Online supporting information for:

Stability and Core-level Signature of Nitrogen Dopants in Carbonaceous Materials

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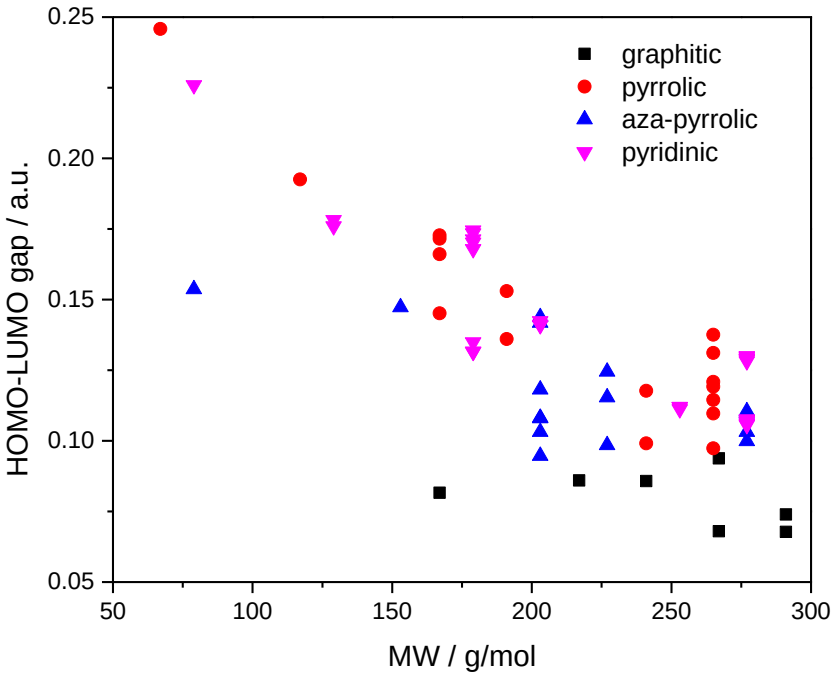

Figure S1. HOMO-LUMO gap versus molecular weight for the 69 model compounds.

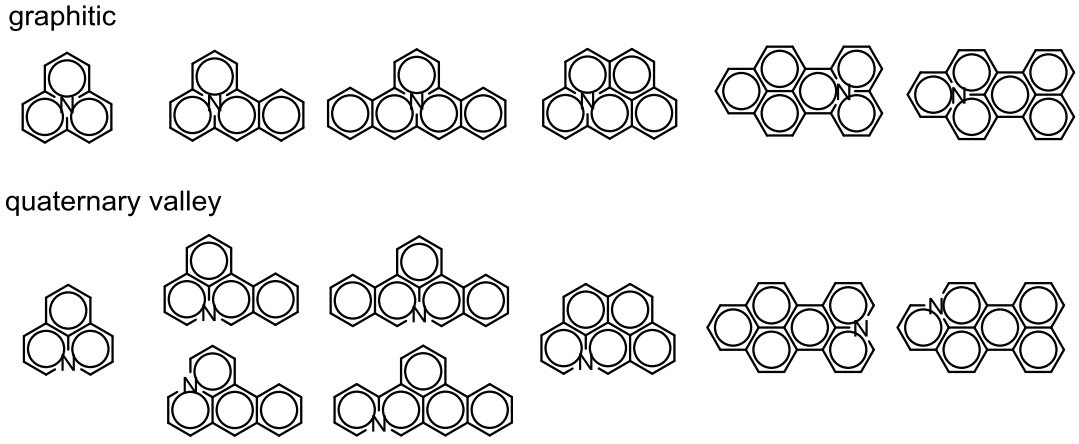

Figure S2. Model compounds containing graphitic and quaternary-valley nitrogen atoms.

