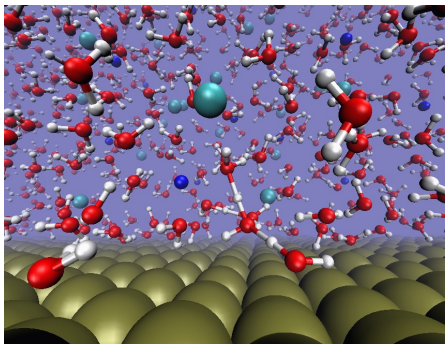
institute for pure & applied mathematics

Workshop I: Embracing Stochasticity in Electrochemical Modeling

SEPTEMBER 15 - 19, 2025



Scientific Overview

Electrochemical systems, in particular electrochemical interfaces, are dynamic ensembles of atoms and molecules, as well as particles that make up the electrode, where stochasticity plays a role. This workshop will focus on modeling techniques that explicitly consider stochasticity, such as ab initio-based molecular dynamics with explicit solvent molecules or stochastic potentiostating and microstructure-scale electrochemical dynamics models. The aim will be to understand which electrochemical quantities/processes are essential in the faithful modeling of electrochemical interfaces, which require an explicit stochastic description and which can serve as benchmarks for the development of new models. Participants will discuss the challenges associated with an atomistic modelling of electrochemical systems such as a proper consideration of the electrode potential. They will furthermore explore the theoretical foundations of interaction kernels and their reduction via mean-field and hydrodynamic limits to effective implicit solvation methods. Crucially the goal is to incorporate fluctuations and randomness into the continuum limits and capture their impact on electrochemical processes. Practical applications of explicit methods in studying charge transfer reactions, ion transport, and electrode kinetics will be demonstrated. The incorporation of these effects into interaction kernels, in particular the requirements for multi-agent kernels, will be pursued. Discussions will revolve around best practices, numerical implementation, and the upscaling of explicit (stochastic) simulations into interaction kernel learning and cell-level models.

Topics include:

- Ab initio molecular simulations with explicitly included water and electric fields
- Advanced mathematical sampling strategies to overcome the limited time scales in ab initio simulations
- Microstructure-scale models for electrochemical dynamics that account for stochasticity
- Approaches in neighboring fields such as bioinformatics, molecular biology and drug design
- Stochastic learning of interaction kernels in potentiostat and thermostat design

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

Axel Gross (Universität Ulm)
Keith Promislow (Michigan State University)
Katsuyo Thornton (University of Michigan)
Mira Todorova (Max-Planck-Institut für Eisenforschung GmbH)

Speakers

Robinson Cortes-Huerto (Max Planck Institute for Polymer Research)
Katharina Doblhoff-Dier (Leiden University)
Axel Gross (Universität Ulm)
Nicolas Hörmann (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Alexei A. Kornyshev (Imperial College London)
KURT KREMER (Max Planck Institute for Polymer Research)
Kari Laasonen (Aalto University)
Jian-Guo Liu (Duke University)
Claudio Margulis (University of Iowa)
Micheal Murillo (Michigan State University)
Keith Promislow (Michigan State University)
Yue Qi Qi (Brown University)
Matthew Rosenzweig (Carnegie Mellon University)
Katsuyo Thornton (University of Michigan)
Mira Todorova (Max-Planck-Institut für Eisenforschung GmbH)
Brian Wetton (University of British Columbia)
Ping Yang (Los Alamos National Laboratory)
Hongbo Zhao (University of California, San Diego (UCSD))

NSF UCLA

For more information, visit the program webpage:
www.ipam.ucla.edu/ECHWS1