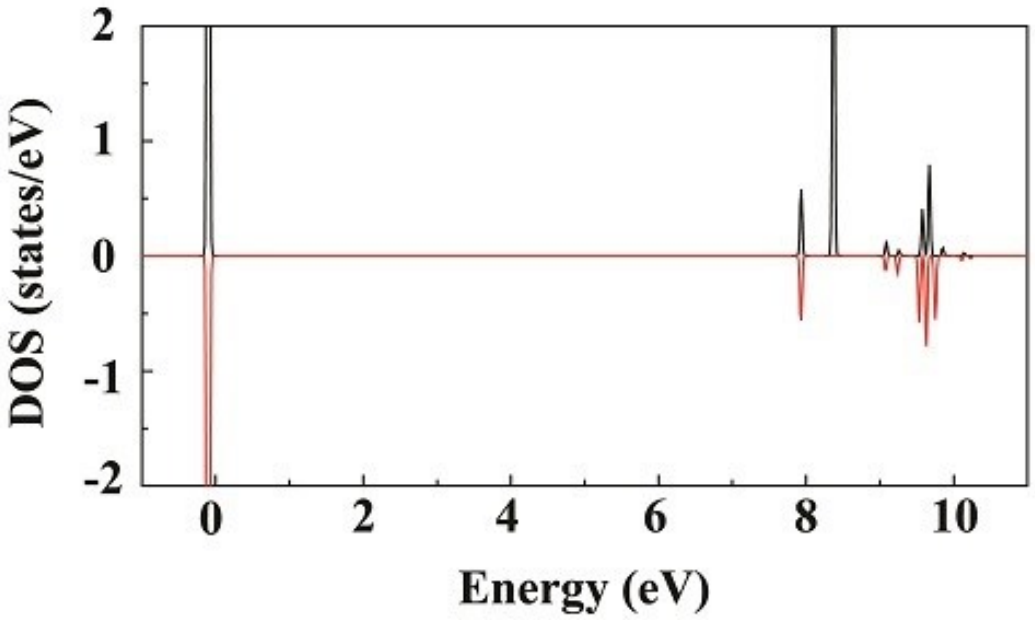

Fig. S4 The *2p* orbitals of the O atom in the isolated CO_2 molecule.