Electronic Supplementary Information for:

Metal-free Catalytic Reduction of 4-Nitrophenol to 4-Aminophenol by N-Doped Graphene**

Xiang-kai Kong, Zhi-yuan Sun, Min Chen, Chang-le Chen, and Qian-wang Chen**

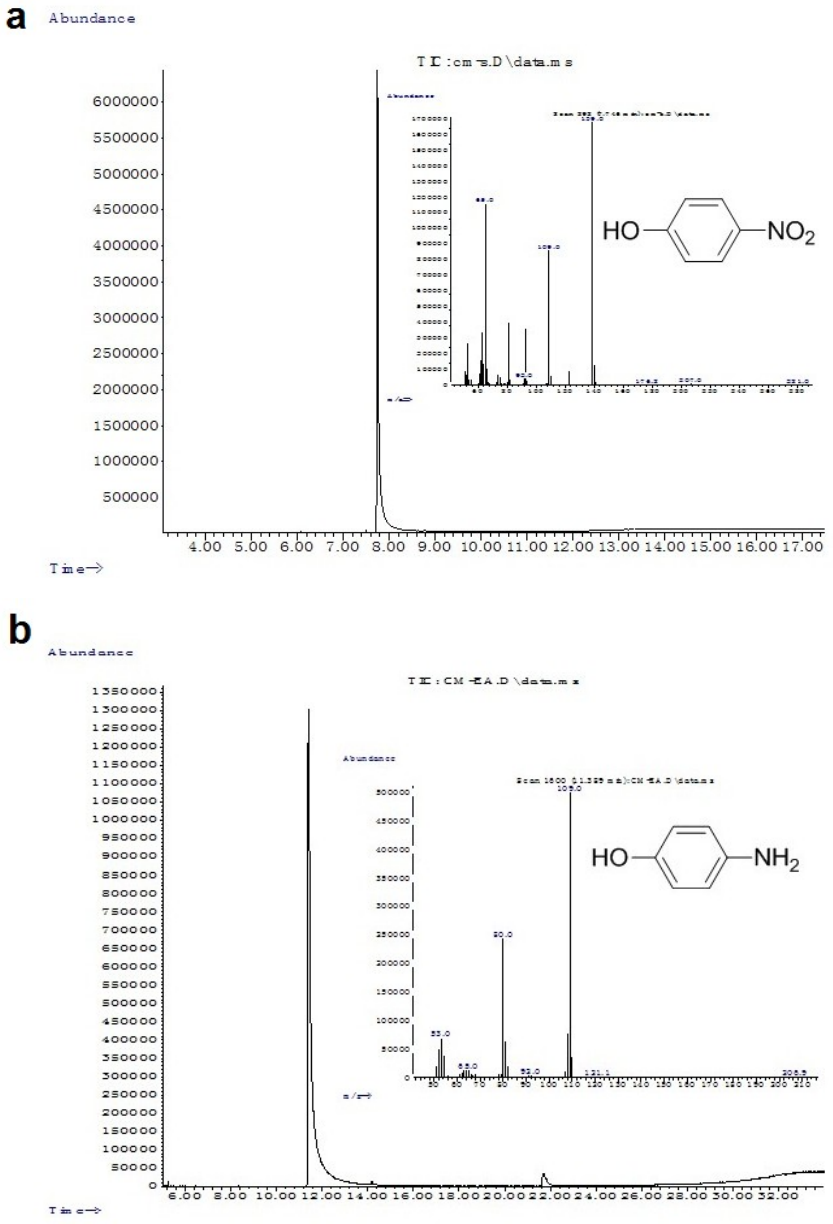

Figure S1. The GC-MS results of (a) the reactant Nip and (b) the Amp product after extracting the reaction mixture with ethyl acetate. (The small peak at retention time ca. 22min is unknown impurity, from the solvent or the small pieces of graphene. However, it is not Nip based on the retention time and the mass spectrum)

