

Supporting Information

Negatively Charged Boron Nitride Nanosheet as a Potential Metal-Free Electrocatalyst for Oxygen Reduction Reaction: a Computational Study

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Figure S1

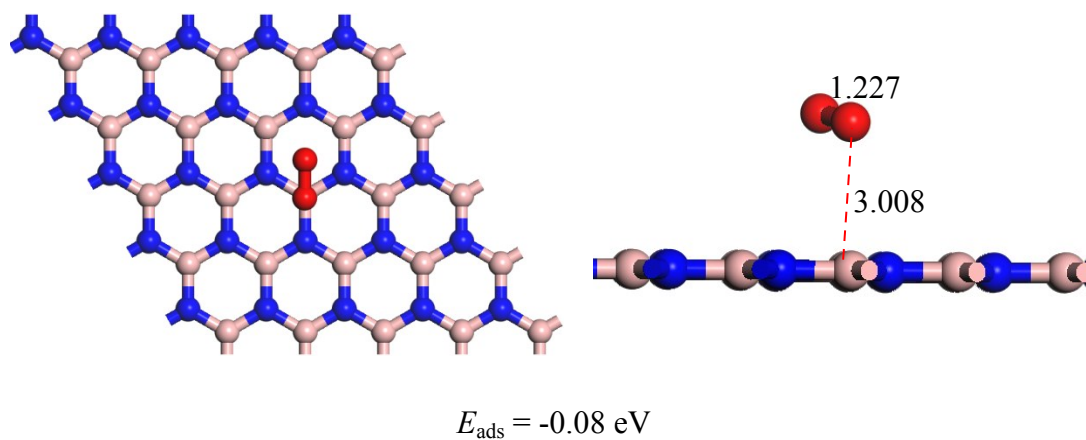


Figure S1. The optimized structures and adsorption energy of the adsorption of O₂ molecule on neutral BN sheet. The bond distance is in angstroms.

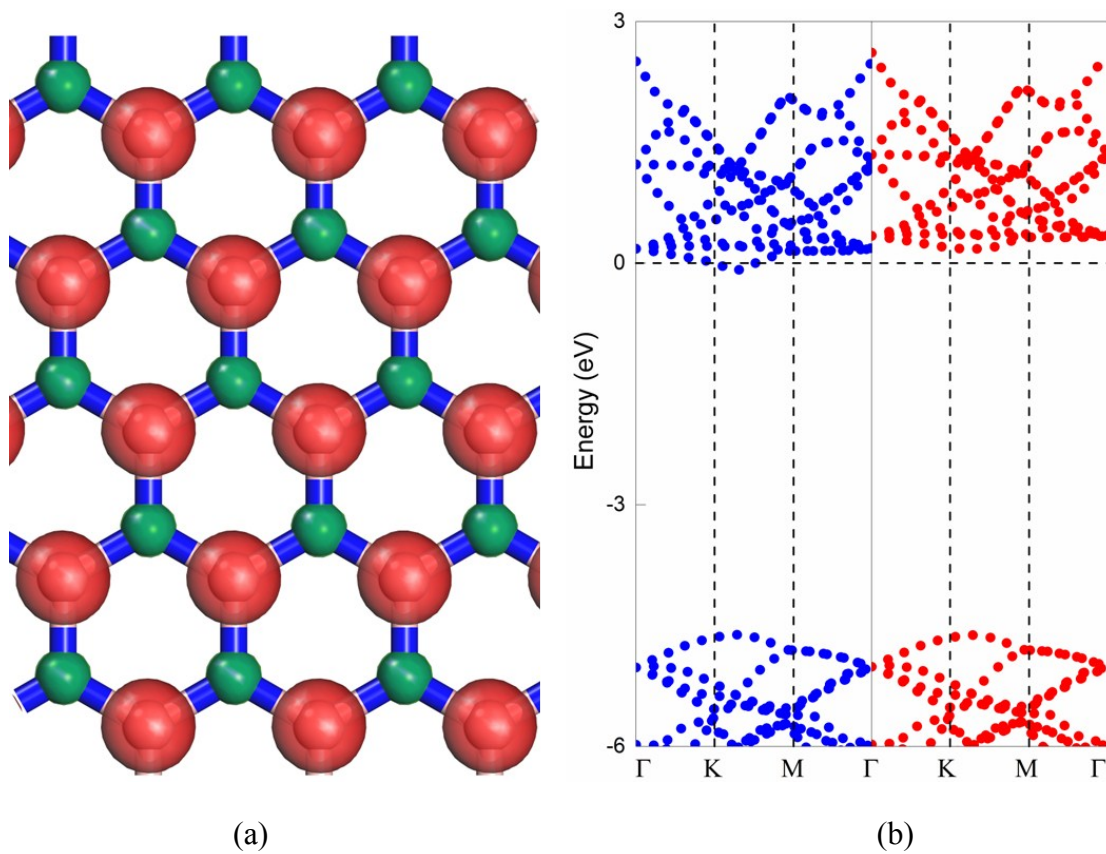


Figure S2. The computed (a) spin density iso-surface and (b) the band structure of negatively charged BN nanosheet. The Fermi level is set as zero in black dotted line.

