

“Supplementary Material”

Electrochemical reduction of NO catalyzed by boron-doped C₆₀ fullerene: a first-principles study

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Figure S1. The adsorption of NO over C atoms of $C_{59}B$, and the corresponding adsorption energy, Gibbs free energy change and PDOS plots. Bond distances are in Å.

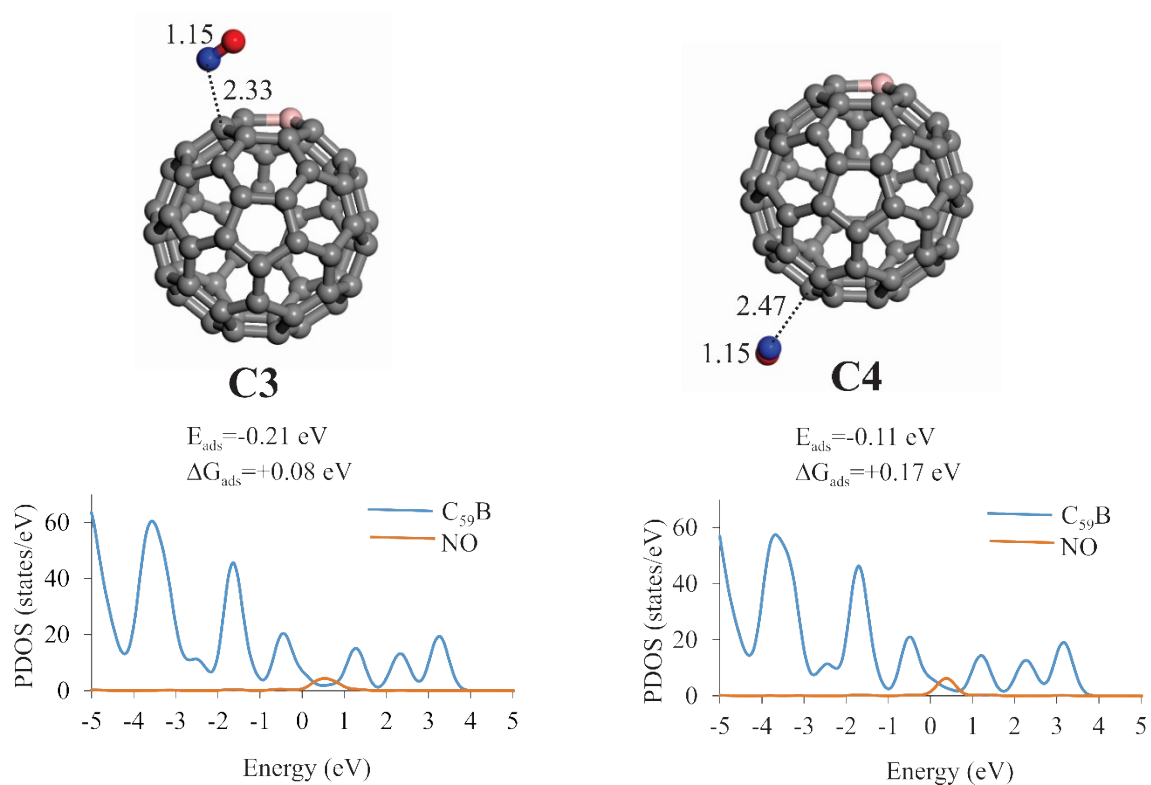
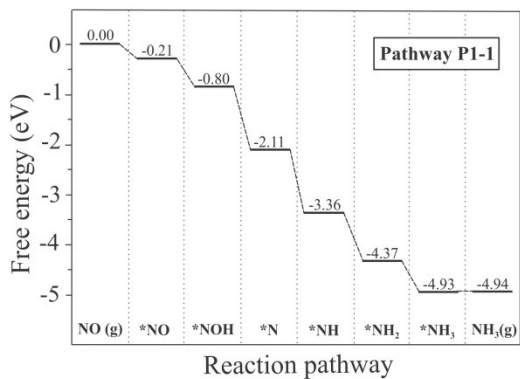
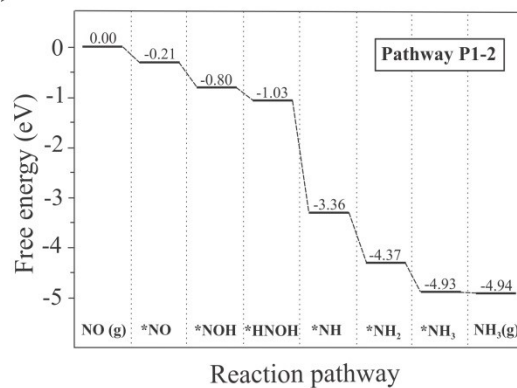


Figure S2. Free energy diagrams for the NOER to NH₃ over C₅₉B at zero and applied potential through (a) P1-1, (b) P1-2, (c) P2-1 and (d) P2-2 pathways

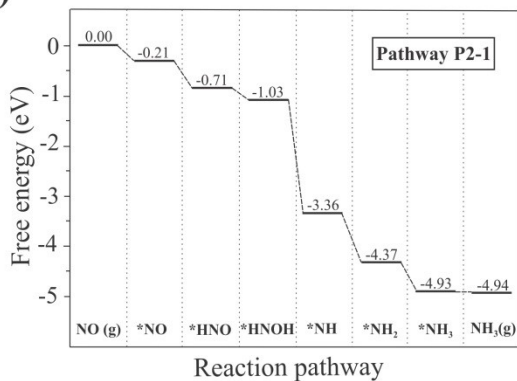
(a)



(b)



