GRAPHENE AND ADATOMS: *AB INITIO* CALCULATIONS AND HYPERFINE INTERACTIONS

A. S. Fenta[1,2,3*], J. N. Gonçalves[1], C. O. Amorim[1], J. G. Correia[3,4], K. Johnston[3], H. Haas[2], V. S. Amaral[1], S. Cottenier [5], L. M. C. Pereira[2]

[1] Department of Physics and CICECO, University of Aveiro, 3810-193 Aveiro, Portugal

[2] KU Leuven, Instituut voor Kern- en Stralingsfysica, Celestijnenlaan 200 D, 3001 Leuven, Belgium

[3] CERN, EP Division, 1211 Geneva 23, Switzerland

[4] Centro de Ciências e Tecnologias Nucleares (C2TN), Instituto Superior Técnico, Universidade de Lisboa, 2686-953 Sacavém, Portugal

[5] Department of Materials Science and Engineering, Ghent University, Technologiepark 903, BE-9052 Zwijnaarde, Belgium

*fenta@ua.pt

Abstract

From the moment it was isolated as a 2-dimensional material, graphene has become a remarkable subject of research, exhibiting novel phenomena that extend to virtually every domain of solid state physics and applications [1,2]. A particularly active domain of graphene research deals with its interaction with atoms which are adsorbed on its surface (*adatoms*) [3,4].

We present *density functional theory* (DFT) calculations of the interaction between graphene and adatoms: atomic positions, binding energies, electronic structure, and hyperfine parameters. While DFT calculations (arguably) lack absolute predictive power in this context, they can provide great insight when combined with experimental studies. Our work is based on the combination of DFT calculations and experimental hyperfine techniques: perturbed angular correlation (PAC) spectroscopy and Mössbauer Spectroscopy (MS). Experimental hyperfine parameters – *electric field gradient* (EFG) and *hyperfine magnetic field* (HMF) – are measured using PAC and MS, and compared to the EFG and HMG values calculated for various structural/electronic/magnetic configurations. The EFG carries the signature of the atomic position with respect to the graphene host, charge state, and type of bonding (ionic, covalent, van der Waals). The HMF provides information on the electronic (and spin) configuration and, in appropriate cases, magnetic phenomena (paramagnetism, magnetic interactions…). As representative examples, we present calculations for Fe, Ta and Hg adatoms, which have suitable MS (Fe) and PAC (Ta, Hg) isotopes and decay schemes.

These calculations form the basis for the experiments which are currently being prepared at the ISOLDE facility at CERN, using ASPIC (Apparatus for Surface Physics and Interfaces at CERN) [5].

References

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