

Workshop I: Embracing Stochasticity in Electrochemical Modeling

Monday September 15, 2025

- 8:00–8:55 *Check-in/Breakfast (hosted by IPAM)*
- 8:55–9:00 *Welcome and Opening Remarks*
- 9:00 *TBA*
- 9:00–9:50 **Axel Gross** (Universität Ulm)
Atomistic Electrochemistry and the Electric Double Layer: Concepts and Simulations
- 10:00–10:15 *Break*
- 10:15–11:05 **Kari Laasonen** (Aalto University)
DFT-Based Constrained MD Simulations of Hydrogen Evolution Activities on Pt(111)
- 11:15–11:30 *Break*
- 11:30–12:20 **Keith Promislow** (Michigan State University)
Correlation in Multiparticle Molecular Models
- 12:30–2:30 *Lunch (on your own)*
- 2:30 *TBA*
- 2:30–3:20 **Michael Murillo** (Michigan State University)
Non-Hydrodynamic Phenomena Near Plasma Interfaces
- 3:30–4:00 *Break*
- 4:00–4:30 *Lightning Poster Round*
- 4:30–6:00 *Poster Session & Reception (Hosted by IPAM)*

Tuesday September 16, 2025

- 8:00–8:55 *Check-in/Breakfast (hosted by IPAM)*
- 9:00 *MODERATOR: Axel Gross*
- 9:00–9:50 **Jian-Guo Liu** (Duke University)
Macroscopic Dynamics for Nonequilibrium Biochemical Reactions from a Hamiltonian Perspective
- 10:00–10:15 *Break*

(Tuesday schedule continued on next page)



(Tuesday schedule continued from previous page)

- 10:15–11:05 **Roman Shvydkoy** (University of Chicago)
On regularity and asymptotics of kinetic alignment models.
- 11:15–11:30 *Break*
- 11:30–12:20 **Alexei A. Kornyshev** (Imperial College London)
When Polyelectrolytes Think: From Electrochemistry to Molecular Genetics (Stochastic Polyelectrolyte Dynamics in Pairing Homologous Genes)
- 12:30–2:30 *Lunch (on your own)*
- 2:30 *MODERATOR: Axel Gross*
- 2:30–3:20 **Matthew Rosenzweig** (Carnegie Mellon University)
Recent progress on mean-field dynamics of Coulomb/Riesz gases
- 3:30–4:00 *Break*
- 4:00–4:50 **Quyuan Lin** (Clemson University)
On the non-isothermal electrodiffusion and Nernst-Planck-Boussinesq system

Wednesday September 17, 2025

- 8:00–8:55 *Check-in/Breakfast (hosted by IPAM)*
- 9:00 *MODERATOR: Keith Promislow*
- 9:00–9:50 **Katharina Doblhoff-Dier** (Leiden University)
Double layer properties at the atomic scale
- 10:00–10:15 *Break*
- 10:15–11:05 **Robinson Cortes-Huerto** (Max Planck Institute for Polymer Research)
The electron transfer process at the electrode/electrolyte solution interface: A stochastic model and its Monte Carlo implementation
- 11:15–11:30 *Break*
- 11:30–12:20 **Nidhi Rajput** (Stony Brook University)
MISPR: An Open-Source Computational Framework for Electrolyte and Electrode-Electrolyte Interfaces
- 12:20–12:30 *Group Photo*
- 12:30–2:30 *Lunch (on your own)*
- 2:30 *MODERATOR: Keith Promislow*
- 2:30–3:20 **Yue Qi** (Brown University)
Incorporating the effect of the electric double layer (EDL) in multicomponent electrolytes on electrochemical reactions
- 3:30–4:00 *Break*

(Wednesday schedule continued on next page)

(Wednesday schedule continued from previous page)

4:00–5:00 **John Lowengrub** (University of California, Irvine (UCI))
Viscous fingering in electro-osmotic flows

Thursday September 18, 2025

8:00–8:55 *Check-in/Breakfast (hosted by IPAM)*

9:00 *MODERATOR: Katsuyo Thornton*

9:00–9:50 **Mira Todorova** (Max Planck Institute for Sustainable Materials)
Fluctuations at electrochemical interfaces and their impact on reactions studied by (ab initio) molecular dynamics calculations

10:00–10:15 *Break*

10:15–11:05 **Nicolas Hörmann** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Bias In, Physics Out: Ab-Initio Insights into Electrified Interfaces

11:15–11:30 *Break*

11:30–12:20 **Ping Yang** (Los Alamos National Laboratory)
Understanding Surface Chemistry and Reactivity of actinide oxides

12:30–2:30 *Lunch (on your own)*

2:30 *MODERATOR: Katsuyo Thornton*

2:30–3:20 *Discussion*

3:30–4:00 *Break*

4:00–5:00 *Discussion*

Friday September 19, 2025

8:00–8:55 *Check-in/Breakfast (hosted by IPAM)*

9:00 *TBA*

9:00–9:50 **Katsuyo Thornton** (University of Michigan)
Phase-Field Modeling of Microstructural Evolution Resulting from Corrosion

10:00–10:15 *Break*

10:15–11:05 **Brian Wetton** (University of British Columbia)
Multiscale Modelling of Electrochemical Systems

11:15–11:30 *Break*

(Friday schedule continued on next page)

(Friday schedule continued from previous page)

11:30–12:20 **Hongbo Zhao** (University of California, San Diego (UCSD))
Learning Physics of Electrochemical Systems from Data

