

Supporting information:

Fig.1. The minimum energy profiles and the configurations of different states for CO oxidation reaction on Fe/DG sheet, including (a) CO + O₂ reaction by the LH mechanism, (b) CO + O₂ = CO₂ + O_{ads} and (c) CO + O_{ads} reaction by the ER mechanism. Red, Green, and black balls represent O, Fe and C atoms, respectively.

Fig.2. The minimum energy profiles and the configurations of different states for CO oxidation reaction on Fe/DG sheet, including (a) CO + O₂ and (b) CO₃ + CO reactions by the ER mechanism. Red, green, and black balls represent O, Fe and C atoms, respectively.

Fig.3. The minimum energy profiles and the configurations of different states for CO oxidation reaction on Fe/DG sheet, including (a) the dissociative adsorption of O₂ molecule and (b) 2CO + 2O_{ads} reactions by the ER mechanism. Red, green, and black balls represent O, Fe and C atoms, respectively.

Table S1. The adsorption energy (E_{ads}, in eV) of individual CO (or O₂) molecule and coadsorbed O₂ + CO molecules on metal embedded graphene sheets (M-gra, M = Al, Au, Cu, Pd and Fe).

| M-gra | CO | O ₂ | O ₂ + CO |
|--------|------|----------------|---------------------|
| Al-gra | 0.83 | 1.57 | 1.95 |
| Au-gra | 1.53 | 1.34 | 1.82 |
| Cu-gra | 1.71 | 2.67 | 3.29 |
| Pd-gra | 1.07 | 1.13 | 1.90 |
| Fe-gra | 1.13 | 1.88 | 2.10 |

