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


Supporting Information for

# Single Pt atom supported on penta-graphene as an efficient catalyst for CO oxidation

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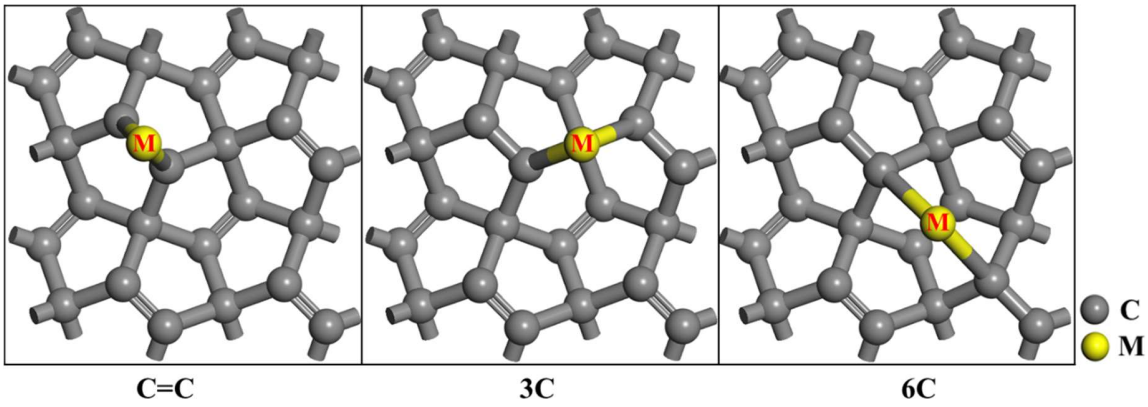


**Figure S1.** Three possible active sites for single-metal atom supported on penta-graphene: C=C, 3C and 6C sites, respectively.

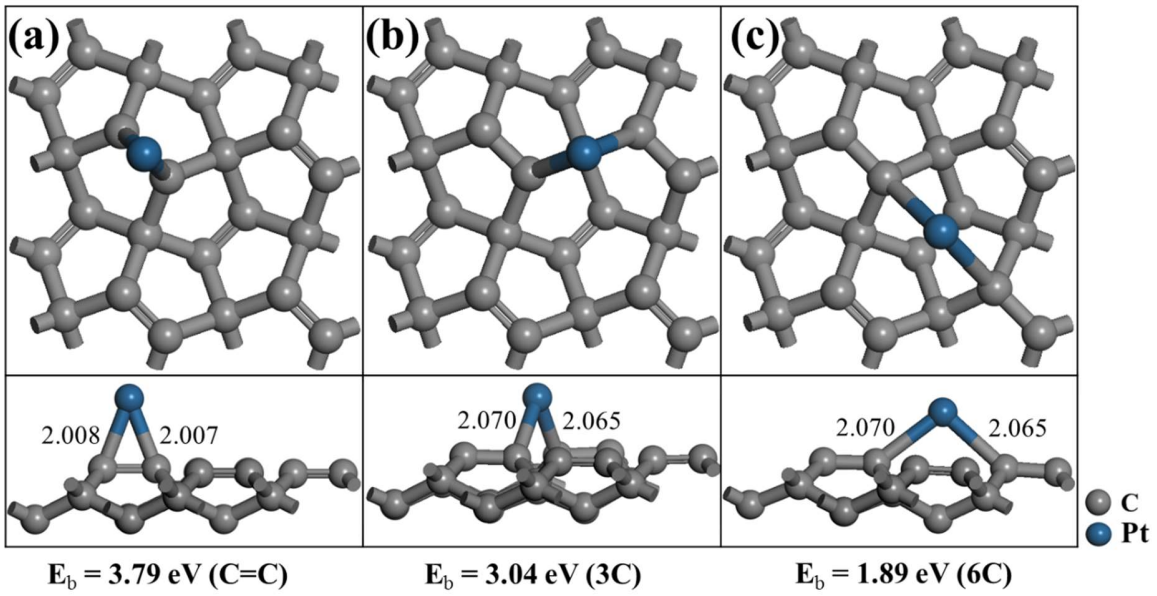


**Figure S2.** Optimized configurations with binding energies for single Pt atom supported on different sites of penta-graphene: (a) C=C site. (b) 3C and (c) 6C, respectively.

