

CONTRATOS PREDOCTORALES 2021 SEVERO OCHOA

PROJECT TITLE / JOB POSITION TITLE:

Optimizing ferroelectric assisted photocatalytic efficiency

RESEARCH PROJECT / RESEARCH GROUP DESCRIPTION:

(2.000 characters – including spaces)

Sunlight induced photocatalytic water splitting is receiving nowadays a lot of interest as a clean energy production technology. However, the efficiency of one of the most promising catalysts, TiO_2 , is largely reduced by fast recombination velocities of the electron-hole pairs produced during illumination. In this context, ferroelectric (FE) films (in this work BaTiO_3 and BiFeO_3), with spontaneous polarization perpendicular to the film, exhibiting an open-circuit photovoltage under illumination, can drive charge carriers to opposite surfaces (bulk photovoltaic effect). The FE-field can thus be used in TiO_2 /FE heterostructures to create spatially separated sites for the reduction and oxidation water reactions yielding H_2 and O_2 , respectively. In this way, the recombination of the photogenerated carriers can be reduced, thus enhancing the photocatalytic efficiency. However, interfacial strain and defects, together with depolarization fields resulting from incomplete charge screening at the TiO_2 /FE interface, can dramatically reduce the polarization strength of the FE layer.

The main objective of this proposal is the analysis of the influence of the FE-polarization on the enhancement of the photo-catalytic efficiency, and assess the influence of the above mentioned drawbacks. To this end, special interest will be paid to the domain configuration and polarization distribution within the FE layer and, particularly, to the atomic structure and defect chemistry of the catalyst/FE interface. These effects will be investigated by combining state of the art Transmission Electron Microscopy imaging and spectroscopy with synchrotron Photo-Electron Emission Microscopy.

ICMAB-CSIC is a prestigious research institute promoting multidisciplinary research in materials science and nanoscience. The Crystallography of Magnetic and Electronic Oxides and the Advanced Characterization and Nanostructured Materials groups at ICMAB, will provide the platform and expertise for the execution of this project.

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 successful candidate will join a multidisciplinary research team devoted to the investigation of functional complex oxide materials, participating in the integration of TiO₂ catalyst films in ferroelectric (FE) epitaxial heterostructures. He/she will develop the investigation of the fundamental structural mechanisms controlling the efficiency of the FE polarization on the splitting of water by the catalyst TiO₂ layer. His/her role will be, in a first stage, the growth of BaTiO₃ and BiFeO₃ FE epitaxial films by Pulsed Laser Deposition, as substrates for the subsequent growth of the TiO₂ catalyst. In a second stage, he/she will focus on the characterization of the heterostructures. This activity will involve a preliminary intensive formation in synchrotron X-ray Photo Electron Emission Microscopy (PEEM), for the characterization of FE domains at the surface of the films, and (Scanning) Transmission Electron Microscopy (TEM) imaging (High Resolution TEM, High Angle Annular Dark Field, Scanning TEM-Bright Field) and spectroscopic (Electron Energy Loss, Energy Dispersive X-ray) techniques for the characterization of the polarization and the investigation of the local structure and defect chemistry of the catalyst/FE interface.

This job position will require availability to attend training courses in any of the areas of his/her research project, such as advanced characterization using synchrotron radiation techniques, advanced transmission electron microscopy, UHV technologies, etc., as well as to attend workshops and conferences.

Part of the experimental work, requiring the use of large facilities such as synchrotron and aberration corrected electron microscopes, will also demand availability to travel within Spain and abroad.

GROUP LEADER:

Title: Dr.

Full names: Felip Sandiumenge, Xavier Torrelles

Email: felip@icmab.es, torrelles@icmab.es

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