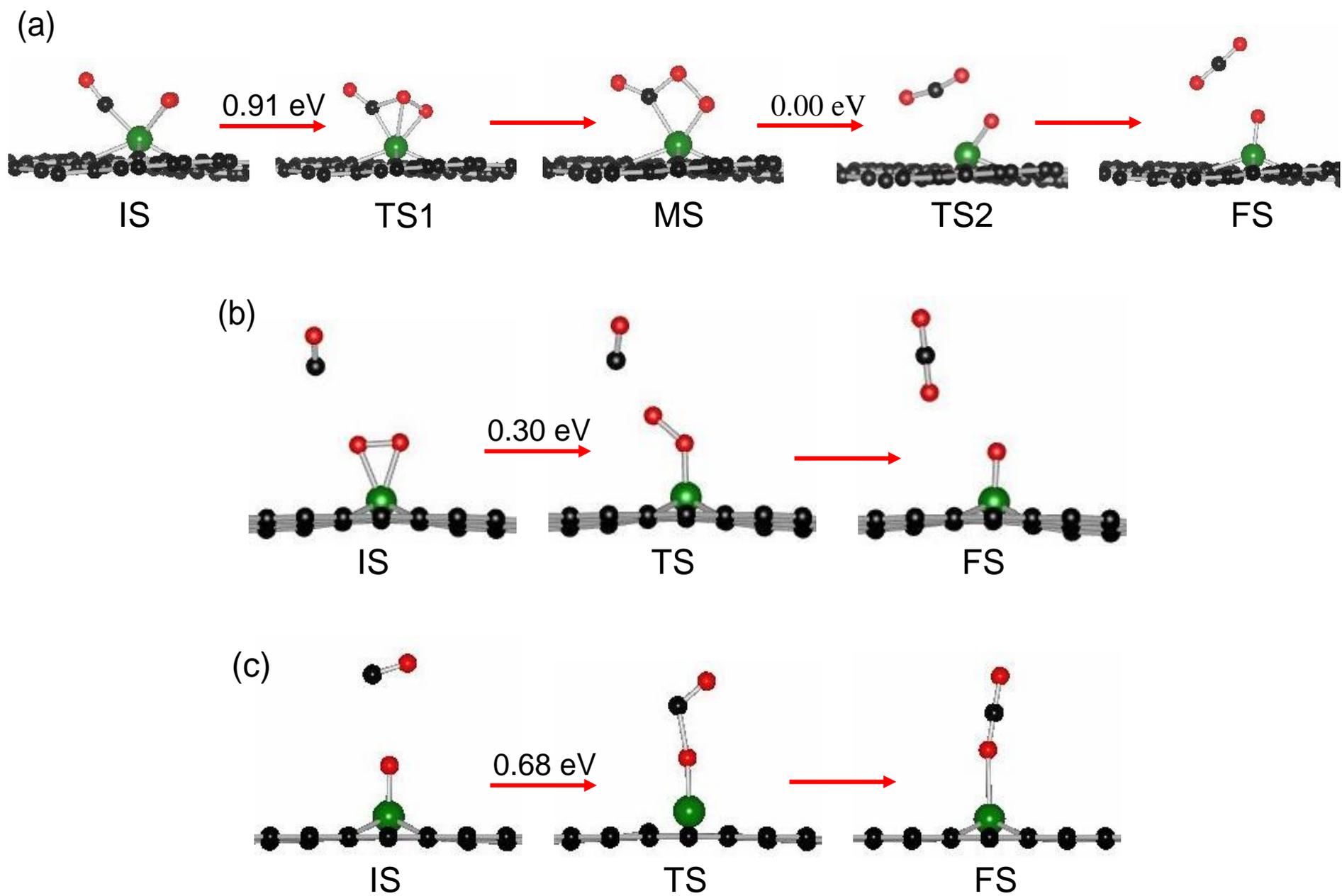


Fig. S1(a)-(c)

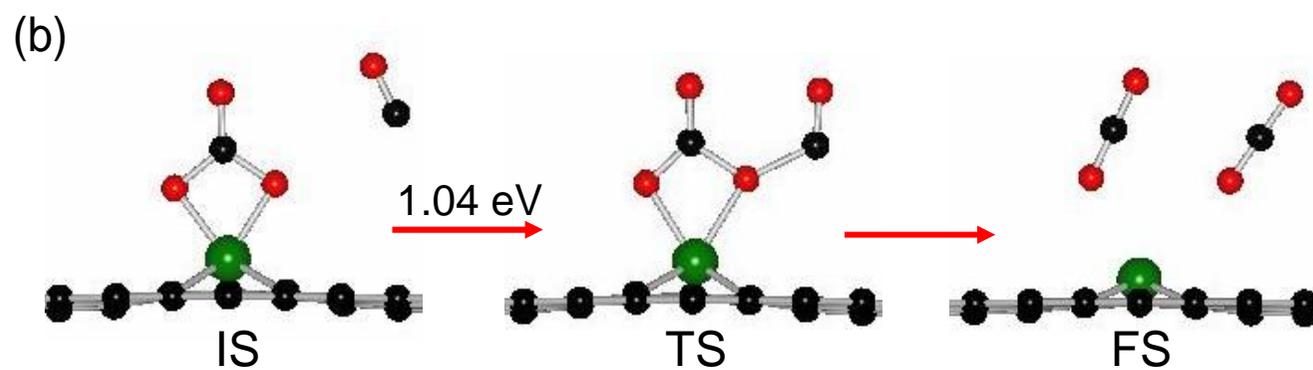
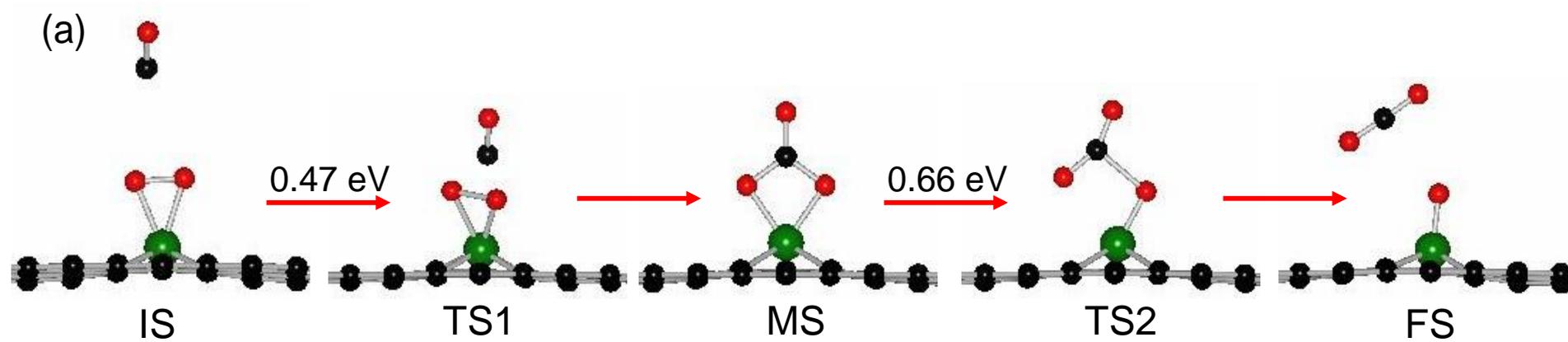


