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Supporting information

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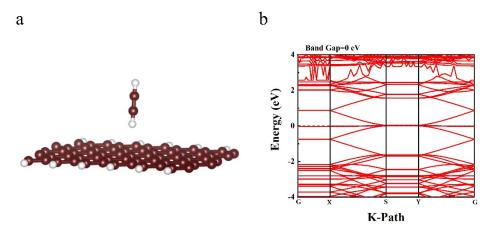


Figure S1. Optimized pristine graphene for C_2H_2 adsorption (a) C_2H_2 molecules attached to pristine graphene (b) band structure of pristine graphene (Color key: Brown-C; White-H)

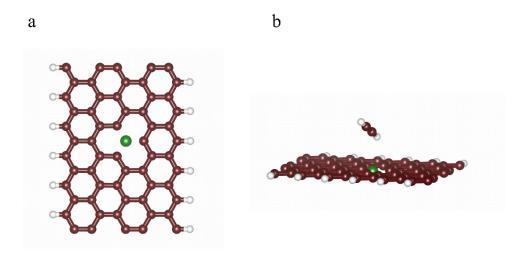


Figure S2. Configuration of single B-doped graphene. (a) B-doped monolayer graphene (b) Optimal configuration of C₂H₂ gas molecule adsorption on B/G.

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