

Annual meeting of the COST Action: Computational materials sciences for efficient water splitting with nanocrystals from abundant elements (CA18234)

“Computational water splitting, where we are now and where to go?”

February 14-15, 2022, on-line event

THE PROGRAM
(final version Feb. 14, 2022)

Monday, Feb. 14

- 9:00-9:05 Welcome (*Tomasz A. Wesolowski*)
9:05-9:25 Introduction by the Action Chair (*Maytal Caspary Toroker*)

Session 1 (WG1) Chair *Francesc Illas*

- 9:30-10:30 **Electrochemical water splitting: state of the art** (keynote talk)
Federico Calle-Vallejo (Barcelona, Spain)
- 10:30-11:00 **Role of Dihydrogen Complexes in Hydrogen Evolution Reaction on Single Atom Catalysts,**
Giovanni di Liberto (Milan, Italy)
- 11:00-11:30 **Oxygen Evolution Reaction with IrO₂ and IrO₂-based hybrid materials**
Xavier Solans (Barcelona, Spain)
- 11:30-12:00 Virtual coffee break

Special session: Chair *Tomasz A. Wesolowski*

- 13:00-14:00 **Transitioning from barrier to porous Al oxides by tuning anodizing parameters,** (invited experimental talk) *Noemie Ott* (EMPA, Dübendorf)

Session 2 (WG1 cnt.) Chair *Francesc Viñes Solana*

- 14:00-14:30 **Water splitting on stepped STO surface: reaction mechanisms**
Yuri. A. Mastrikov (Riga, Latvia)
- 14:30-15:00 **On the role of dopants and defects in tuning Oxygen electrocatalysis at transition metal oxide surfaces,**
Michele Pavone (Naples, Italy)
- 15:00-15:30 Virtual coffee break

Management Committee Meeting

- 15:30-17:00 MC breakout room

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Session 3 (WG2) Chair Nicu Goga

- 9:00-9:30 **Black Titania – Insights from ab initio simulations,**
F. Mayrhofer (Freiburg, Germany)
- 9:30-10:00 **Stability of the hematite supported oxide nanoclusters from MD**
simulations, *Bartłomiej Szyja* (Wrocław, Poland)
- 10:00-10:30 **Biomass reforming into hydrogen production with ZrO₂ using ReaxFF,**
Veerapandian Ponnuchamy (Izola, Slovenia)
- 10:30-11:00 Virtual coffee break

Session 4 (WG1+WG4) Chair Anja Bierberle-Hütter

- 11:00-11:30 **Simulating thermodynamic and kinetic properties of surface states for**
OER catalysis,
Nadav Snir (Technion, Israel)
- 11:30-12:00 **Description: Variance-based Global Sensitivity Analysis: A Methodological**
Framework and Case Study for Microkinetic Modelling,
Bart van den Boorn (Eindhoven, The Netherlands)
- 12:00-12:05 Closing the conference

Meetings of the Working Groups

- 13:00-13:30 WG1
- 13:30-14:00 WG4
- 14:00-14:30 WG5