Workshop III: Batteries and Fuel Cells

Monday November 4, 2013

8:00–9:00	*Check-In/Light Breakfast (Hosted by IPAM)*
9:00	*Session Chair: G. Henkelman*
9:00–9:15	*Welcome and Opening Remarks*
9:15–9:55	**Chris Wolverton** (Northwestern University) *Predicting Novel Materials for Li-ion and Li-O2 Batteries*
10:15–10:30	*Break*
10:30–11:10	**Klaus-Dieter Kreuer** (Max-Planck-Institut für Festkörperforschung (Solid State Research)) *Proton and Hydroxide Ion Conducting Polymer Membranes for Fuel Cells: Fundamentals, Research Strategies and Implications for the Development of Separator Membranes for Redox-Flow and Alkaline-Ion Batteries*
11:30–11:45	*Break*
11:45–12:25	**Axel Gross** (Universität Ulm) *Towards a first-principles description of structures and processes in electrochemical energy storage and conversion*
12:30–2:30	*Lunch (on your own)*
2:30	*Session Chair: C. Wolverton*
2:30–3:10	**Adam Weber** (Lawrence Berkeley Laboratory) *Macroscopic Modeling of Performance Concerns in Proton-Exchange-Membrane Fuel-Cell Catalyst Layers*
3:30–4:00	*Pre-Poster Session Introductions: Presenters will give brief introductions of their posters for Tuesday's Session*
4:30	*4:30 PM: IPAM Public Lecture: Korn Convocation Hall, Anderson School (UCLA)*
4:30–5:30	**Emily Carter** (Princeton University) *Public Lecture: Quantum Mechanics and the Future of the Planet*
6:00–7:00	*Private Reception (by invitation only)*

Tuesday November 5, 2013

8:00–9:00 *Continental Breakfast*

9:00 *Session Chair: A. Gross*

9:00–9:40 **Bruce Dunn** (University of California, Los Angeles (UCLA))
Three-Dimensional Battery Architectures

10:00–10:15 *Break*

10:15–10:55 **Anton van der Ven** (University of California, Santa Barbara (UC Santa Barbara))
Connecting electronic structure to phenomenological descriptions of dynamic processes in electrodes

11:15–11:30 *Break*

11:30–12:10 **Emily Carter** (Princeton University)
First Principles Quantum Mechanics Methods for Simulating Fundamental Phenomena in Batteries and Fuel Cells

12:30–2:30 *Lunch (on your own)*

2:30 *Session Chair: M. Tuckerman*

2:30–3:10 **Troy Farrell** (Queensland University of Technology)
Mathematical Modelling and Numerical simulation of LiFePO4 Cathodes

3:30–4:00 *Break*

4:00–4:40 **Keith Promislow** (Michigan State University)
Network Structures in Amphiphilic Materials: Morphology and Transport

5:00–6:00 *Reception and Poster Session (Hosted by IPAM)*

Wednesday November 6, 2013

8:00–9:00 *Continental Breakfast*

9:00 *Session Chair: K. Persson*

9:00–9:40 **Venkat Subramanian** (Washington University in St. Louis)
Mathematics in the Driver's Seat

10:00–10:15 *Break*

10:15–10:55 **Richard Braatz** (Massachusetts Institute of Technology)
A Roadmap for the Multiscale Simulation of Lithium-ion Batteries

11:15–11:30 *Break*

(Wednesday schedule continued on next page)

(Wednesday schedule continued from previous page)

11:30–12:10 **Vidvuds Ozolins** (University of California, Los Angeles (UCLA))
Sparse physics and its applications to energy materials

12:30–2:30 *Lunch (on your own)*

2:30 *Session Chair: B. Wetton*

2:30–3:10 **Kristin Persson** (Lawrence Berkeley Laboratory)
The Coupling Between Cation Ordering And Phase Evolution And Its Implications For Single-Phase Cathode Design: A case study of the high-voltage Lixni0.5 Mn1.5 O4 spinel from first-principles modeling

3:30–4:00 *Break*

4:00–4:40 **Katsuyo Thornton** (University of Michigan)
Smoothed-Boundary-Method Electrochemical Simulation Framework for Battery Materials

Thursday November 7, 2013

8:00–9:00 *Continental Breakfast*

9:00 *Session Chair: K.D. Kreuer*

9:00–9:40 **Jacob White** (Massachusetts Institute of Technology)
Model Reduction Based Battery Modeling for Simulating Vehicle Cooling Systems

10:00–10:15 *Break*

10:15–10:55 **Stephen Paddison** (University of Tennessee)
Structure/function modeling of Polymer Electrolytes: Effects of confinement and hydrophobicity

11:15–11:30 *Break*

11:30–12:10 **Brian Wetton** (University of British Columbia)
Modelling fuel cells in start-up and reactant starvation conditions

12:30–2:30 *Lunch (on your own)*

2:30 *Session Chair: M. Bazant*

2:30–3:10 **Edwin Garcia** (Purdue University)
Spatially-Resolved Modeling of Three-Dimensionally Reconstructed Li-Ion Battery Electrode Microstructures

3:30–4:00 *Break*

4:00–4:40 **Martin Bazant** (Massachusetts Institute of Technology)
Nonequilibrium Thermodynamics of Li-ion Batteries

Friday November 8, 2013

8:00–9:00	*Continental Breakfast*
9:00	*Session Chair: K. Promislow*
9:00–9:40	**Mark Tuckerman** (New York University) *Understanding the mechanisms of proton transport in hydrogen bonded media from first-principle molecular dynamics*
10:00–10:15	*Break*
10:15–10:55	**Daniel Cogswell** (Samsung Advanced Inst. of Technology) *Modeling non-equilibrium microstructure in electrochemistry*
11:15–11:30	*Break*
11:30–12:10	**Richard Hennig** (Cornell University) *Computational Methods for Structure Prediction and Solid/Liquid Interfaces for Energy Materials*
12:30	*Conclusion*