

## Supporting Information

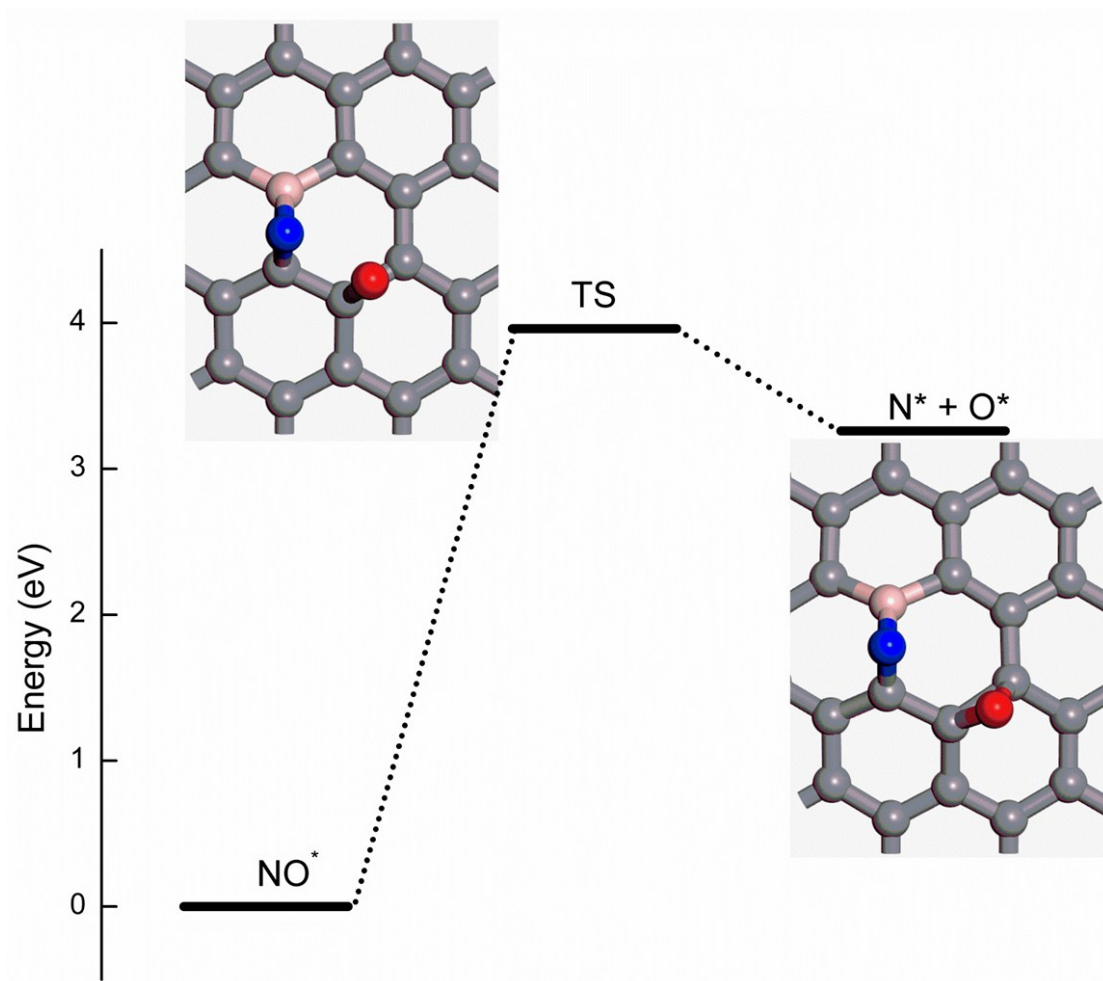
### **Boron-Doped Graphene as a Promising Electrocatalyst for NO Electrochemical Reduction: a Computational Study**

