

Bridging the Gap: Transitioning from Deterministic to Stochastic Interaction Modeling in Electrochemistry Tutorials

Thursday September 4, 2025

- 8:00–8:55 *Check-In/Breakfast (Hosted by IPAM)*
- 8:55–9:00 *Welcome and Opening Remarks*
- 9:00–10:15 **Jörg Neugebauer** (Max-Planck-Institut für Eisenforschung)
DFT for Electrochemistry: Part 2
- 10:15–10:45 *Break*
- 10:45–12:00 **Katsuyo Thornton** (University of Michigan)
The Role of Materials and Microstructures in Electrochemical Energy Storage; Part 1
- 12:00–2:00 *Lunch (on your own)*
- 2:00–3:15 **Keith Promislow** (Michigan State University)
Correlation as a Source of Stochasticity in Continuum Models: Part 1
- 3:15–3:45 *Break*
- 3:45–5:00 **Mira Todorova** (Max-Planck-Institut für Eisenforschung GmbH)
Molecular Level Modeling: Part 2

Friday September 5, 2025

- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00–10:15 *Jörg Neugebauer: Hands-on tutorial DFT and MD*
- 10:15–10:45 *Break*
- 10:45–12:00 **Katsuyo Thornton** (University of Michigan)
The Role of Materials and Microstructures in Electrochemical Energy Storage; Part 2
- 12:00–2:00 *Lunch (on your own)*
- 2:00–3:15 **Keith Promislow** (Michigan State University)
Correlation as a Source of Stochasticity in Continuum Models: Part 2
- 3:15–3:45 *Break*
- 3:45–5:00 **Jörg Neugebauer** (Max-Planck-Institut für Eisenforschung)
DFT for Electrochemistry: Part 2



Monday September 8, 2025

- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00–10:15 **Mira Todorova** (Max-Planck-Institut für Eisenforschung GmbH)
Molecular Level Modeling: Part 2
- 10:15–10:45 *Break*
- 10:45–12:00 **Manuel Landstorfer** (Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS))
Modeling Electrochemistry with Continuum Non-Equilibrium Thermodynamics: Part 1
- 12:00–2:00 *Lunch (on your own)*
- 2:00–3:15 **Mauro Maggioni** (John Hopkins University)
Learning Interaction Kernels in Interacting Particle Systems
- 3:15–3:45 *Break*
- 3:45–5:00 **Richard Hennig** (University of Florida)
Continuum Solvation Models for Solid-Liquid Interfaces: Theory, Assumptions, and Pathways Beyond

Tuesday September 9, 2025

- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00–10:15 **Juergen Fuhrmann** (Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS))
Thermodynamically Consistent Finite Volume Methods for Generalized Nernst-Planck-Poisson Problems
- 10:15–10:45 *Break*
- 10:45–12:00 **Manuel Landstorfer** (Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS))
Modeling Electrochemistry with Continuum Non-Equilibrium Thermodynamics: Part 2
- 12:00–2:00 *Lunch (on your own)*
- 2:00–3:15 **Richard Hennig** (University of Florida)
Continuum Solvation Models for Solid-Liquid Interfaces: Theory, Assumptions, and Pathways Beyond
- 3:15–3:45 *Break*
- 3:45–5:00 **Katsuyo Thornton** (University of Michigan)
Hands-on Tutorial: Phase Fields

