

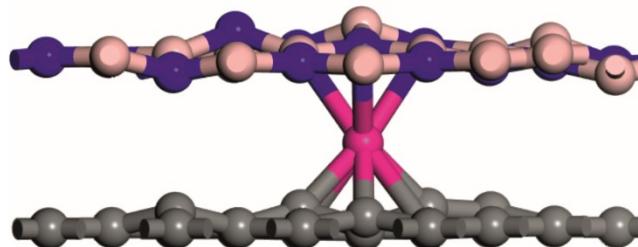
# “Supporting Information”

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

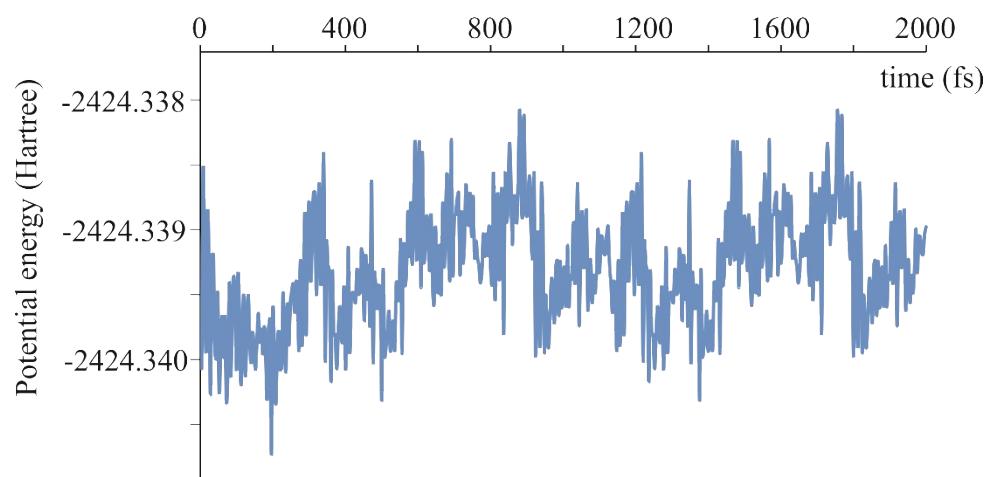
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**Figure S1.** (a) Final structure of BN/V/Gr after the AIMD simulations, and (b) potential energy diagram versus time during the AIMD simulations

(a)



(b)



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

