

PhD position on Chemical-physics properties of new 2D materials

Research Center: FUNDACION IMDEA NANOCIENCIA - <http://www.nanociencia.imdea.org/>

Center Description: IMDEA Nanociencia is a young interdisciplinary research centre dedicated to the exploration of basic nanoscience and the development of applications of nanotechnology in connection with innovative industries. IMDEA Nanociencia has been recently selected as Severo Ochoa Centre of Excellence.

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

Project Title: Chemical-physics properties of new 2D materials

Group leader: Prof. Fernando Martín García.

<http://nanociencia.imdea.org/fernando-martin-s-group/group-home>

Research project / Research Group description:

Two-dimensional (2D) materials have received a big deal of attention during the last decade, these materials include not only a free-standing monolayer, or a monolayer adsorbed on isolating materials, but also a monolayer adsorbed on semiconductors or metals that allow to functionalize these 2D materials, changing, modifying or altering their chemical-physics properties. Our aim within this project is to propose new 2D materials with specific properties suitable for specific practical applications, using as working tool computational modeling. Our group has been working in this field for the last decade, and as a result of this effort we have made important contributions to the knowledge, such as an exhaustive study of graphene properties adsorbed on a metal surface [Nat. Physics 9, 368 (2013); ACS Nano 2, 2927 (2013); Nano Lett. 14, 4560 (2014); Nanoscale 6, 15271 (2014)], and a detailed description of the electronic structure of 'Antimonene' [Adv. Mater. 28, 6332 (2016)]. The PhD student will work in the study of the properties of these new 2D materials.

Job position description:

The PhD student working on this project will be responsible for the computational modeling of new 2D materials, and for the analysis of their chemical-physics properties, with the aim of proposing structural changes that result in specific turned 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 those provided by the Computational Center of the Universidad Autonoma de Madrid (UAM) and the Spanish Supercomputing Network (RES). He/she will have the opportunity of collaborate with top (theoretical and experimental) groups in the area. The candidate will work in close collaboration with researchers from the Campus theoretical group at UAM (<https://campusys.qui.uam.es/>).

The ideal candidate should have a master in Condense Matter Physics, in Theoretical Chemistry, or similar area. Knowledge of PBC simulation packages and programming skills are desirable but not mandatory. Good knowledge of English and teamwork skills are required.

Related link to the position:

Campus theoretical research group: <https://campusys.qui.uam.es/>