Calculating core level binding energies for graphene and azafullerenes

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X-ray photoelectron spectroscopy (XPS) combined with first principles modeling is a powerful tool for determining the chemical composition of novel materials, such as graphene and carbon nanotubes doped with heteroatoms [1].

As a model system, we calculated the C1s binding energy of graphene using two methods based on density functional theory total energy differences: a calculation with an explicit core-hole [2], and an all-electron extension of the delta self-consistent field method [3], with the latter giving absolute energies close to graphite measurements.

Furthermore, we analyzed spectra of C_{60} and $C_{59}N$ fullerene powders [4], elucidating the identity of the oxygen signal. The calculations also allow us to quantify the effect of $C_{59}N$ dimerization on its N1s core-level shift (0.4 eV), with implications for interpreting other nitrogen-doped systems.

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