(c)



(d)

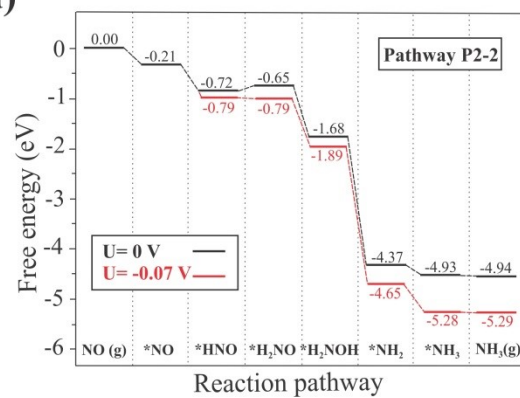


Figure S3. Reaction energy diagrams of NOER process over $C_{59}B$ along (a) P1-1, (b) P1-2, (c) P2-1 and (d) P2-2 pathways at low NO coverage

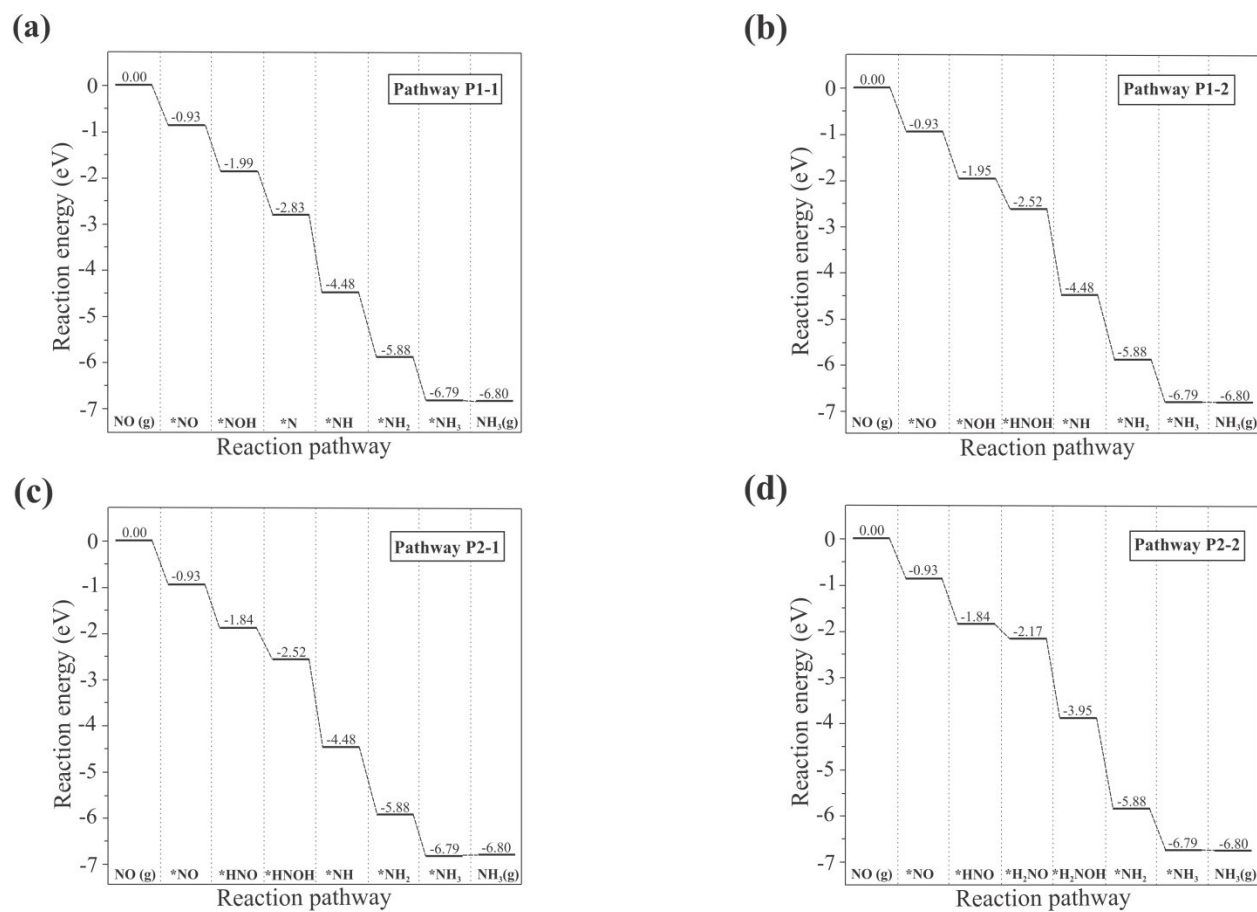
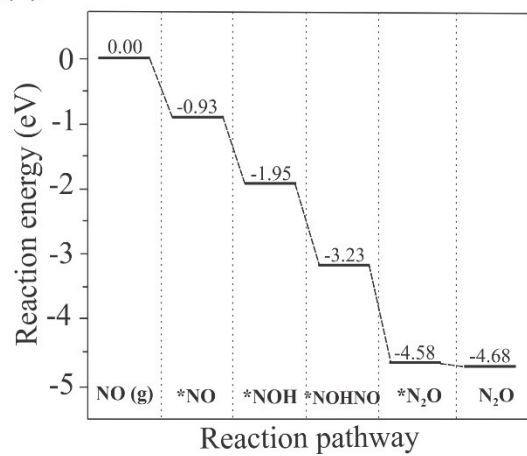


Figure S4. Reaction energy and free energy diagrams for NO conversion to N₂O catalyzed by C₅₉B

(a)



(b)

