Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

A density function theory study on the NO reduction on nitrogen doped graphene

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Supporting information 1:

Table S1: The vibrational frequencies of the transition states for the main reaction steps.

Reaction step	Vibrational frequencies (cm^{-1})
$NO \rightarrow N + O$	i514.83, 177.39, 257.18, 264.77, 359.79, 53.41, 745.31, 866.05,
$(NO)_2 \rightarrow N_2O + O_{ads}$	i196.09, 114.14, 146.46, 200.09, 246.53, 415.45, 580.19, 1089.55, 1340.12, 1903.21, 2383.35, 2425.07
$O_{ads} + NO \rightarrow NO_2$	i72.57, 73.80, 114.80, 138.75, 201.33, 233.71, 664.34, 952.20, 1788.35

Supporting information 2:

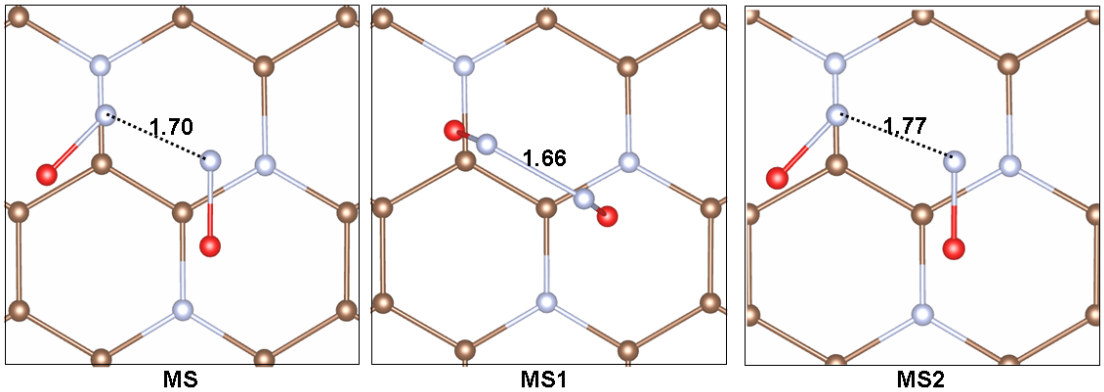

Figure S1: The metastable state structures for the co-adsorption of two NO molecules on the NG support. The E_t represent the total energy of the system and the MS2 represent the structure with the VdW correction.