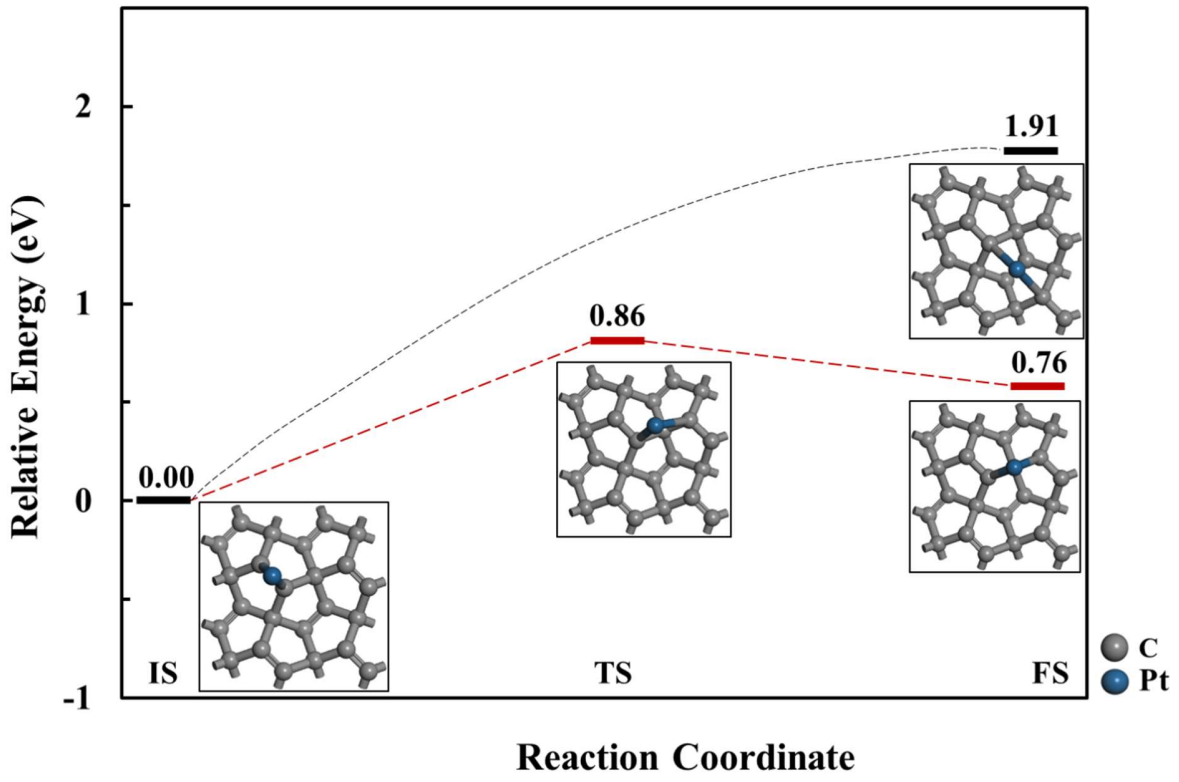


**Figure S3.** The diffusion paths of Pt on penta-graphene. Red line (Path A) and black line (Path B) represent Pt atom diffuses from C=C site to 3C site and 6C site, respectively.

**Table S1.** The predicted binding energy $E_b$ (eV), Bader charge and diffusion barriers (eV) for single Pt, Cu and Fe atoms supported on penta-graphene.

| Atoms | Sites | $E_b$ (eV) | Bader charge \|*e*\| | Diffusion barriers (eV) |
|---|---|---|---|---|
| Pt | C=C | 3.79 | 0.1 | |
| | 3C | 3.04 | 0.24 | 0.86 red line (Path A) |
| | 6C | 1.89 | 0.2 | 1.84 black line (Path B) |
| Cu | C=C | 1.25 | 0.28 | |
| | 3C | 1.24 | 0.43 | 0.06 red line (Path A) |
| | 6C | 1.13 | 0.43 | 0.11 black line (Path B) |
| Fe | C=C | 2.3 | 0.7 | |
| | 3C | 2.37 | 0.83 | 0.20 red line (Path A) |
| | 6C | 1.6 | 0.85 | 0.93 black line (Path B) |

