NANOWS 2022 - Achievements and Challenges of Multiscale Modelling of Nanocrystals for Efficient Water Splitting

11-12 July 2022, University of Aveiro, Portugal

NANOWS 2022 aims at bringing together researchers and scientists, who are pioneering the development and/or application of computer simulations approaches to the understanding of the photocatalytic water splitting with nanocrystals from abundant elements, to discuss advances and difficulties in this field of research, to identify new issues, and to shape the future directions concerning the multiscale modelling of this important reaction in the framework of COST Action 18234.

NANOWS 2022 is a two-day venue that will take place at the University of Aveiro, Aveiro, Portugal on the 11-12 July 2022.

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International Scientific Committee

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Francesc Illas	University of Barcelona, Spain
Eugene Kotomin	University of Latvia, Latvia
Florian Libisch	Vienna University of Technology, Austria
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Local Organizing Committee

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SCIENTIFIC PROGRAM

11th of July, 2022

Time	Speaker / Title
9:00	Registration and Opening Session
9:15	Filipe FIGUEIREDO / Transition metal perovskites as electrocatalysts for OER and ORR: electrochemistry and chemical stability
10:00	Ricardo GRAU-CRESPO / Modelling spinel materials for photocatalysis
10:30	Rafaela Maria GIAPPA / Modelling catalyst materials for CO_2 reduction reaction
10:45	**COFFEE BREAK**
11:15	Veera KRASNENKO / Water Splitting on Multifaceted $SrTiO_3$ Nanocrystals: Calculations of Raman Vibrational Spectrum
11:45	Bartek SZYJA / On the stability of hematite supported TiO_2 nanoparticles
12:15	Veerapandian PONNUCHAMY / Evaluation of nanoparticles for biomass reforming process into hydrogen
12:30	**LIGHT-LUNCH**
13:45	Core Group Meeting (for COST Action 18234 core group members ONLY!)
14:30	Ángel MORALES-GARCÍA / Understanding the influence of water on the properties of photoactive titania nanoparticles
15:00	Sergejs PISKUNOVS / TDDFT simulations of modified TiO_2 nanofilms for photocatalytic water splitting
15:15	Mihai BUTOLO / The process of water splitting using photocatalytic semiconductor nanoparticles
15:30	Klemen BOHINC / Charging of Nanoparticles
15:45	Said HAMAD / Computational design of photocatalytic nanoporous materials for water splitting and carbon dioxide reduction
16:15	**COFFEE BREAK**
16:45	Management Committee Meeting
20:00	**DINNER**

12th of July, 2022

Time	Speaker / Title
9:00	Maytal CASPARY TOROKER / Extended models for charge transport calculations across materials
9:45	Ugur BOSKAYA / A Combined Cluster-in-Molecules and Systematic Molecular Fragmentation Approach for Electronic Structure Theories
10:00	Yair REICHMAN / Electronic properties and simulated dynamics of mismatched zinc-blende semiconductor heterostructures
10:15	Alex COMES-VIVES / Modelling the Dynamics of Heterogeneous Catalysts: Challenges and Opportunities
10:45	**COFFEE BREAK**
11:15	Vesselin TONCHEV / How to distinguish between crystallization and aggregation?
11:45	Sean PACHMANOV DVIR / Machine learning based adsorption sites searching
12:00	Amit VURGAFT / Predictive Maintenance: When Materials Science and Data Science come together
12:30	**LIGHT-LUNCH**
14:30	Emmanouil PERVOLARAKIS / Machine Learning for the edge energies of nanoparticles for catalysis applications
14:45	Florian LIBISCH / Machine Learning defect parameters for tight-binding calculations
15:15	Assembly Discussion + Closing Session
16:15	**COFFEE BREAK**