Theoretical Study of Nitrogen-Doped Graphene Nanoflakes: Stability and Spectroscopic Properties Depending on Dopant Types and Flake Sizes

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The physical chemical properties of nitrogen-doped hexagonal and rectangular graphene nanoflakes (GNFs), which are affected by substitutional dopant types, positions, and numbers as well as flake shapes and sizes, have been investigated by using DFT calculations. It shows that nitrogen atoms locating on zig-zag edges are generally more stable than those on armchair edges or inside flakes. Interplay between multiple nitrogen dopants in the same flake is more complicated examined by their frontier molecular orbitals. The UV-visible absorption spectra of these nitrogen-doped GNFs display strong dependence on flake sizes, where the larger flakes have their major peaks in lower energy ranges. Moreover, the spectra exhibit different connections to various dopant types and positions: the graphitic-type (simple substitution) dopant species present large variety in absorption profiles, while the pyridinic-type ones show extraordinary uniform stability and spectra independent of dopant positions/numbers and hence are hardly distinguishable from each other.

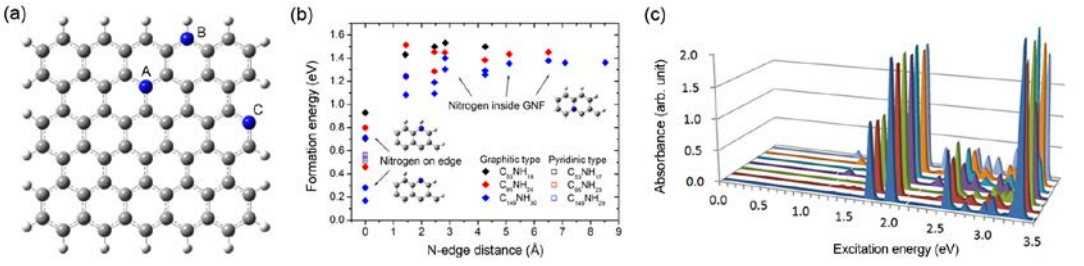

Figure 1. (a) Various nitrogen dopant types and positions in graphene nanoflakes. (b) Formation energies of single-nitrogen-doped models depending on nitrogen-edge distance. (c) UV-visible absorption spectra of pyridine-type models showing position-independent features.

References:

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