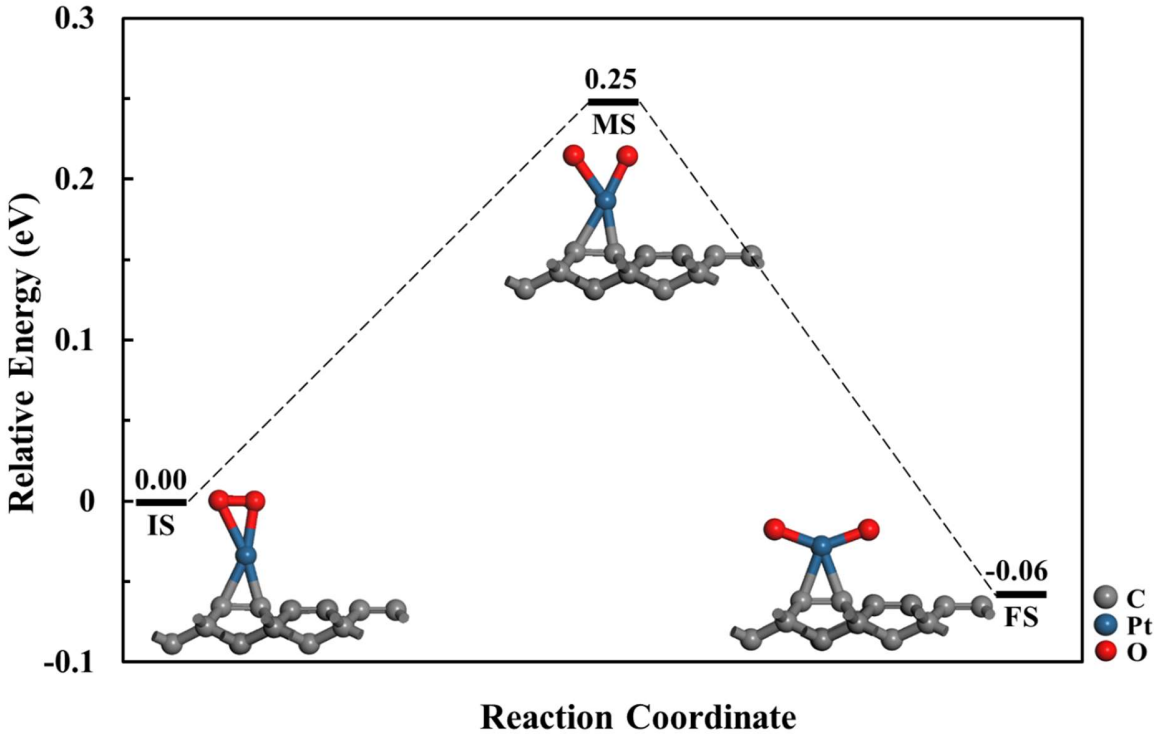


**Figure S4.** Energy profile for $O_2$ dissociation on the Pt/PG involving the initial state (IS), the transition state (TS) and the final state (FS).

