

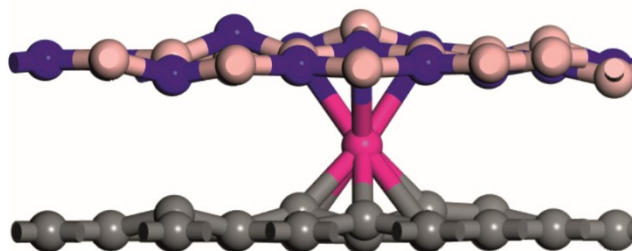
“Supporting Information”

A Vanadium Atom Sandwiched by Boron Nitride and Graphene Sheets for Electrochemical Reduction of Nitric Oxide: Insights from First-Principles Calculations

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Figure S1. (a) Final structure of BN/V/Gr after the AIMD simulations, and (b) potential energy diagram versus time during the AIMD simulations

(a)



(b)

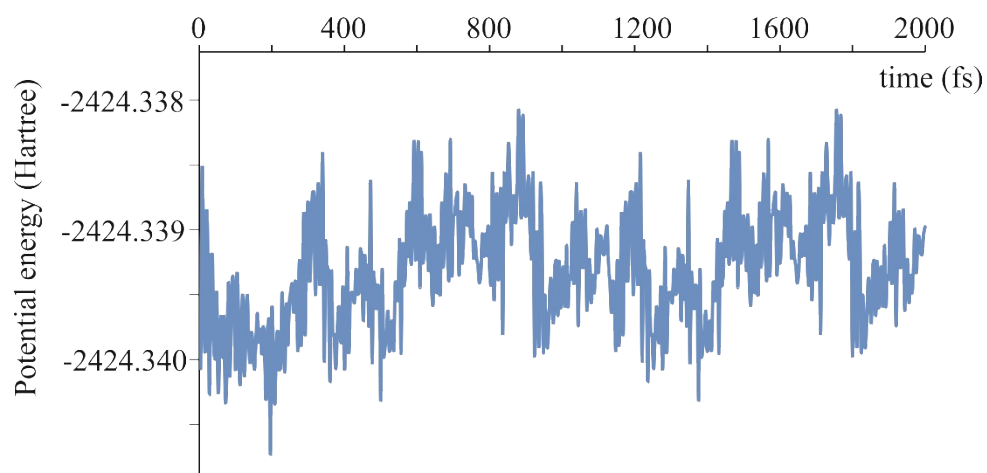


Figure S2. Interaction of NO molecule with the V atom of BN/V/Gr

