

# Core level binding energies of defected and functionalized graphene

T. Susi<sup>1</sup>, M. Kaukonen<sup>1</sup>, M. Ljungberg<sup>2</sup>, P. Ayala<sup>3</sup>, E. I. Kauppinen<sup>1</sup>

<sup>1</sup>*NanoMaterials Group, Department of Applied Physics, Aalto University School of Science, Finland*

<sup>2</sup>*Chemical Physics Group, Department of Physics, Faculty of Science, Stockholm University, Sweden*

<sup>3</sup>*Faculty of Physics, University of Vienna, Austria*

X-ray photoelectron spectroscopy (XPS) is a widely used tool for probing carbon-based nanomaterials. To interpret the binding energies measured by XPS, references to which such energies can be compared is needed. We have employed core-hole calculations utilizing a Delta Kohn-Sham total energy differences method recently implemented [1] in the real-space grid-based projector-augmented wave (GPAW [2]) DFT code to calculate reference core level energies for defected and functionalized graphene.

Our graphene system had a 9x9 unit cell with periodic boundary conditions, treated with 3x3x1 k-points. Using the PBE functional, we calculated C1s and O1s core level energies for simple oxygen and hydrogen functionalities such as the hydroxide, epoxide and carboxylic groups. In addition, we considered the elementary atomic defects [3]: single and double vacancies, and the Stone-Thrower-Wales defect. Finally, modifications of the reactive single vacancy with O and H containing groups were considered. The calculated C1s and formation energies were compared to data in the literature, and Bader analysis [4] employed to elucidate the effect of charge transfer to the observed shifts.

[1] M.P. Ljungberg, J.J. Mortensen, and L.G.M. Pettersson, *J. Electron Spectros. Related Phenom.* 10.1016/j.elspec.2011.05.004 (2011)

[2] J. Mortensen, L. Hansen, and K. Jacobsen, *Phys. Rev. B* 71 (2005) 035109

[3] W. Tang, E. Sanville, and G. Henkelman, *J. Phys. Condens. Matter* 21 (2009) 084204

[4] F. Banhart, J. Kotakoski, and A.V. Krasheninnikov, *ACS Nano* 5 (2011) 26