

Supporting Information:

Pt atoms Stabilized on Hexagonal Boron Nitride as
Efficient Single-Atom Catalysts for CO Oxidation:
A First-principles Investigation

Xin Liu^{†,*}, *Ting Duan*[†], *Changgong Meng*[†], *Yu Han*[‡]

[†] School of Chemistry, Dalian University of Technology, Dalian, 116024, P. R. China

[‡] Advanced Membranes and Porous Materials Center, King Abdullah University of Science and
Technology, Thuwal, 23955-6900, Kingdom of Saudi Arabia

*Corresponding Author:

Dr. Xin Liu

Tel: +86-411-84986343

Email: xliu@dlut.edu.cn

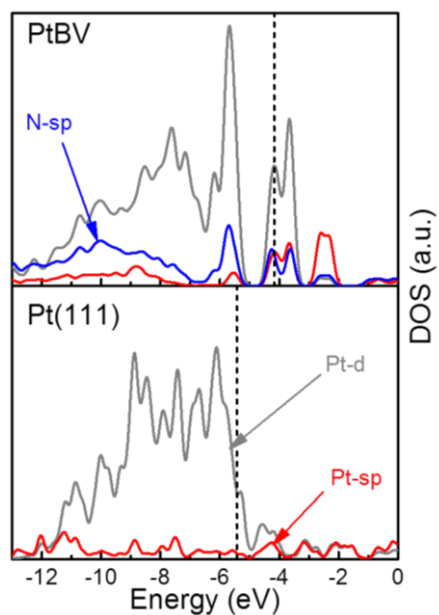


Figure S1. The DOS of PtBV and Pt(111). The DOS curves are aligned by the calculated vacuum level which is set as 0 and the E_F of each system is marked with the dashed lines.

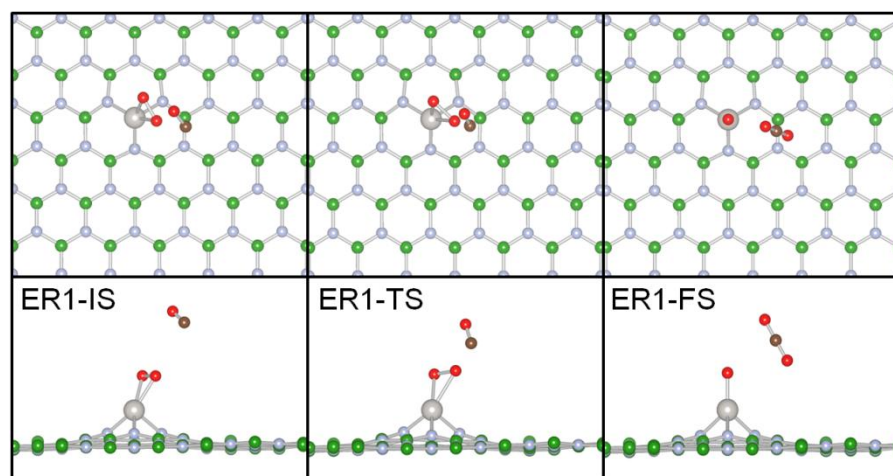


Figure S2. Top views (Top panel) and side views (Bottom panel) of local configurations of the adsorbates on the PtBV at various states along the minimum-energy pathway via the one-step ER mechanism, including the initial state (ER1-IS), transition state (ER1-TS) and final state (ER1-FS). (C: Brown; O: Red; N: Light blue; B: Green; Pt: Silver.)

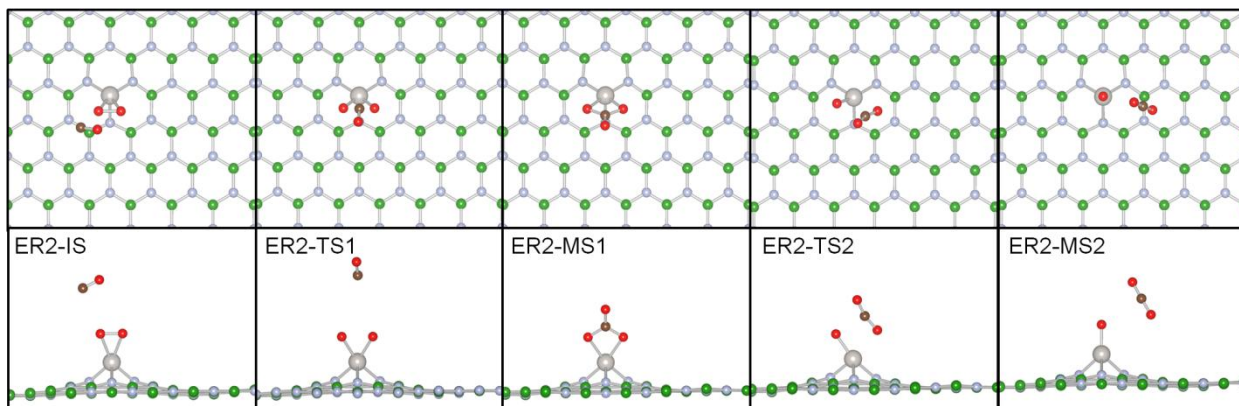


Figure S3. Top views (Top panel) and side views (Bottom panel) of local configurations of the adsorbates on the PtBV at various states along the minimum-energy pathway via the 2-step ER mechanism, including the initial state (ER2-IS), transition states (ER2-TS1 and ER2-TS2), intermediate state (ER2-MS1) and final state (ER2-MS2). (C: Brown; O: Red; N: Light blue; B: Green; Pt: Silver.)

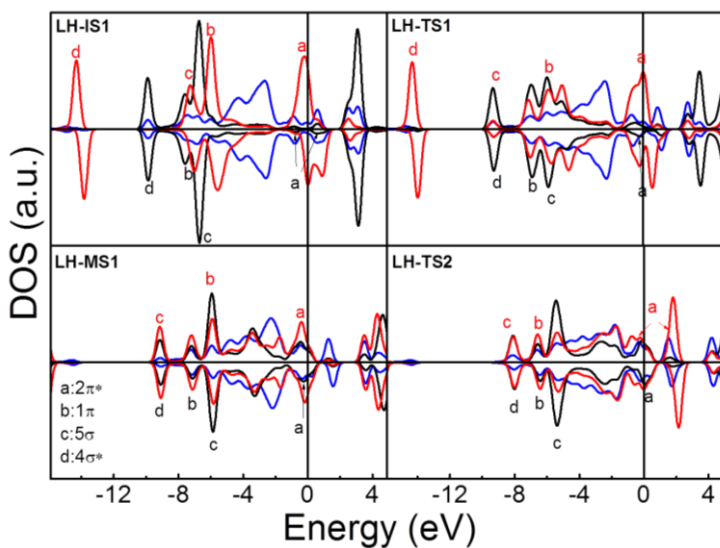


Figure S4. PDOS of CO, O₂ and Pt atom in LH-IS1, LH-TS1, LH-MS1 and LH-TS2. The DOS plots were aligned by the calculated E_F . DOS curves of Pt-d, CO and O₂ are in blue, black and red, respectively.