Electronic Supplementary Material (ESI) for ChemComm.
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# Supporting Information
# Iron oxide cluster induced barrier–free conversion of nitric oxide to ammonia

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(Dated: January 18, 2015)

## I. SUPPORTING INFORMATION: COMPUTATIONAL METHOD

The grid-based projector-augmented wave (GPAW) method within the density functional theory is implemented [1]. The reactions over the gas phase $Fe_4$ are calculated within $\gamma$ point where 10 Å of vacuum condition is applied for all directions. Finite difference mode within GPAW is implemented. The grid spacing is set to 0.18 Å and 0.00 eV of smearing is applied. The exchange correlation of PBE exchange is applied with spin polarization calculations [2].

The reactions over supported $Fe_4$ cluster calculations are done within periodic condition with 15 Å of vacuum in z direction. Linear combination of atomic orbitals method within GPAW is implemented for supported clusters [3]. $2 \times 2 \times 1$ k points within the Brillouin zone sampling coupled with the Monkhorst-Pack scheme is applied along 0.1 eV of smearing [4]. Grid spacing is set to 0.22 Å and the spin polarization calculation is also applied. vdW-DF exchange correlation is implemented for supported case as the effect of Van Der Waals forces play an important role within the graphene calculation [5, 6].

The ground state structure of gas phase and supported $Fe_4$ clusters are searched by implementing the basin-hopping algorithm [7, 8]. Bader analysis is implemented for charge transfer analysis [9, 10]. Nudge elastic band method is implemented for calculating the activation barriers [11].

The adsorption energies ($E_{ad}$) of adsorbate on clusters is calculated by Equation (1):

$$E_{ad} = E(Cluster + Adsorbate) - E(Cluster) - E(Adsorbate) \quad (1)$$

Note that a negative sign indicates an exothermic reaction. The effect of the zero point energy of hydrogen is included in all cases.

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