PhD position on Graphene-based materials: Exploring new physical properties based on theoretical simulations

Research Center: Condensed Matter Physics Center (IFIMAC) - http://www.ifimac.uam.es/-

Center Description: The IFIMAC Center is a new María de Maeztu Excellence Research Unit located in the campus of the Universidad Autónoma de Madrid pursuing cutting-edge research and scientific excellence.

Area of knowledge and discipline: PHYSICAL SCIENCES, MATHEMATICS and ENGINEERING panel. PHYSICS

Project Title: Graphene-based materials: Exploring new physical properties based on theoretical simulations

Group leader: Dr. Cristina Díaz Blanco. CampuS Theoretical Group.
https://campusys.qui.uam.es/ (Computations in Atomic and Molecular Physics of Unbound Systems)

Research project / Research Group description:

Since 2004, when synthesized for the first time, graphene and graphene-base materials have received a big deal of attention within condensed matter and surface science community. However, discrepancies still persist related to their structural, geometrical and electronic properties. Within this project the PhD student will carrie out a detailed study of graphene-based materials, focused on functionalized graphene, using state-of-the-art computational tools, from electronic structure to dynamics methods. Theoretical simulations will also allow us to proposed new functionalized graphene-based materials, with specific properties suitable for specific practical applications. Our group has been working with these theoretical tools for the last decade, and as a result of this effort, we have made quite relevant contributions to the knowledge, for both dynamics [Science 326, 832 (2009); Phys. Rev. Lett. 108, 236104 (2012); Chem. Soc. Rev 45 3658 (2016)] and geometrical [Phys. Rev. Lett. 106, 186102 (2011); ACS Nano 2, 2927 (2013)], electronic [Nanoscale 6, 15271 (2014)], and magnetic [[Nat. Physics 9, 368 (2013); Nano lett. 14, 4560 (2014)] properties.

Job position description:

The PhD student working on this project will be responsible for the computational modeling of functionalized graphene, and for the analysis of their geometrical and electronic properties. The student will receive specialized training in the research area, specifically in density functional theory and in periodic boundary conditions (PBC) simulations. He/she will have access to vast technological resources, including the Computational Center of the UAM and the Spanish Supercomputing Network. He/she will have the opportunity of collaborate with top (theoretical and experimental) groups in the area.

The ideal candidate should have a master in condensed matter Physics, theoretical Chemistry, or equivalent, and a solid background in solid state physics. Experience with PBC simulations packages and programming skill will be evaluated positively, but not mandatory. He/she should have a strong commitment towards critical and independent thinking, as well as, towards teamwork. Good knowledge of English, both written and oral, is required.

Related link to the position:
http://www.uam.es/departamentos/ciencias/quimica/spline/cristina/index.html