Workshop III: Boundary Conditions for Atomistic Simulations in Macroscopic Electrochemical Cells

Monday October 27, 2025

8:00–8:55 *Check-In/Breakfast (Hosted by IPAM)*

8:55–9:00 *Welcome and Opening Remarks*

9:00 *Session Chair: Clotilde Cucinotta*

9:00–9:50 **Giulia Galli** (University of Chicago & Flatiron Institute)
Interfaces between water and semiconductors from first principles

10:00–10:15 *Break*

10:15–11:05 **Jörg Neugebauer** (Max Planck Institute for Sustainable Materials)
Boundary conditions for atomistic simulations: Insights, solutions and challenges

11:15–11:30 *Break*

11:30–12:20 **Michael Eikerling** (RWTH Aachen University)
The Local Reaction Environment in Electrocatalytic Media: Infusing Interface Theory with Realism and Complexity

12:30–2:30 *Lunch (on your own)*

2:30 *Session Chair: Clotilde Cucinotta*

2:30–3:20 **Jun Cheng** (Xiamen (Amoy) University)
AI acceleration of AIMD simulation of electrochemical interfaces

3:30–4:00 *Break*

4:00–4:30 *Lightning Poster Round*

4:30–6:00 *Poster Session & Reception (Hosted by IPAM)*

Tuesday October 28, 2025

8:00–8:55 *Check-In/Breakfast (Hosted by IPAM)*

9:00 *Session Chair: Chris Anderson*

9:00–9:50 **Clotilde Cucinotta** (Imperial College)
Advancing Ab Initio Molecular Dynamics for Electrified Interfaces

10:00–10:15 *Break*

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10:15–11:05 **Stefan Wippermann** (Philipps-Universität Marburg)
Capturing Electrode Potential Dynamics in Ab initio Electrochemical Simulations

11:15–11:30 *Break*

11:30–12:20 **Mark Tuckerman** (New York University)
Beating the viscosity-conductivity inverse relation barrier to create a breakthrough electrolyte for emerging battery applications

12:30–2:30 *Lunch (on your own)*

2:30 *Session Chair: Chris Anderson*

2:30–3:20 **Davide Donadio** (University of California, Davis)
Molecular Dynamics of Solutions out of Equilibrium

3:30–4:00 *Break*

4:00–5:00 **Leslie Greengard** (New York University)
A periodic fast multipole method and a new version of fast Ewald summation

Wednesday October 29, 2025

8:00–8:55 *Check-In/Breakfast (Hosted by IPAM)*

9:00 *Session Chair: Stefan Ringe*

9:00–9:50 **Thomas Swinburne** (University of Michigan and CNRS)
Functional simulations for uncertainty quantification and inverse problems

10:00–10:15 *Break*

10:15–11:05 **Phillip Colella** (Lawrence Berkeley Laboratory)
Embedded Boundary Methods for Conservation Laws in Complex Geometries

11:15–11:30 *Break*

11:30–12:20 **Carlos Garcia-Cervera** (University of California, Santa Barbara (UCSB))
Electronic Structure Models with 2d Symmetries in the presence of a uniform magnetic field

12:30 *Group Photo*

12:30–2:30 *Lunch (on your own)*

2:30 *Working Group Reports*

2:30–2:50 *Group 1: Machine Learnt Force Fields for Electrochemistry*

2:50–3:10 *Group 2: Bridging the Gap Between Atomistic and Mesoscale Models*

3:10–3:30 *Group 3: Fluctuations and Correlations in Mesoscopic Dynamics*

3:30–3:45 *Break*

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3:45–4:05 *Group 4: Method Bridging*

4:05–4:25 *Group 5: cDFT and Var frameworks update*

4:25–4:45 *Group 6: Generative AI and Configuration Sampling*

Thursday October 30, 2025

8:00–8:55 *Check-In/Breakfast (Hosted by IPAM)*

9:00 *Session Chair: Christoph Freysoldt*

9:00–9:50 **Alfredo Pasquarello** (École Polytechnique Fédérale de Lausanne (EPFL))
Electron Transfer at Transition-Metal-Oxide/Water Interfaces

10:00–10:15 *Break*

10:15–11:05 **Annabella Selloni** (Princeton University)
Insights into the Chemistry of Aqueous Oxide Interfaces from Machine Learning Molecular Dynamics

11:15–11:30 *Break*

11:30–12:20 **Jing Yang** (Max Planck Institute for Iron Research)
Molecular dynamics simulation for electrochemical systems: challenges of the field fluctuation

12:30–2:30 *Lunch (on your own)*

2:30 *Session Chair: Christoph Freysoldt*

2:30–3:20 **Stefan Ringe** (Korea University)
Continuum modeling meets quantum chemistry: Multi-scale modeling of electrochemical processes

3:20–4:00 *Discussions*

Friday October 31, 2025

8:00–8:55 *Check-In/Breakfast (Hosted by IPAM)*

9:00 *Session Chair: Thomas Swinburne*

9:00–9:50 **Christoph Freysoldt** (Max Planck Institute for Sustainable Materials)
Correcting for electrostatic boundary artifacts in simulations of charged systems

10:00–10:15 *Break*

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10:15–11:05 **Bin Wang** (University of Oklahoma)
Modeling interfacial charge transfer in thermochemical and electrochemical reactions and their analogy

11:15–11:30 *Break*

11:30–12:20 **Chris Anderson** (University of California, Los Angeles (UCLA))
Domain decomposition and parameterized effective boundary conditions for Poisson's equation.