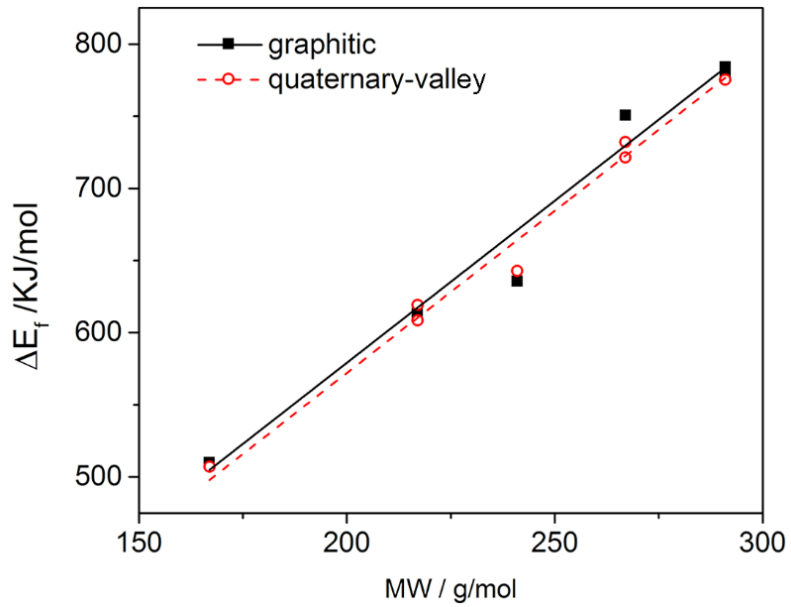

Figure S3. Calculated formation energies of compounds containing graphitic and quaternary-valley nitrogen dopants.

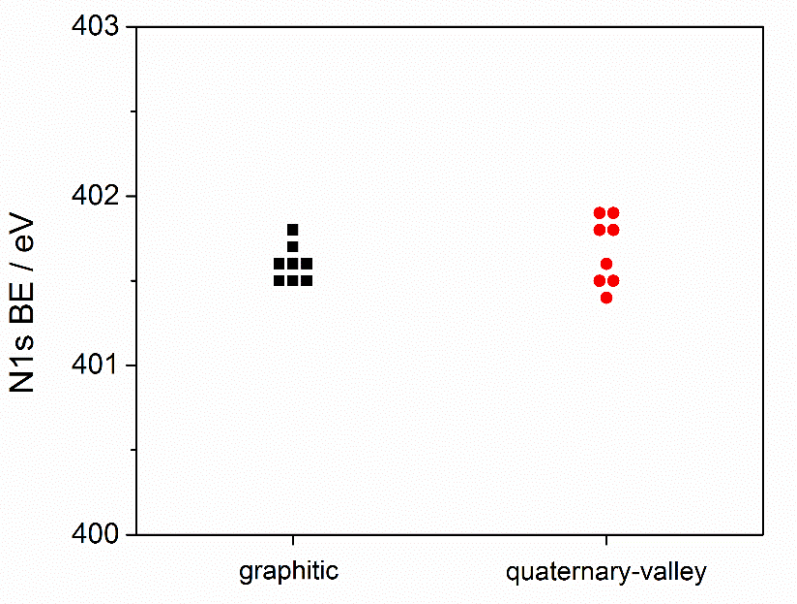

Figure S4. Comparison of simulated N 1s binding energies of graphitic and quaternary-valley nitrogen atoms.

How we chose the small N-containing molecules for their experimental N 1s binding energies: In the National Institute of Standards and Technology (NIST) X-ray Photoelectron Spectroscopy Database online,[1] there are hundreds of nitrogen-containing compounds whose experimental XPS spectra and N 1s binding energies are available. Most of the compounds are organometallic. For this study, we picked from the database those N-containing organic compounds (shown in Figure 4 of the main text) similar to our model compounds (Figure 1 of the main text), such as pyrrole, pyridine, porphyrin, amine, azobenzene and nitrobenzene molecules. Their experimental N 1s binding energies range from 397.9 to 405.9 eV.[1]

Reference:

1. Naumkin, A. V.; Kraut-Vass, A.; Gaarenstroom, S. W. and Powell, C. J. NIST X-ray Photoelectron Spectroscopy Database, http://srdata.nist.gov/xps/; last accessed, June 9, 2015.