COST action 18234 conference

Designing The Future: Electro-, Photo- And Thermo-Chemical Water Splitting

Brussels 20-22 February 2023

Website and program: https://tess-db.com/h2o/

Local organizing committee:

Ionut **Tranca**	Vrije Universiteit Brussel
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Sponsors and Partners:

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International Scientific Committee

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Tomasz **Wesolowski**	University of Geneva, Switzerland

20 February, Monday

8:30 – 9:30	Registration and Opening Session (**Ionut Tranca**)
9:30 – 10:00	**Maytal Caspary Toroker** / TBA
10:00 – 10:30	**Marc Koper** / Mechanisms of electrochemical hydrogen evolution
10:30 – 10:45	**Dorota Rutkowska Zbik** / DFT studies of Vanadium-based systems for electro- and photochemistry
10:45 – 11:00	**Diana Bergmann** *(online)* / TBA
11:00 – 11:15	COFFEE BREAK
11:15 – 11:30	**Xavier Solans Monfort** / Supported Ru and RuO_2@Ru nanoparticles for electrocatalytic hydrogen evolution: structural and electronic effects on their catalytic activity
11:30 – 11:45	**Peter Vancso** / Quasi-flat Pt nanoclusters on MoS_2 for efficient hydrogen evolution
11:45 – 12:15	**Jose Gomes** / Chemical reactions at the surface of MXenes
12:15 – 13:45	LIGHT LUNCH (13:15 – 13:45 COST Core Group meeting)
13:45 – 14:15	**Monica Calatayud** / Hydrogen and TiO_2: surface or subsurface
14:15 – 14:45	**Konstantin Neyman** / Surprising oxidation of platinum in subnano-state: Insights from catalytic experiments and DFT modelling
14:45 – 15:15	**Gianfranco Pacchioni** / DFT modelling of electrocatalysis by single-atoms: handle with care
15:15 – 15:30	COFFEE BREAK
15:30 – 15:45	**Giovanni di Liberto** / Role of Superoxo and Peroxo Complexes in the Oxygen Evolution Reaction on Single-Atom Catalysts
15:45 – 16:00	**Leonhard Mayrhofer** / DFT investigations of interfacial contact charge separation
16:00 – 16:15	**Isabela Man** / Effect of surface protonation of TiO_2 (101) / (100) anatase surfaces on water splitting overpotentials
16:15 – 16:30	**Bartłomiej Szyja** / Active sites and mechanism of water splitting on mixed oxides from DFT level MD simulations
16:30 – 18:00	COST MC (Management Committee) meeting

21 February, Tuesday

9:00 – 9:30	**Remo Schäppi** / Fuel from sunlight and air – demonstration of the thermochemical pathway
9:30 – 10:00	**Wojciech Lipiński** *(online)* / Mixed metal oxides for enhanced solar fuel production via thermochemical redox cycling
10:00 – 10:30	**Raul Molina Gil** / Macroscopic structures of non-stoichiometric mixed oxides for hydrogen production by low temperature thermochemical water splitting
10:30 – 10:45	COFFEE BREAK
10:45 – 11:00	**Veerapandian Ponnuchamy** *(online)* / ReaxFF study of dehydration mechanism of surface doped salt hydrates for thermochemical heat storage
11:00 – 11:30	**Martin Roeb** / Status and Trends in Solar Thermochemical Fuel Generation
11:30 – 12:00	**Farid Safari** / TBC
12:00 – 13:00	LIGHT LUNCH
13:00 – 13:30	**Eugene Kotomin** / The perovskite band engineering for photostimulated water splitting
13:30 – 14:00	**Said Hamad Gomez** / Tuning the properties of photocatalytic ZIFs: mixing and nucleation
14:00 – 14:30	**Ricardo Grau-Crespo** / Spinel oxides for photocatalysis: DFT modelling and experimental characterization
14:30 – 14:45	**Yuri Mastrikov** / Water splitting on stepped STO surface
14:45 – 15:00	**Veera Krasnenko** / Ab Initio Calculations of the Raman Spectra of Thin Strontium Titanate Films
15:00 – 15:15	**Stanislav Záliš** / Modelling of excited-state dynamics of Re photo-sensitizer
15:15 – 15:30	COFFEE BREAK
15:30 – 17:30	POSTER SESSION

