Calculating core level binding energies for graphene and azafullerenes

Toma Susi 1, Duncan J Mowbray 2, Mathias P Ljungberg 2, Dogan Erbahar 3, Carla Bittencourt 4, Christopher P Ewels 3, Paola Ayala 5

1 Faculty of Physics, University of Vienna, Austria
2 Donostia International Physics Center, San Sebastian, Spain
3 Institut des Materiaux Jean Rouxel, Universite de Nantes, France
4 Chemistry of Interaction Plasma-Surface, University of Mons, Belgium
5 paola.ayala@univie.ac.at

Contact e-mail: toma.susi@univie.ac.at

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 C60 and C59N fullerene powders [4], elucidating the identity of the oxygen signal. The calculations also allow us to quantify the effect of C59N dimerization on its N1s core-level shift (0.4 eV), with implications for interpreting other nitrogen-doped systems.