Workshop II: Bridging Scales from Atomistic to Continuum in Electrochemical Systems

Monday October 6, 2025

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

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

9:00 *SESSION CHAIR: Katsuyo Thornton*

9:00–9:50 **Karsten Reuter** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
First-Principles based Modelling of Electrocatalysis Beyond the Potential of Zero Charge

10:00–10:15 *Break*

10:15–11:05 **Richard Hennig** (University of Florida)
Enhancing VASPsol Accuracy for Non-Qqueous Solvents via Active Learning

11:15–11:30 *Break*

11:30–12:20 **Craig Plaisance** (Louisiana State University)
Modeling Electrocatalysis Without the Pain: Past, Present, and Future

12:30–2:30 *Lunch (on your own)*

2:30 *SESSION CHAIR: Katsuyo Thornton*

2:30–3:20 **Mauro Maggioni** (Johns Hopkins University)
learning interaction laws in particle-based systems

3:30–4:00 *Break*

4:00–4:30 *Lightning Poster Round*

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

Tuesday October 7, 2025

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

9:00 *SESSION CHAIR: Richard Henning*

9:00–9:50 **Graeme Henkelman** (University of Texas at Austin)
Correlating structure and function for nanoparticle catalysts

10:00–10:15 *Break*

(Tuesday schedule continued on next page)

(Tuesday schedule continued from previous page)

10:15–11:05 **Salvatore Torquato** (Princeton University)
Virtual Talk: Sensitive Microstructural Descriptors of Disordered Heterogeneous Materials Across Length Scales for Materials Discovery

11:15–11:30 *Break*

11:30–12:20 **Ilenia Battiato** (Stanford University)
Upscaling and Automation: Pushing the Boundaries of Multiscale Modeling of Battery Systems through Symbolic-Numeric Computing

12:30–2:30 *Lunch (on your own)*

2:30 *SESSION CHAIR: Richard Henning*

2:30–3:20 **Peter Voorhees** (Northwestern University)
Dendrite Formation in Batteries: Dead Lithium and Thermodiffusion

3:30–4:00 *Break*

4:00–4:50 **David Bortz** (University of Colorado Boulder)
Virtual Talk: Weak form SciML for Learning Models on Different Scales

Wednesday October 8, 2025

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

9:00 *SESSION CHAIR: Mauro Maggioni*

9:00–9:50 **Manuel Landstorfer** (Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS))
Continuum Thermodynamic Models for Electrochemical Interfaces

10:00–10:15 *Break*

10:15–11:05 **Jun Huang** (Forschungszentrum Jülich)
Hybrid density-potential functional approach to bridge atomistic scale and continuum

11:15–11:30 *Break*

11:30–12:20 **Juergen Fuhrmann** (Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS))
Continuum scale electrolyte simulations based on finite volume methods

12:30–12:40 *Group Photo*

12:40–2:30 *Lunch (on your own)*

2:30 *SESSION CHAIR: Mauro Maggioni*

2:30–3:20 **Huan Lei** (Michigan State University)
An energy-stable machine-learning model of non-Newtonian hydrodynamics with molecular fidelity

3:30–4:00 *Break*

(Wednesday schedule continued on next page)

(Wednesday schedule continued from previous page)

4:00–5:00 **Martin Bazant** (Massachusetts Institute of Technology)
Unified quantum theory of electrochemical kinetics by coupled ion-electron transfer

Thursday October 9, 2025

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

9:00 *SESSION CHAIR: Juergen Fuhrmann*

9:00–9:50 **Michael Herbst** (École Polytechnique Fédérale de Lausanne (EPFL))
Algorithmic differentiation (AD) for plane-wave DFT

10:00–10:15 *Break*

10:15–11:05 **Rachel Kurchin** (Carnegie Mellon University)
Non-equilibrium Electrochemical Phase Maps with Automatic Differentiation

11:15–11:30 *Break*

11:30–12:20 **Yunan Yang** (Cornell University)
Virtual Talk: The Distributional Koopman Operator for Random Dynamical Systems

12:30–2:30 *Lunch (on your own)*

2:30 *SESSION CHAIR: Juergen Fuhrmann*

2:30–3:20 **Daniel Schwalbe-Koda** (University of California, Los Angeles (UCLA))
Bridging Scales in Materials Modeling with Atomistic Simulations, Information Theory, and Generative Models

3:30–4:00 *Break*

4:00–5:00 *Discussion*

Friday October 10, 2025

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

9:00 *SESSION CHAIR: Graeme Henkelman*

9:00–9:50 **Roman Grigoriev** (Georgia Institute of Technology)
Bridging scales using physically-informed machine learning

10:00–10:15 *Break*

10:15–11:05 **Danny Perez** (Los Alamos National Laboratory)
Modeling metallic interfaces under high electric fields for particle accelerators

11:15–11:30 *Break*

(Friday schedule continued on next page)

(Friday schedule continued from previous page)

11:30–12:20 **Chong Liu** (University of California, Los Angeles (UCLA))
An experimentalist's (primitive) view of stochasticity in electrochemistry