22 February, Wednesday

9:00 – 9:30	**Thomas Bligaard** / Accelerating catalysis simulations with surrogate machine learning models
9:30 – 10:00	**Florian Libisch** / Machine learning for ab-initio defect parametrization
10:00 – 10:30	**Matthijs van Berkel** / Microkinetic modeling from a systems and control perspective
10:30 – 10:45	COFFEE BREAK
10:45 – 11:05	**Fedor Goumans** / Parametrizing DFTB, ReaxFF, and machine learned potentials with ParAMS
11:05 – 11:20	**Sean Pachmanov-Dvir /** TBA
11:20 – 11:50	**Toon Verstraelen** / Physical constraints on polarization and charge transport in machine-learning potentials.
11:50 – 13:00	LIGHT LUNCH
13:00 – 13:30	**Francesc Illas /** Modeling and understanding hydroxylation of TiO_2 nanoparticles: One more step towards approaching realistic systems
13:30 – 14:00	**Kai Exner** / Theoretical Description of Energy Storage and Conversion Processes
14:00 – 14:30	**Bryan Goldsmith** *(online)* / Interpretable "transparent box" machine learning to understand materials and catalytic properties
14:30 – 14:45	**Hannu-Pekka Komsa** *(online)* / Machine-learning force fields and polarizability models for Raman spectra of complex systems
14:45 – 15:00	COFFEE BREAK
15:00 – 15:30	**Uğur Bozkaya** / Molecular Fragmentation Approaches for Electron Correlation Methods
15:30 – 16:00	**Shyue Ping Ong** *(online)* / The Materials 3-body Graph Network (M3GNet) Universal Potential for Materials Design
16:00 – 16:30	**Jim Lutsko** / Understanding crystallization pathways using classical DFT
16:30 – 16:45	**Vesselin Tonchev** *(online)* / Studying crystallization between 2 and 3D: Cellular Automata vs. analytical model
16:45 – 17:15	Closing remarks (**Frederik Tielens**)

Poster session

Veton Haziri	*A gateway for ion transport on gas bubbles pinned onto solids*
Yuheng Zhao	*DFT Investigation of interactions between poly(adp-ribose) and metal ions in biomineralizatio*
Shohreh Faridi	*Computational Study on MXenes as Bifunctional Catalyst for Metal-Air Batteries.*
Fileto Rodriguez	*TBA*
Rafał Stottko	*Procedure to indicate stable CuNi clusters based on machine learning methods*
María Orfila Del Hoyo	*Macroscopic shaping of mixed metal oxides for thermochemical hydrogen production*
Ali Moussadik	*Effects of W/Mo co-doping on the photoelectrochemical properties of $BiVO_4$ photoanodes for solar water splitting: A density functional theory study*
Loic Dumortier	*BalancedLoss: A Weightless Cost-Function for ReaxFF Optimization*
Eleonora Romeo	*Electrochemical symmetry in the oxygen evolution reaction*
Jose Luis Nunez	*DFT Studies of H_2O dissociation on Iridium Oxide-modified CNTs.*
Samad Razzaq	*Method to determine bifunctional index of the oxygen electrocatalysis*
Vipin Kumar	*Oxygen reduction reaction on pristine and N-doped nanosheet comparison study by implicit and explicit solvent model*
Miguel Recio	*Crystal properties without crystallinity? Influence of surface hydroxylation on the structure and properties of small TiO2 nanoparticles*
Diwakar Singh	*Theoretical Study of Nitrogen reduction over MXenes*

Muhammad Usama	*Comprehending the Oxygen and Chlorine Evolution Reactions over IrO_2-Based Electrode Materials on the Atomic Scale*