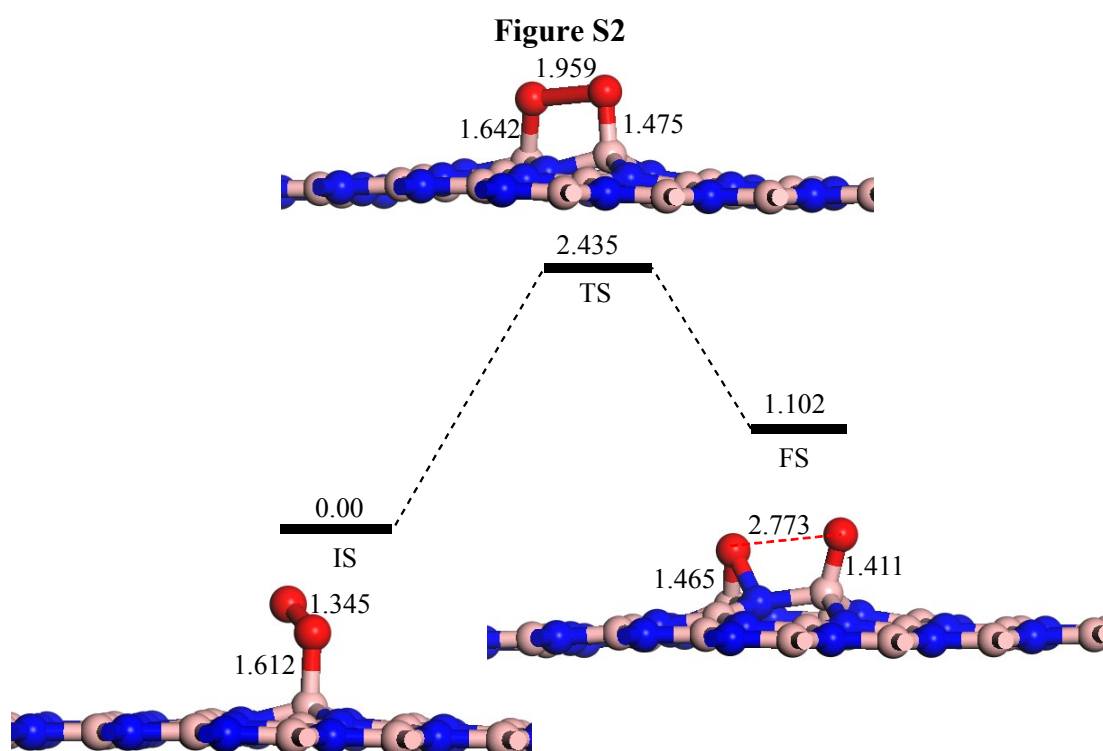


Figure S3. The MEP profile with the optimized geometries of reactants, transition states, and products for (a) $O_{2(ads)} \rightarrow 2O_{(ads)}$ on negatively charged BN sheets. The bond distances are in angstroms.

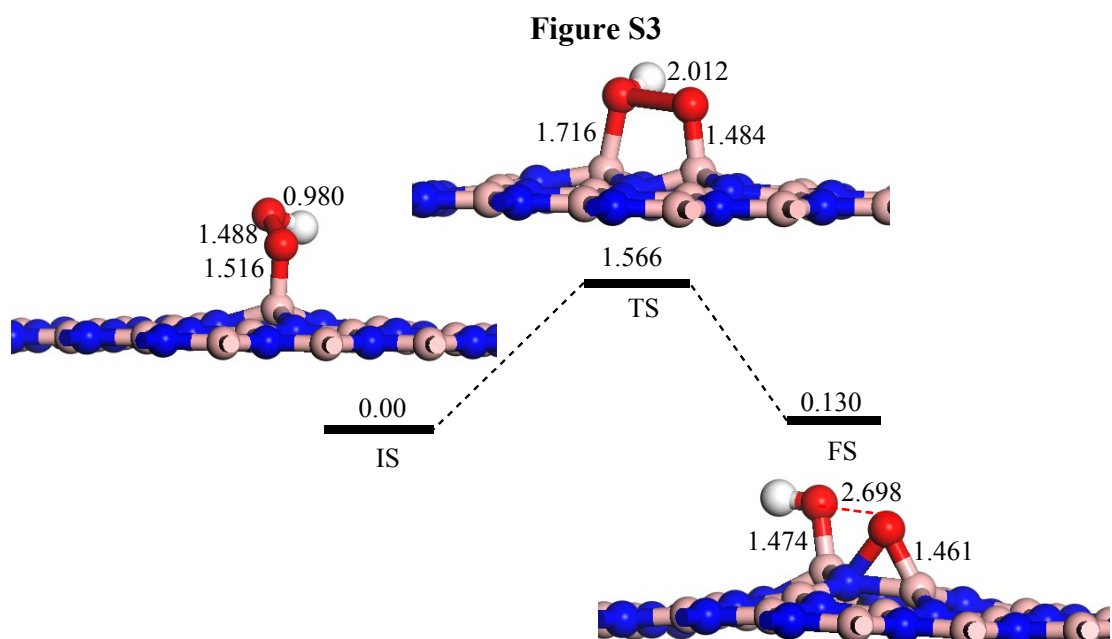


Figure S4. The MEP profile with the optimized geometries of reactants, transition states, and products for (a) $\text{OOH}_{(\text{ads})} \rightarrow \text{O}_{(\text{ads})} + \text{OH}_{(\text{ads})}$ on negatively charged BN sheets. The bond distances are in angstroms.