

Supporting information

Tianzi Cai^a, Zilong Zhang^a, Xingyu Gai^a, Fangmin Zuo^a, Fengkai Gao^a, Bolin Wang^a,
* and Haifeng Zhang^a,*

¹ School of Chemical Engineering, Northeast Electric Power University, Jilin 132012, China;

* bolinwang@neepu.edu.cn; zhfeepu@163.com

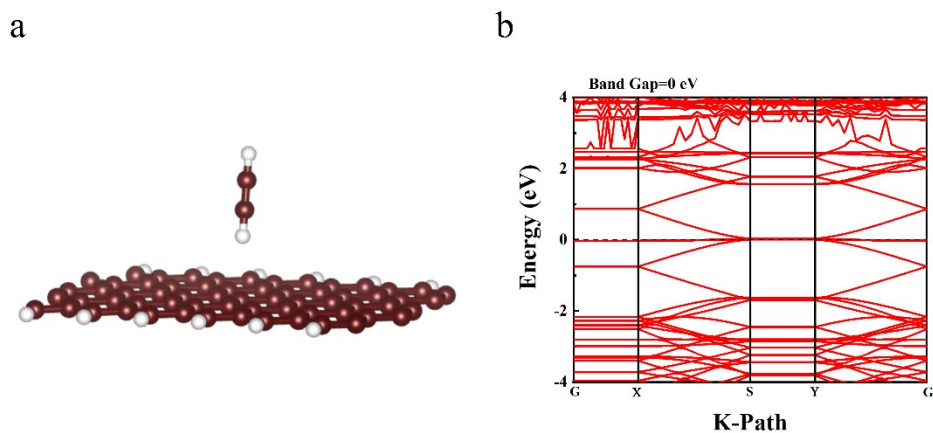


Figure S1. Optimized pristine graphene for C₂H₂ adsorption (a) C₂H₂ molecules attached to pristine graphene (b) band structure of pristine graphene (Color key: Brown-C; White-H)

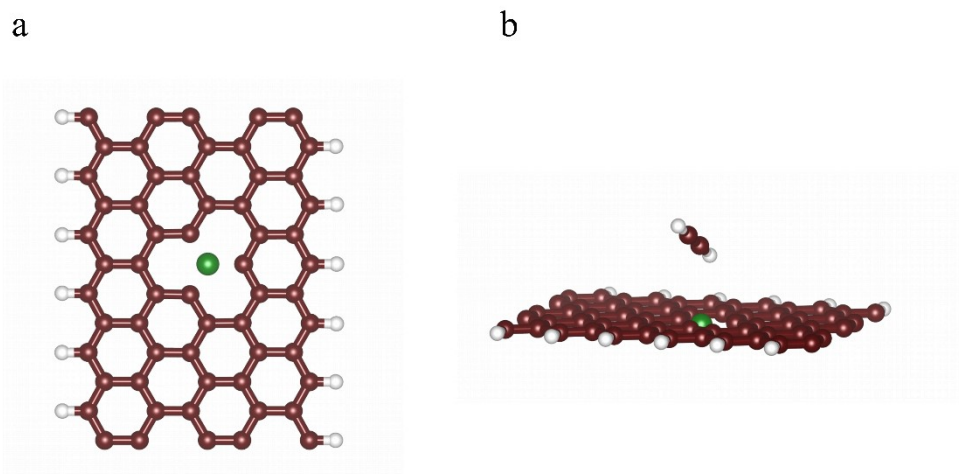


Figure S2. Configuration of single B-doped graphene. (a) B-doped monolayer graphene (b) Optimal configuration of C₂H₂ gas molecule adsorption on B/G.