UNIVERSITÀ CATTOLICA del Sacro Cuore | UNIVERSITY OF NOTRE DAME | KU LEUVEN | PONTIFICIA UNIVERSIDAD CATÓLICA DE CHILE

International Doctoral Program in Science Position

Supersonic cluster beam synthesis of innovative transition metal oxides photoelectrodes for hydrogen production

Background and motivation

The need for efficient devices converting renewable energies to fuels such as H_2 may be tackled by photoelectrochemical water splitting: electron/hole pairs generated at two photoelectrodes (PE) drive the half-reactions producing H_2 and O_2. The state of the art PE built with ternary metal oxides (TMOs) like $CuFe_2O_4$ face major limitations like scant efficiency, photocorrosion and instability. They are ascribed to ***the low charge transfer*** induced by the small polarons due to the TMO hybrid valence band orbitals, and to ***the high recombination rate of charge carriers*** at the TMO surface and bulk states. Moreover, current PE lacks a comprehensive investigation of different TMO phases, stoichiometries and transport properties for sizes below 50 nm. The project strategy is to overcome the current limits by: 1) ***reducing the TMO sizes*** by producing PE of $ZnFe_2O_4$, $CuFe_2O_4$ and $BiFeO_3$ with a ***nanogranular morphology (NG-TMO) at scales below 50 nm*** by supersonic cluster beam deposition (SCBD); 2) determining the ***PE morphological, optical and electrochemical behavior*** for three different NG-TMO compounds; 3) determining the ***PE transport behavior*** from the reaction kinetic constants (k_t for the hopping process and k_r for recombination process), as a function of TMO selected stoichiometries, phases and sizes.

The expected project breakthroughs are: 1) **a new class of nanostructured PE for electrochemistry, NG-TMOs**; 2) **morphological, optical and stoichiometric properties correlation with PE thickness and annealing temperature**; 3) **Electrochemical properties correlation with the PE thickness and annealing temperature**; 4) **charge transport correlation with morphology, optical response, stoichiometry**; 5) **reveal the role of small polarons and surface recombination in NG-TMOs at scales below 50 nm**.

The student will be tutored by three experienced tutors at the Università Cattolica (UCSC) for the PE synthesis and physical properties characterization, at the university of Padova (UPD) and university of Notre Dame (ND) for the PE electrochemical characterizations.

Profile

- Master's degree or comparable qualification in Physics, Chemistry, Material Science or adjacent fields. The title must be obtained before OCTOBER 31ST 2022.
- Previous experience in characterization or synthess of nanostructured materials is a plus.
- Good knowledge of the English language, both spoken and written, is essential.
- Strong commitment, ability to work in a team, and eagerness for international mobility is desired.

Opportunities

- Experimental research participating to the international collaboration between UCSC, ND (USA) and UPD, with at least one year spent in Notre Dame.
- **Double degree opportunity.**

Supervisors

- Prof. Luca Gavioli, UCSC, Italy luca.gavioli@unicatt.it
- Prof. Prashant Kamat, ND, USA pkamat@nd.edu
- Prof. Gian Andrea Rizzi, UPD, Italy gianandrea.rizzi@unipd.it