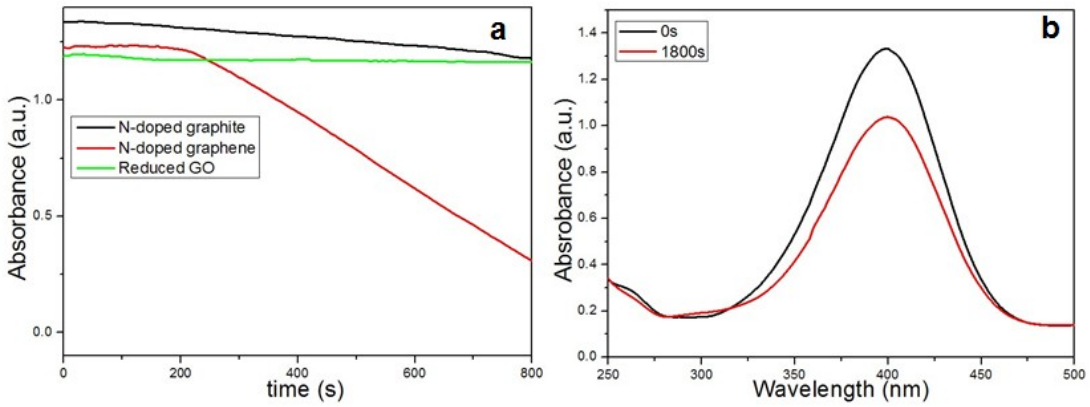

Figure S2. (a) The measured curves of absorbance at 400 nm vs. time for N-doped graphene, N-doped graphite and reduced GO; (b) The UV/Vis spectra of reduction Nip for N-doped graphite.

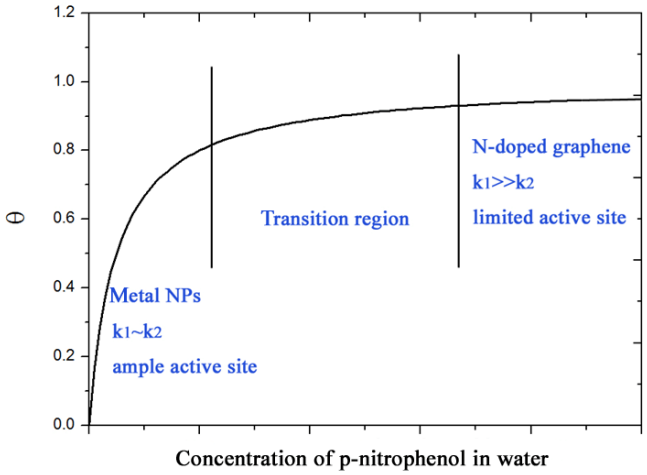

Figure S3. Diagram of Langmuir adsorption isotherm for metallic nanoparticles and N-doped graphene.

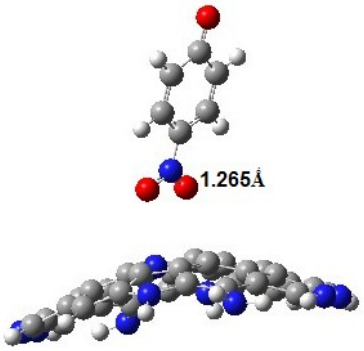

Figure S4. The optimized structure of Nip ion absorbed on the N-doped graphene sheet via its nitro group, and the large separated distance indicates a weak interaction at the interface. The N-O bond length has been marked directly.

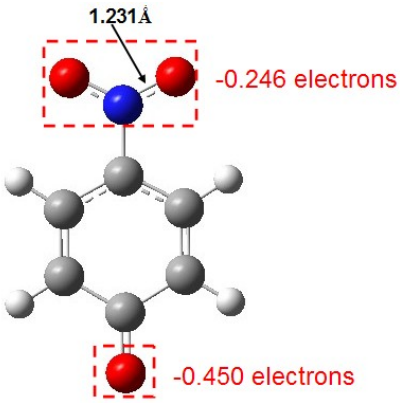

Figure S5. The calculated charge distributions for the nitro group and the O atom (adsorption site) of one free Nip ion, with the N-O bond marked directly.

Models	E_{ads} (Hartree)
N-doped graphene	-0.0665
N-doped graphene via nitro group adsorption	-0.0282
pristine graphene with center adsorption	0.0006
pristine graphene with edge adsorption	-0.0009
graphene doped with pyridinic N atoms	-0.0082
graphene doped with pyrrolic N atoms	-0.0173
graphene doped with amine like N atoms	-0.0752
graphene doped with graphitic N atoms	-0.0549

Table S1. The calculated Nip adsorption energies for these discussed graphene models.