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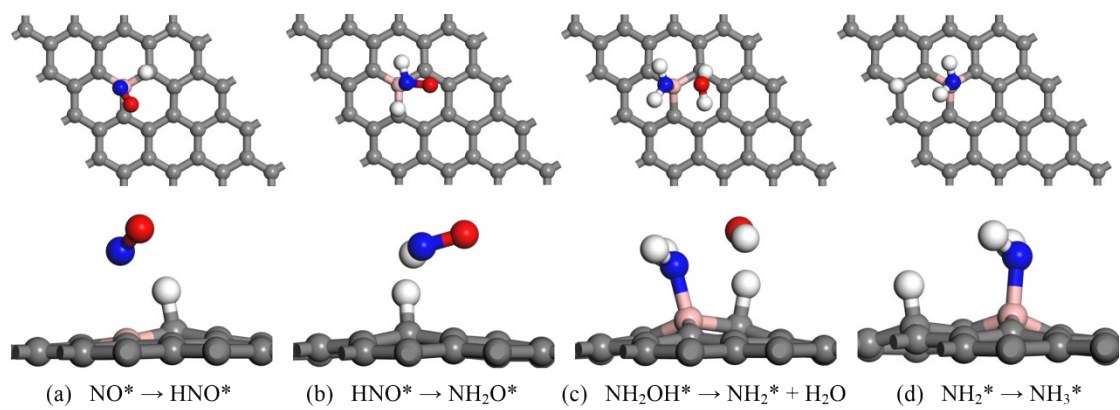
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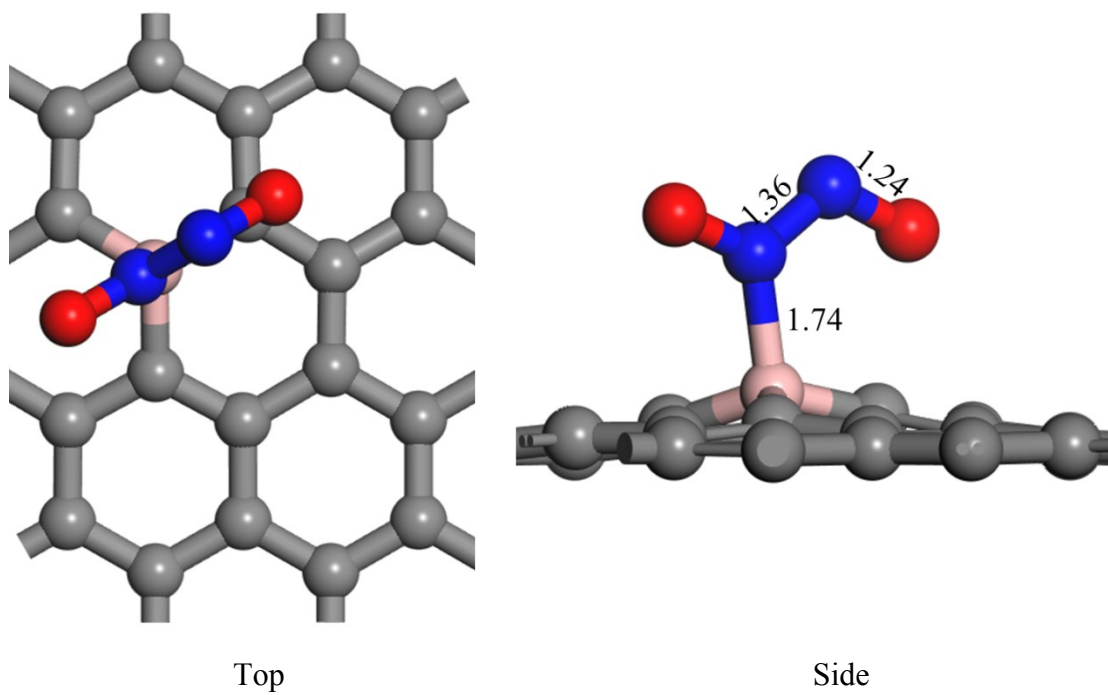
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**Fig. S1.** The dissociation pathway of the adsorbed NO species on BG.



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



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