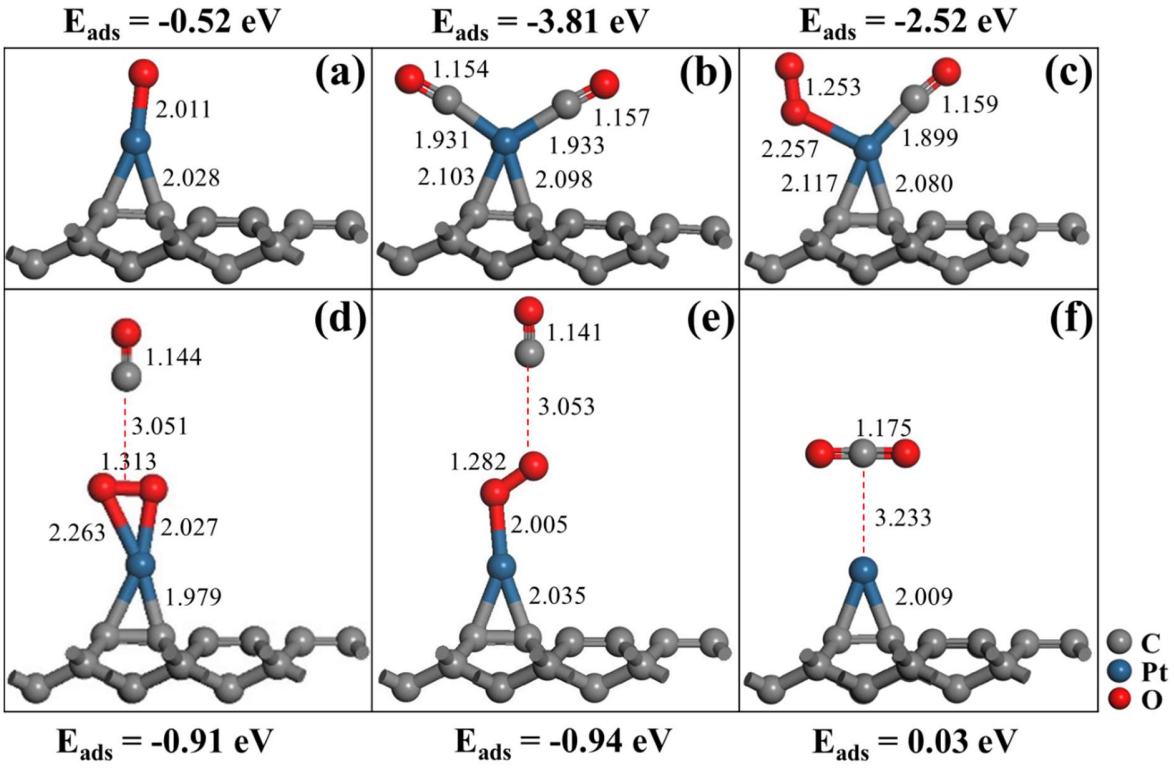


**Figure S5.** Optimized adsorption configurations with calculated adsorption energies: (a) atomic O, (b) co-adsorption of 2CO, (c) co-adsorption of $O_2$ and CO, (d) pre-adsorption of CO on adsorbed $O_2$ (side-on) (e) pre-adsorption of CO on adsorbed $O_2$ (end-on) and (f) $CO_2$ adsorption on the Pt/PG.

