



CONTRATO PREDOCTORAL 2018 - ICMAB Severo Ochoa

PROJECT TITLE / JOB POSITION TITLE:

Use of highly ordered switchable ferroelectric films to enhance the water splitting activity of TiO₂ photo-catalysts

RESEARCH PROJECT / RESEARCH GROUP DESCRIPTION:

One of the most promising technologies capable of providing high energy yield without pollutant byproducts is the photocatalytic water splitting (PWS) using sunlight.

To achieve overall water splitting the redox reactions of water splitting are first initiated by photon absorption to generate electron-hole pairs. The charge carriers migrate to the surface of the catalysts and react with surface active sites to reduce water to form hydrogen, while the holes oxidize water molecules to give oxygen.

TiO₂ is one of the most studied photocatalysts, however, its fast charge carrier recombination (electron-hole pairs) results in the release of unproductive energy.

Ferroelectric (FE) film systems showing spontaneous polarization (SP) oriented along the film normal direction exhibiting an open-circuit photovoltage under illumination can drive charge carriers to opposite surfaces (bulk photovoltaic effect). The FE-field acts to drive electrons and holes to different locations on the surface, thus creating spatially separate sites for reduction and oxidation reactions. The FE's dipolar field can be exploited covering the FE with the appropriate photocatalyst (TiO₂). Assuming that the Fe-field is not completely screened by charge at the interface, it will influence carriers in the film. BiFeO₃ and BaTiO₃ are semiconductors with a relatively narrow band gap (2.5, 3.42 eV) and well defined SP along their pseudo-cubic <111> and <001> directions, respectively. Their internal polarization will reduce recombination of the photogenerated carriers and will enhance the photocatalytic efficiency.

The TiO₂ films will be grown on BaTiO₃(001) and/or BiFeO₃(111) films over SrTiO₃(001) and SrTiO₃(111), respectively. Several TiO₂ film thicknesses will be grown by PLD to understand: the evolution of the TiO₂ film structure, its interface, polarization decay dependence with film thickness, surface and electronic film properties under operando electrochemical conditions with external applied bias.

JOB POSITION DESCRIPTION:

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

As part of the Advanced Structural and Functional Characterization research group, the Crystallography of Magnetic and Electronic Oxides (CMEOS) group provides the platform and expertise for sample preparation (thin films by Pulsed Laser Deposition and powder oxides) and characterization using conventional techniques (high resolution X-ray diffraction, local probe microscopy, electron microscopy and UHV



sample characterization in ALBA partner laboratory) as well as advanced surface structural and electronic characterization using synchrotron radiation techniques.

As PhD involved in the project “Use of highly ordered switchable ferroelectric films to enhance the water splitting activity of TiO₂ photo-catalysts” for the CMEOS group, your missions will be the following:

- Play and active role in the synthesis of the thin films specified in the project by PLD
- Play an active role in the accomplishment of all those measures that are necessary for the correct characterization of the samples
- Play an active role in the electrochemical characterization of the selected compounds
- Availability to attend training courses in any of the areas of the group: advanced characterization in synchrotron radiation techniques, training in UHV technologies...
- Availability to travel (participation in experiments carried out in large facilities, training courses, attendance to workshops and or conferences, ...)
- Active collaboration in the design and testing of a photoelectrochemical cell

Profile, skills and experience

- You should hold a BSc in Physics, Materials Science or Chemistry with a Master's degree in Materials Science or preferably in Electrochemistry
- Experience in conventional characterization tools, knowledge on diffraction techniques is advisable.
- Experience or be willing to learn in thin film synthesis using PLD (RHEED assisted).
- Ability to work in group and methodical in laboratory work.
- Good level of English.

Candidates should submit their CV and the following academic documents: academic records and the credits earned in the Master's program.

If you are interested, please send the previous information to torrelles@icmab.es by January 15th 2018

GROUP LEADER:

Title: Dr.

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Research project / Research Group website: <https://departments.icmab.es/cmeos/>
<https://departments.icmab.es/crystallography/>