

Agenda of the International Conference

COST CA 18234 Meeting

"Electrode materials of earth-abundant elements for water splitting"

Institute of Solid State Physics, University of Latvia

(Location: Wellton Riverside SPA Hotel, 33, 11. Novembra krastmala, Riga, LV-1050, Riga, Latvia)

April 25th, 2022

| Start | End | Duration | Speaker | Affiliation | Title of the presentation |
|-------|-------|----------|---|---|---|
| 9:00 | 9:30 | 0:30 | Organizers / Maytal Caspary Toroker* | Institute of Solid State Physics, University of Latvia / Technion – Israel Institute of Technology | A word from the Organizers and the Leader of the Action. |
| 9:30 | 10:00 | 0:30 | Yuval Elbaz | Technion – Israel Institute of Technology | "A cross-disciplinary study of oxides properties: DFT, tight-binding, and machine learning methods" |
| 10:00 | 10:30 | 0:30 | LauraLaverdure | University of Jyväskylä | All about that base: electro-oxidation of glycerol on gold |
| 10:30 | 10:45 | 0:15 | Break | | |
| 10:45 | 11:15 | 0:30 | Toni Kiljunen | University of Jyväskylä | Choosing a proper thermostat in DFT-MD evaluations of a water--nanocrystal system is crucial for reliable modelling of catalytic performance |
| 11:15 | 11:45 | 0:30 | Manuel Jerome Kolb | Universitat de BarcelonaFacultat de Quimica | Thermodynamic Limits for Bifunctional Oxygen Evolution and Reduction Catalysts from Scaling Relations |
| 11:45 | 13:15 | 1:30 | Lunch | | |
| 13:15 | 13:45 | 0:30 | Kai Exner* | University of Duisburg-Essen | Theoretical modeling of the oxygen evolution Reaction: Quo vadis |
| 13:45 | 14:15 | 0:30 | Maxim Sokolov | University of Duisburg-Essen | Oxygen evolution reaction on faceted strontium titanate surfaces |
| 14:15 | 14:45 | 0:30 | Shohreh Faridi* | University of Duisburg-Essen | MXenes as earth-abundant electrode materials for oxygen evolution |
| 14:45 | 15:00 | 0:15 | Break | | |

| | | | | | |
|-------|-------|------|-------------------------|---|--|
| 15:00 | 15:30 | 0:30 | Francesca Fasulo* | University of Naples Federico II Comp. Univ. MSA | Dynamics of water TiO ₂ interface at low coverages |
| 15:30 | 16:00 | 0:30 | Adriana Pecoraro* | University of Naples Federico II Comp. Univ. MSA | Oxygen evolution reaction at Mo-/W- doped BiVO ₄ |
| 16:00 | 16:15 | 0:15 | Break | | |
| 16:15 | 16:45 | 0:30 | Federico Calle-Vallejo* | Universitat de Barcelona Facultat de Quimica | Impact of gas-phase errors on the computational modelling of oxygen electrocatalysis |
| 16:45 | 17:15 | 0:30 | Marko Melander* | University of Jyväskylä | Experiments, theory, and simulations to understand outer-sphere electron transfer on model 2D electrodes |
| 17:15 | 17:30 | 0:15 | Organizers | Institute of Solid State Physics, University of Latvia | Conclusion of the Meeting |

*Remote participation