

## Chemical-physics properties of new 2D materials

**IMDEA - Nanociencia Institute**

[www.nanociencia.imdea.org](http://www.nanociencia.imdea.org)

### **CENTRE 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.

Our purpose-built building was inaugurated in 2014 and features state-of-the-art facilities for 21st century science, where the frontiers between fields disappear and Physics, Chemistry, Biology, Engineering, and Medicine merge. It features more than 30 operative laboratories with over € 16 M worth of equipment - including the Centre for Micro and Nanofabrication. We are located at the UAM Campus, with access to all the facilities of one of Spain's largest and most prestigious Universities. The UAM Campus is just a few minutes away from Madrid's lively city centre, connected by "cercanías" trains and several bus lines.

We are over 150 scientists, with different professional and personal backgrounds. Approximately 40% of our PhD and postdocs come from outside Spain, representing every corner of the world, from Germany to China, from the USA to Singapore –a true international environment in which to develop your scientific career. Women make up 36% of our scientific and 62% of our management staff. No matter who you are or where you come from, you will feel welcome from the very first minute.

We take science seriously and value quality over quantity. Our scientists enjoy tackling complex multidisciplinary problems, often within in-house collaborations, so all of our students receive truly interdisciplinary training. We also enjoy publishing in the very best journals, with >200 publications a year, and an institutional h index of 79. Check out our webpage <http://nanociencia.imdea.org/>, facebook @IMDEANanociencia or twitter @IMDEA\_Nano for more information.

So if you are a talented, hard-working individual with a real interest in Science, IMDEA Nanociencia is the right place for you! Come work with us!

### **ADDRESS**

Faraday 9, 28049 Madrid, Madrid

### **AREA OF KNOWLEDGE**

Physical Sciences, Mathematics and Engineering

### **GROUP OF DISCIPLINES**

Physics

## GROUP LEADER

Prof. Fernando Martín García

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**Research Group Website:** <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), *Sciences Advances* (2018)], 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.

## OTHER RELEVANT WEBSITES

Campus theoretical research group

<https://campusys.qui.uam.es/>