The Lorentz Center organizes international workshops for researchers in all scientific disciplines. Its aim is to create an atmosphere that fosters collaborative work, discussions, and interactions.

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This workshop is part of the CECAM-Lorentz collaboration to stimulate innovative computational simulation and modeling.

Atomistic Modelling of Solid-Liquid Interfaces in Electrocatalysis

8 - 12 January 2024, Leiden, the Netherlands

Scientific Organizers

- Giancarlo Cicero, Politecnico di Torino
- Max García-Melchor, Trinity College Dublin
- Hannes Jónsson, University of Iceland
- Marc Koper, Leiden University
- Nuria López, Institut Català d’Investigació Química

Topics

- Improvement of Implicit Solvation Models
- The Inclusion of the Explicit Liquid Phase in the Simulations
- Study of the Effect of the Electrolyte Solution on the Catalysis
- The Inclusion of an External Applied Potential in the Simulations
- Use of Machine Learning Algorithms

"The intricate nature of solid/liquid interfaces, sketching various features and phenomena." Image by Dr. Michelle Re Finovert (Politecnico di Torino). Poster design: SuperNova Studios NL.
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<td>10.30-11.00</td>
<td>A. Gross (Ulm University): Formation and structure of electric double layers from an atomistic point of view</td>
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<td>11.00-11.30</td>
<td>M. Caspary-Toroker (Technion): Computational methods for modeling materials for H2O splitting</td>
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<td>11:30-12:00</td>
<td>G. Kastlunger (Technical University of Denmark): The role of the electrochemical driving forces in electrocatalytic reaction energetics</td>
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<td>A. Muñoz-García (University of Naples Federico II): Exploring the boundaries of first-principles methods in heterogenous functional interfaces</td>
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<td>14.30-15.00</td>
<td>F. Calle-Vallejo (University of the Basque Country): Gas-phase errors in computational electrocatalysis models</td>
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<td>15.00-15.30</td>
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<td>16.30-17.00</td>
<td>G. Cicero (Politecnico di Torino): Survey Analysis</td>
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<td>09.00-09.30</td>
<td><strong>K. Schwarz</strong> <em>(National Institute of Standards and Technology)</em>: Ingredients for implicit solvation recipes: moving beyond SaLSA</td>
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<td>09.30-10.00</td>
<td><strong>S. Ringe</strong> <em>(Korea University)</em>: Importance of a charge-transfer descriptor for the computational screening of electrocatalysts</td>
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<td><strong>T. Rahman</strong> <em>(University of Central Florida)</em>: Enhancements in the implicit solvent model for simulations of the electrochemical environment for CO2RR</td>
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<td>11.00-11.30</td>
<td><strong>M. Melander</strong> <em>(University of Jyväskylä)</em>: Combining electronic DFT with statistical liquid state theories to model electrochemical interfaces</td>
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<td>11.30-12.00</td>
<td><strong>J. Cheng</strong> <em>(Xiamen University)</em>: Towards AI2 Electrochemistry</td>
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<td><strong>S. Vijay</strong> <em>(VASP Software GmbH)</em>: Linking models of the electrochemical interface with the Vienna ab-initio simulation package</td>
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<td><strong>D. Le</strong> <em>(University of Central Florida)</em>: Improving the Computational Efficiency of Explicit-Implicit Hybrid Solvent Model for Simulations of the Electrochemical</td>
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<td>09.00-09.30</td>
<td>I. McCrum (Clarkson University)</td>
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<td>K. Doblhoff-Dier (Leiden University)</td>
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<td>M. Sulpizi (Ruhr Universität Bochum)</td>
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<td>G. Melani (CNR)</td>
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<td>S-J. Shin (Imperial College London)</td>
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<td>K. Honkala (University of Jyväskylä): Grand-canonical ensemble DFT calculations for understanding electrocatalytic reactions at atomic scale</td>
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<td>N. G. Hörmann (Fritz-Haber-Institut): Divergent Paths, Convergent Insights: Constant Charge vs. Constant Potential Methods</td>
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<td>J. Mark Martínez (Princeton University): Can embedded multiconfigurational wavefunction methods reveal fresh insights into the electrochemical CO2</td>
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<td>C. Cucinotta (Imperial College London): Exploring the Pt(111)-Electrolyte Interface Under Applied Potentials: A First Principles Approach</td>
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<td>J. Rossmeisl (University of Copenhagen): Electrocatalysis on high entropy alloys</td>
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<td>L. Li (Fritz-Haber-Institut): The Response of Interfacial Water at an Electrified Pt(111) Surface</td>
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<td>J-X. Zhu (Xiamen University): Machine Learning-Accelerated Simulation of Electrochemical Interfaces</td>
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<td>N. López (ICIQ): HPC opportunities</td>
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<td><strong>M. Caro (Aalto University)</strong>: Atomistic machine learning for a unified description of bulk, surfaces, liquids and molecules with force field computational cost and</td>
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