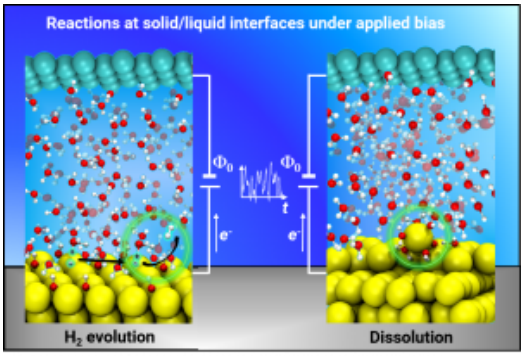
institute for pure & applied mathematics

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

October 27-31, 2025



Scientific Overview

This workshop will delve into the challenges and opportunities associated with modeling electrochemical systems in a periodic supercell, which is a prerequisite for almost all practical density functional theory simulations when addressing electrochemical phenomena. Participants will explore efficient boundary conditions that accurately describe ion transport to and from the electrochemical interface within a grand canonical and thermodynamically consistent framework. Additionally, they will investigate boundary conditions and implicit solvent models for the inclusion of long-range electrostatic fields, a characteristic feature of electrochemical systems, to enhance the realism and precision of the simulations. The workshop will also revolve around the analysis of interfacial phenomena, charge transport and electron transfer across interfaces, the impact of supercell size on electrochemical behavior, and the implementation of potentiostats that are able to consistently reproduce potential fluctuations in the small supercells. This event aims to empower researchers to overcome scale-bridging challenges, advancing the precision of atomistic simulations within macroscopic electrochemical cell models.

Topics include:

- Explore extensions to advance DFT codes for realistic electrochemical simulations within periodic supercells
- Design of efficient boundary conditions to realistically capture the long-range nature of Coulomb interactions at electrochemical interfaces
- Creation of new generation of ML potentials which accurately capture charge transfer and polarization
- Efficient algorithms to make underlying PDEs to capture atomic-scale fluctuations
- Training of interaction kernels from periodic supercell simulations

Long Program Schedule

This workshop is part of the long program Bridging the Gap: Transitioning from Deterministic to Stochastic Interaction Modeling in Electrochemistry

- Bridging the Gap: Transitioning from Deterministic to Stochastic Interaction Modeling in Electrochemistry Opening Day : September 3, 2025
- Bridging the Gap: Transitioning from Deterministic to Stochastic Interaction Modeling in Electrochemistry Tutorials : September 4-9, 2025
- Workshop I: Embracing Stochasticity in Electrochemical Modeling : September 15-19, 2025
- Workshop II: Bridging Scales from Atomistic to Continuum in Electrochemical Systems: October 6-10, 2025
- Workshop III: Boundary Conditions for Atomistic Simulations in Macroscopic Electrochemical Cells : October 27-31, 2025
- Workshop IV: Electrochemistry Hackathon: Bridging the Gap Between Implicit and Explicit Methods: November 17-21, 2025
- Bridging the Gap: Transitioning from Deterministic to Stochastic Interaction Modeling in Electrochemistry Culminating Workshop at Lake Arrowhead : December 7-12, 2025

Participation

Additional information about this workshop including links to register and to apply for funding, can be found on the web page listed below. Encouraging the careers of women and minority mathematicians and scientists is an important component of IPAM's mission, and we welcome their applications.

Organizers

Chris Anderson (UCLA)
Clotilde Cucinotta (Imperial College)
Virginie Ehrlacher (École Nationale des Ponts-et Chaussées)
Jörg Neugebauer (Max-Planck-Institut für Eisenforschung)
Bilge Yildiz (Massachusetts Institute of Technology)

Speakers

Chris Anderson (University of California, Los Angeles (UCLA))
Paul Cazeaux (Virginia Polytechnic Institute and State University)
Jun Cheng Cheng (Xiamen (Amoy) University)
Phillip Colella (Lawrence Berkeley Laboratory)
Clotilde Cucinotta (Imperial College)
Davide Donadio (University of California, Davis)
Virginie Ehrlacher (École Nationale des Ponts-et-Chaussées)
Michael Eikerling (RWTH Aachen University)
Christoph Freysoldt (Max-Planck-Institut für Eisenforschung GmbH)
Giulia Galli (University of Chicago & Flatiron Institute)
Carlos Garcia-Cervera (University of California, Santa Barbara (UCSB))
Leslie Greengard (New York University)
Francois Gygi (University of California, Davis (UC Davis))
Jörg Neugebauer (Max-Planck-Institut für Eisenforschung)
Christoph Ortner (University of British Columbia)
Alfredo Pasquarello (École Polytechnique Fédérale de Lausanne(EPFL))
Stefan Ringe (Korea University)
Annabella Selloni (Princeton University)
Mark Tuckerman (New York University)
Bin Wang (University of Oklahoma)
Stefan Wippermann (Philipps-Universität Marburg)
Jing Yang (Max Planck Institute for Iron Research)
Bilge Yildiz (Massachusetts Institute of Technology)

NSF UCLA

For more information, visit the program webpage:
www.ipam.ucla.edu/ECHWS3