Supporting Information

Co-N_4 Moiety Embedded into Graphene as an Efficient Single-Atom-Catalyst for NO Electrochemical Reduction: a Computational Study

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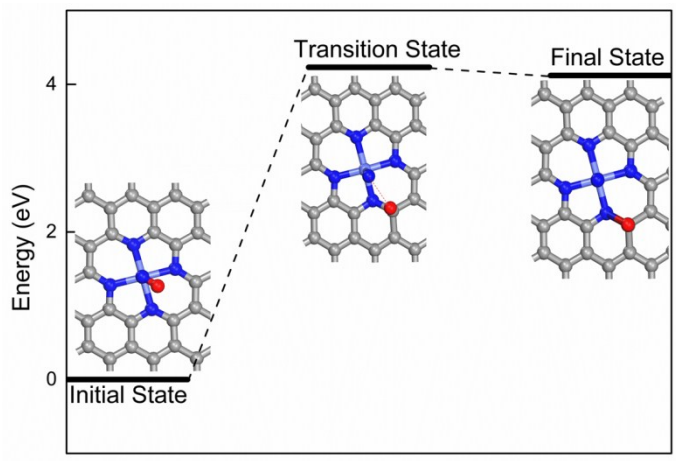

Figure S1. The minimum energy path (MEP) of NO dissociation on the Co-N_4 moiety embedded into graphene.

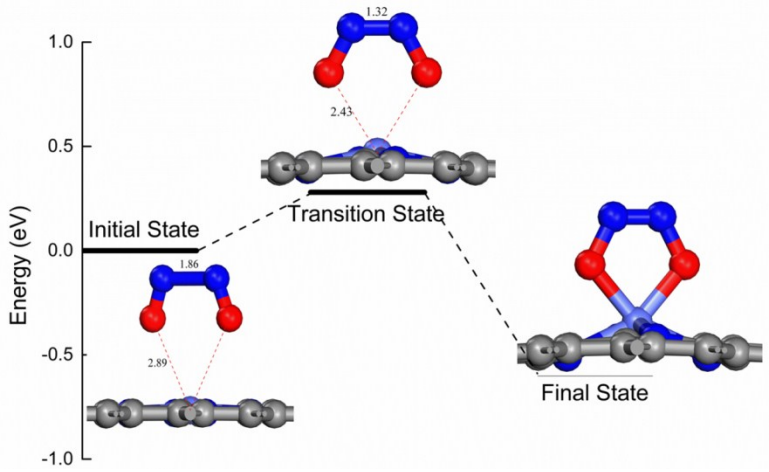

Figure S2. The minimum energy path (MEP) to form the energetically most favorable $(NO)_2$ dimer on the Co-N_4 moiety embedded into graphene.

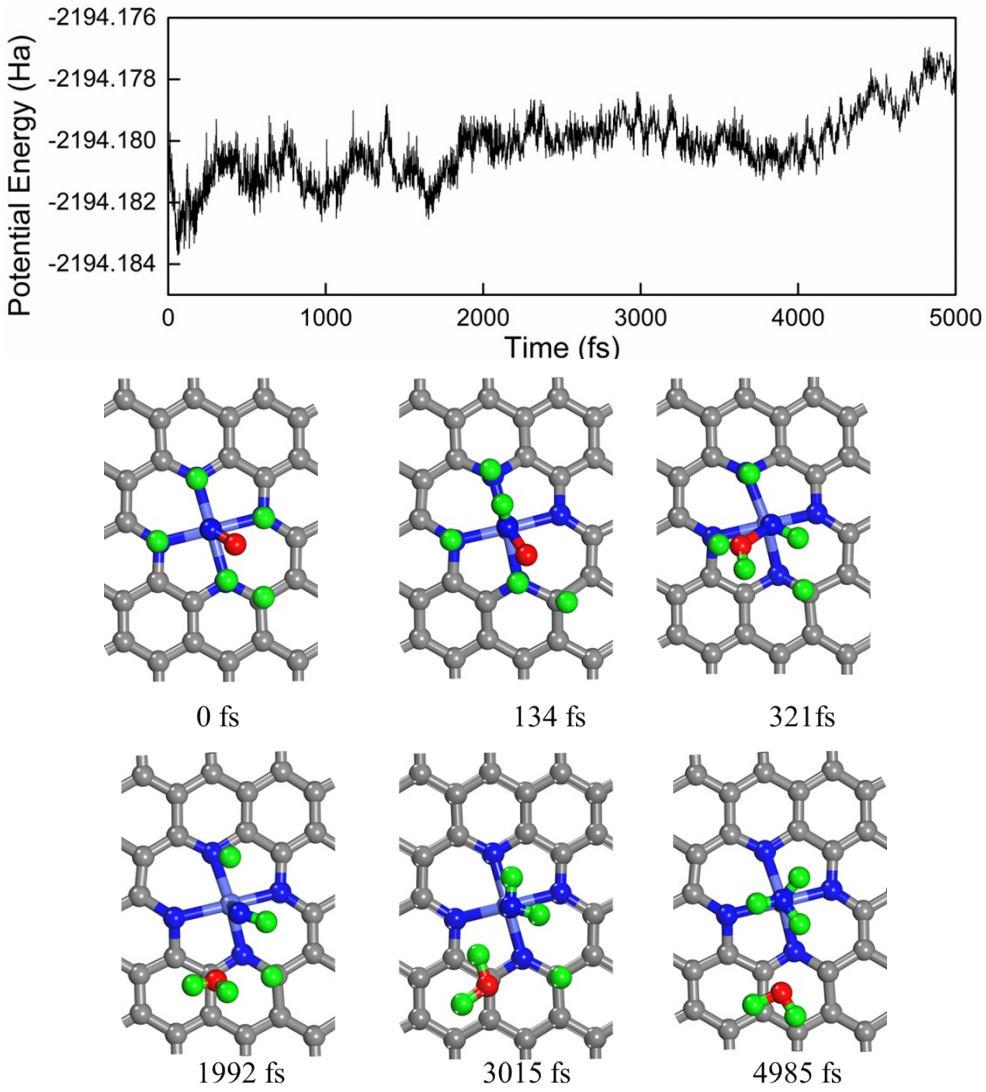

Figure S3. Some key snapshots during the trajectories of the first principles MD simulations of NO reduction on Co-N_4/graphene at 300 K.