

CONTRATOS PREDOCTORALES 2020 SEVERO OCHOA

PROJECT TITLE / JOB POSITION TITLE:

Innovative strategies to fabricate 2D covalent materials for energy and environmental applications

RESEARCH PROJECT / RESEARCH GROUP DESCRIPTION: (2.000 characters – including spaces)

The success of organic semiconductors (OSCs) in photovoltaic devices boosts optimization of OSC properties for operation as photo-electrodes in solar energy conversion to electricity or chemical energy. These materials are also extremely promising for gas storage, catalysis, sensing and environmental applications (e.g. reduction of CO₂ and photo-degradation of pollutants). A new alternative for miniaturized model OSC systems relies on two-dimensional covalent organic frameworks (2D-COFs) where different π -conjugated molecules are covalently bonded to form 2D layers. Because the large choice of available commercial and synthetic molecules (building blocks), COFs have an enormous chemical versatility and modularity, in which functionalization and tunable pore size can be used to control their physical and chemical properties. An unprecedented achievement would be demonstrating how confinement of water in nanometer size pores affects the water splitting capability of the COFs. The limiting factors are the difficulties to have COFs as well ordered, oriented and continuous thin films. However, improved control over film formation may be possible using the innovative bottom-up synthesis on surfaces. This strategy (see **“On-surface synthesis: a guide for explorers”**) uses small precursors that confined on a surface react to form single molecular layers. *The PhD candidate will fabricate of 2D-COFs by on-surface synthesis with a systematic variation of the pore size and functionalization by selecting the appropriate precursors and characterize them by surface science techniques. To that end, diverse molecular lengths will vary the pore size, and diverse side groups (hydrophobic or hydrophilic) will influence the interaction of the 2D-COF with water. Main goal: obtaining ordered 2D layers in clean environments by pulsed layer injection using molecular solutions and by deposition from sublimation. Characterization by Scanning Tunneling Microscopy, X-ray diffraction, X-ray and UV spectroscopies.*

“On-surface synthesis: a guide for explorers”

<https://mappingignorance.org/2019/05/23/on-surface-synthesis-a-guide-for-explorers/>

JOB POSITION DESCRIPTION:

(2.000 characters – including spaces)

Include all the relevant information about the position, role, responsibilities and skills required within the project/group

The research fellow will be integrated in an international community and benefit of a collaborative and friendly atmosphere, with physicists and chemists, in the Institute of Materials Science of Barcelona (ICMAB). *The proposal develops within highly synergetic collaborations established with other ICMAB groups, in particular those led by Dr. J. Farauo (Theory group) and Dr. N. Aliaga in the same Research Unit (Functional Surfaces and Interfaces).*

The young researcher will be trained to use, in an autonomous way, standard surface science techniques in the group laboratories, including advanced scanning probe microscopy methods as Scanning Tunneling and Atomic Force Microscopies (STM and nc-AFM) in ultra-high-vacuum (UHV). In addition, the fellow will have the opportunity to employ photoelectron spectroscopy and perform sophisticated measurements (XPS, UPS, GIXD, NEXAFS, PEEM-LEEM...) in synchrotron radiation facilities around Europe. The main tasks in the project include deposition on clean surfaces using a novel atomic layer injection system (to deposit molecules by liquid micro-droplets and evaporation facilities (to deposit molecules by sublimation), both in clean UHV conditions. The on-surface processing will employ thermal activation polymerization of the building blocks (confined on the surface) to induce supramolecular growth by covalent bonding. The molecular-scale structure and chemical and electronic properties of the obtained 2D-COF layers will be investigated by the surface science techniques mentioned above. We are looking for a highly motivated candidate with good academic record holding a Master degree in Materials Science/Engineering, Nanoscience/Nanotechnology, Chemical Engineering, Chemistry or Physics. Curiosity for research and interest in experimental investigation are essential. Good English skills will be positively considered.

GROUP LEADER:

Title: Prof.

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Research project: Photochemistry and stability of organic/water model interfaces for water splitting (ref: PID2019-110907GB-I00) /

Research Group website: Physical Chemistry of Surfaces and Interfaces group

<https://departments.icmab.es/surfaces/>

RELATED LINKS TO THE POSITION (optional)

URL: <https://departments.icmab.es/surfaces/phd-fellowship-severo-ochoa-2020/>

Title link: Open positions. PhD fellowship Severo Ochoa 2020