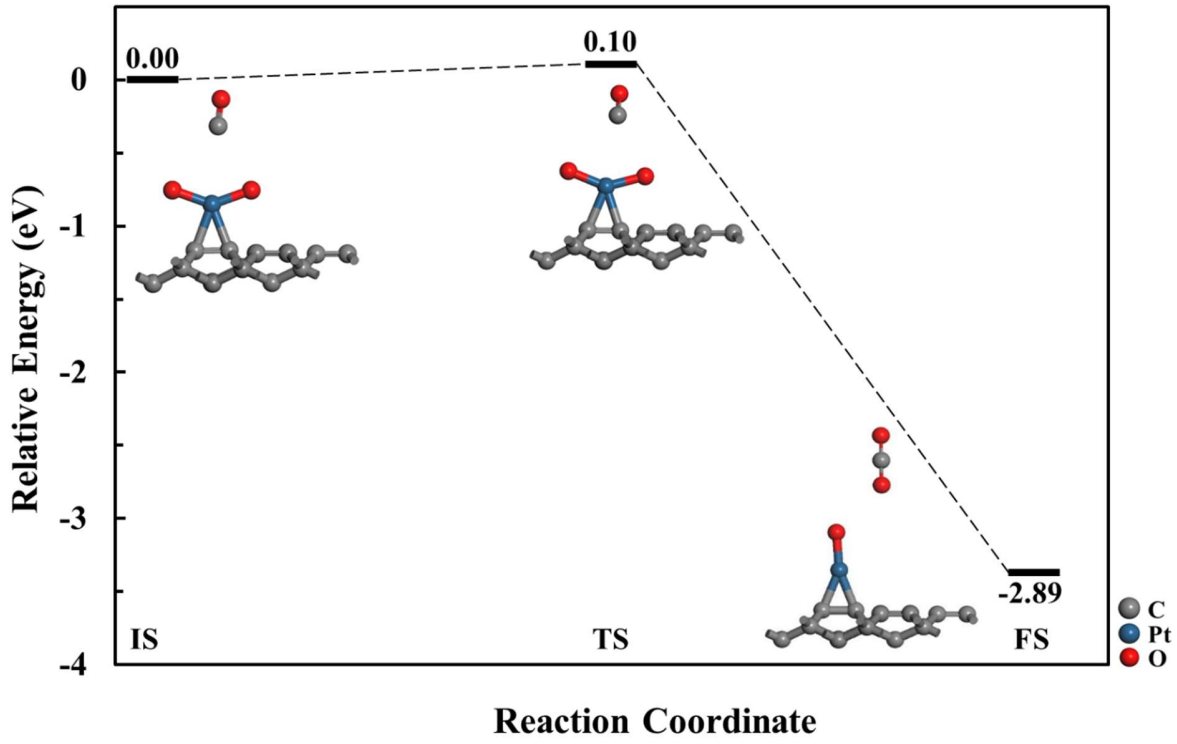


**Figure S6.** Energy profile for ER direct reaction mechanism of CO oxidation by dissociative adsorption of $O_2$ on the Pt/PG involving the initial state (IS), the transition state (TS) and the final state (FS).

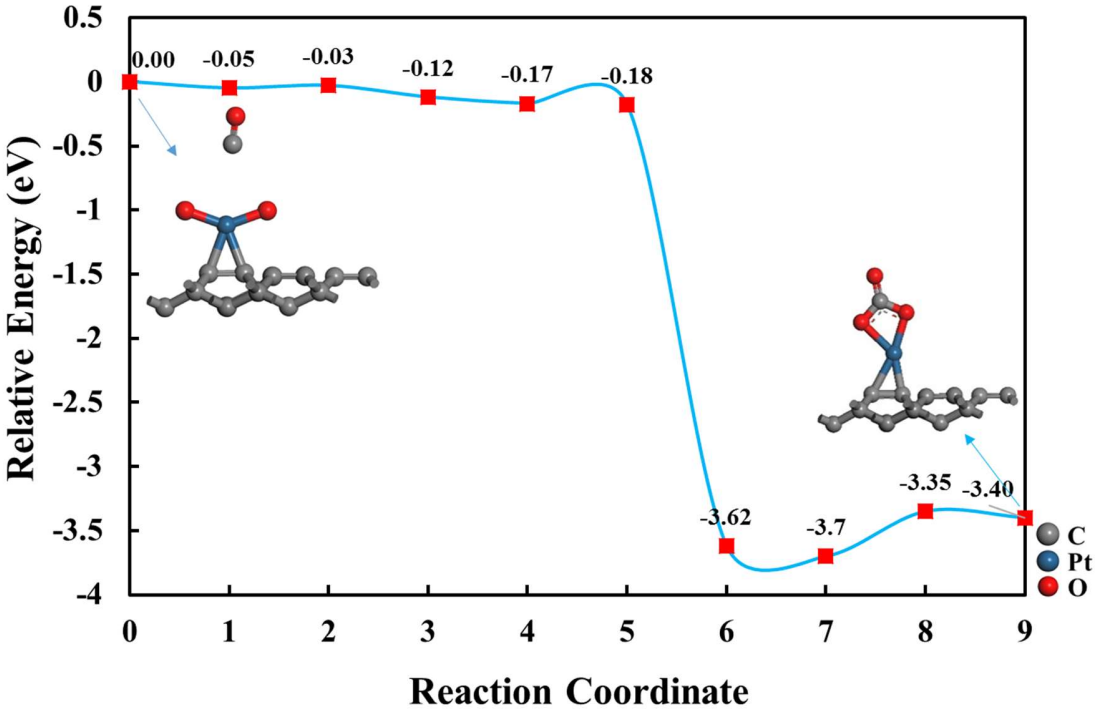


**Figure S7.** Energy profile for ER intermediate formation mechanism by dissociative adsorption of $O_2$ on the Pt/PG involving the initial state (IS), the transition state (TS) and the final state (FS).