Fig. S2(a)-(b)

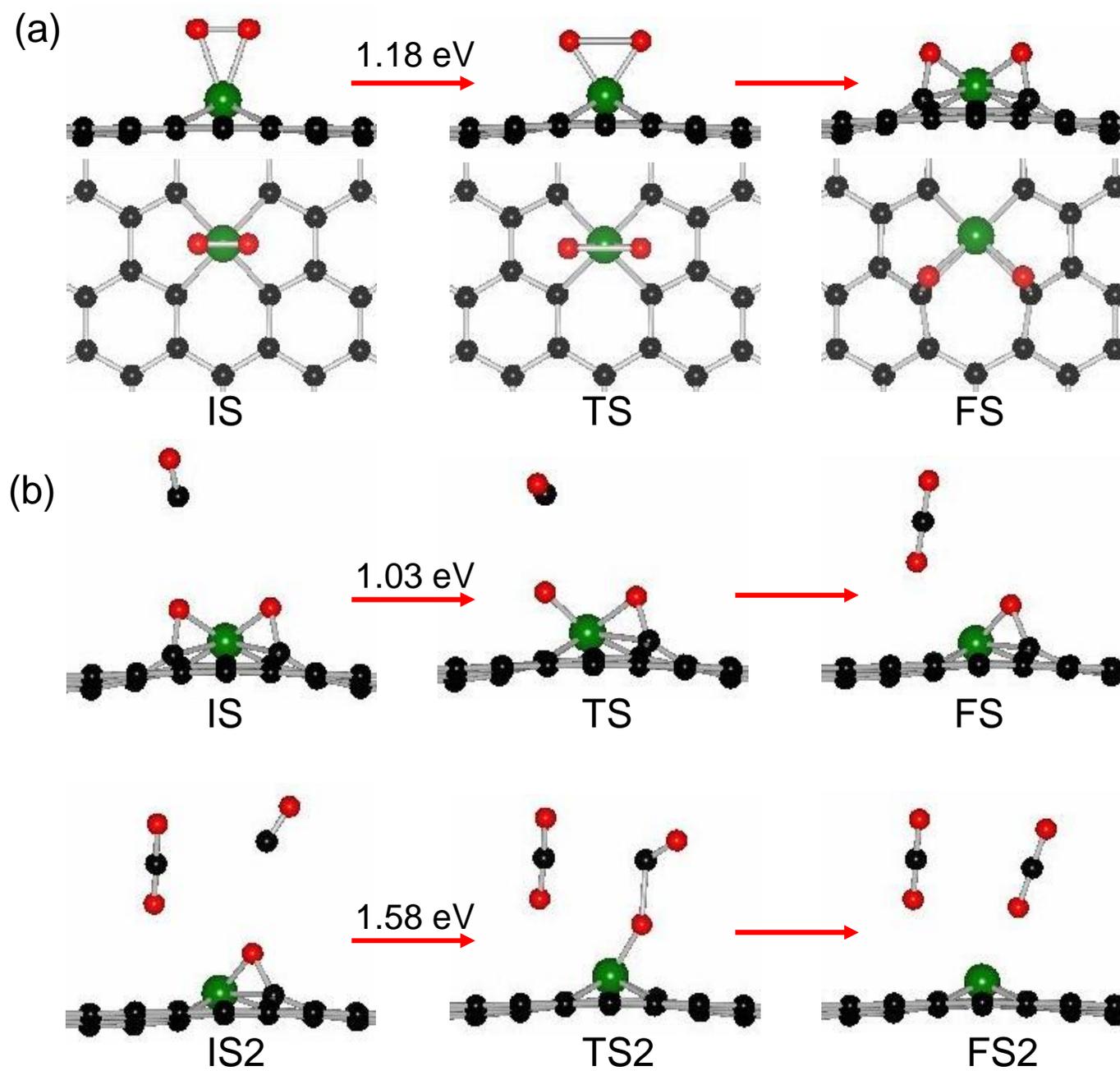


Fig. S3(a)-(c)