Workshop III: Materials Design in Chemical Compound Space

Monday May 2, 2011

8:00–8:50 *Check-In/Light Breakfast (Hosted by IPAM)*

8:50–9:00 *Welcome & Opening Remarks: Dean Miguel García-Garibay (Dean of Physical Sciences, UCLA) and Dima Shlyakhtenko (Director, IPAM)*

9:00–9:50 **Gerbrand Ceder** (Massachusetts Institute of Technology)

10:00–10:15 *Break*

10:15–11:05 **Chris Wolverton** (Northwestern University)

11:15–11:30 *Break*

11:30–12:20 **Stefano Curtarolo** (Duke University)

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Alex Zunger** (National Renewable Energy Laboratory)
The Inverse Problem: Finding structures with Target Electronic Properties

3:30–4:00 *Break*

4:00–4:50 **Matthias Scheffler** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Screening the Chemical Compound Space from First Principles: Accessing the Accuracy and Reliability of the Base of Multi-Scale Modeling

5:00–7:00 *Reception and Poster Session (Hosted by IPAM)*

Tuesday May 3, 2011

8:00–9:00 *Continental Breakfast*

9:00–9:50 **Tamar Seideman** (Northwestern University)
Toward Coherent Control in the Nanoscale

10:00–10:15 *Break*

10:15–11:05 **Bjork Hammer** (Aarhus University)
A genetic algorithmic approach to structural optimization of supported metal particles.

11:15–11:30 *Break*

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11:30–12:20 **Joachim Sauer** (Humboldt-Universität)
The support effect and the chemical composition and structure space of solid oxide catalysts

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Suljo Linic** (University of Michigan)
Using electronic structure descriptors to identify new catalysts

3:30–4:00 *Break*

4:00–4:50 **Kristin Persson** (Lawrence Berkeley Laboratory)

Wednesday May 4, 2011

8:00–9:00 *Continental Breakfast*

9:00–9:50 **Vincent Crespi** (Pennsylvania State University)
Materials Design: Lessons from Photonics, Entropy and Good Old-fashioned Experience

10:00–10:15 *Break*

10:15–11:05 **Ralf Drautz** (Ruhr-Universität Bochum)
Phase stability in complex alloys

11:15–11:30 *Break*

11:30–12:20 **Adri van Duin** (Pennsylvania State University)
The ReaxFF reactive force field method: concepts, development and applications

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Richard Hennig** (Cornell University)
Predicting structure formation across length scales - from crystal structures to nanoscale assembly of hybrid materials.

3:30–4:00 *Break*

4:00–4:50 **Volker Blum** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Pushing all-electron DFT past some old limits: Large-scale surface structure, molecules, and some serial predictions

Thursday May 5, 2011

8:00–9:00 *Continental Breakfast*

9:00–9:50 **Kristen Fichthorn** (Pennsylvania State University)
Multi-Scale Simulations of the Growth and Assembly of Colloidal Nanoscale Materials

10:00–10:15 *Break*

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10:15–11:05 **Denis Andrienko** (Max Planck Institute for Polymer Research)

11:15–11:30 *Break*

11:30–12:20 **Vidvuds Ozolins** (University of California, Los Angeles (UCLA))

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Emily Carter** (Princeton University)
Quantum Mechanical Evaluation of Energy Conversion Materials

3:30–4:00 *Break*

4:00–4:50 **David Sholl** (Georgia Institute of Technology)
Computationally-aided development of membranes for high performance gas separations

Friday May 6, 2011

8:00–9:00 *Continental Breakfast*

9:00–9:50 **Steven Lustig** (DuPont Central Research and Development)

10:00–10:15 *Break*

10:15–11:05 **Jutta Rogal** (Ruhr-Universitaet Bochum)
Analysing reaction coordinates within the reweighted path ensemble

11:15–11:30 *Break*

11:30–12:35 **Graeme Henkelman** (University of Texas at Austin)

12:45–2:30 *Lunch (on your own)*

2:30–3:20 **David Rogers** (Sandia National Laboratories)
Organizing Desalination Membrane Design Using Thermodynamic Cycles

3:30–4:00 *Break*

4:00–4:50 **Sidney Yip** (Massachusetts Institute of Technology)
Toward Materials Ageing