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Supporting Information

Boron-Doped Graphene as a Promising Electrocatalyst for NO Electrochemical

Reduction: a Computational Study

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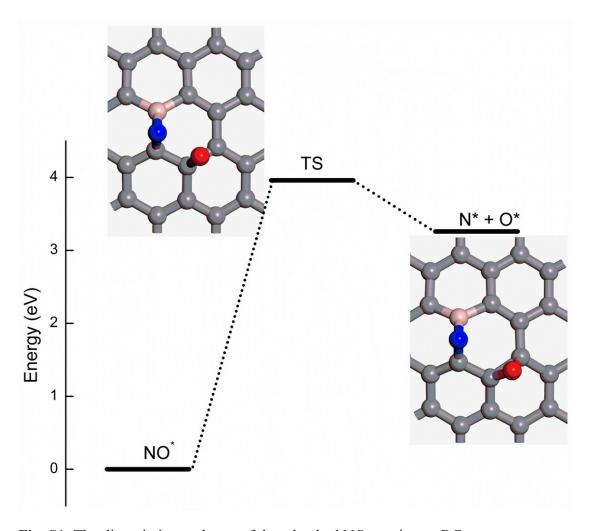


Fig. S1. The dissociation pathway of the adsorbed NO species on BG.

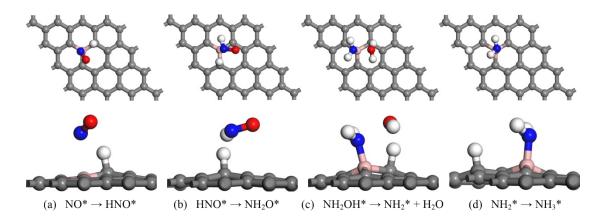


Fig. S2. Some key transition states involved into the NOER on BG.

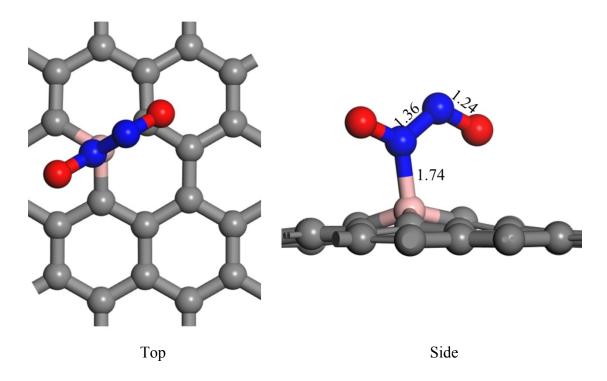


Fig. S3. The optimized configurations of NO dimer adsorption on BG.