

Materials for a Sustainable Energy Future Tutorials

Monday September 9, 2013

3:00 *Monday, September 9, 2013: Opening Day at Temescal Canyon, including talks by Shirley Meng (Batteries), Aleksandra Vojvodic (Catalysis), and Nate Lewis (Solar Cells). This is an invitation only event. Please contact us if interested in attending.*

Tuesday September 10, 2013

- 8:00–9:00 *Check-In/Light Breakfast (Hosted by IPAM)*
- 9:00–10:15 **Kieron Burke** (University of California, Irvine (UCI))
The ABC of DFT
- 10:15–10:45 *Break*
- 10:45–12:00 **Keith Promislow** (Michigan State University)
Continuum Level Transport and Morphology 1
- 12:00–12:30 *IPAM Orientation*
- 12:30–2:00 *Lunch (on your own)*
- 2:00–3:15 **Mark Tuckerman** (New York University)
Enhanced sampling in molecular dynamics: Targeting specific collective variables
- 3:15–3:45 *Break*
- 3:45–5:00 **Carlos Garcia-Cervera** (University of California, Santa Barbara (UC Santa Barbara))
Mathematical Foundations of DFT 1

Wednesday September 11, 2013

- 8:00–9:00 *Continental Breakfast*
- 9:00–10:15 **Kieron Burke** (University of California, Irvine (UCI))
The XYZ of DFT
- 10:15–10:45 *Break*

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- 10:45–12:00 **Keith Promislow** (Michigan State University)
Continuum Level Transport and Morphology 2
- 12:00–2:00 *Lunch (on your own)*
- 2:00–3:15 **Mark Tuckerman** (New York University)
Enhanced sampling in molecular dynamics: Unbiased approaches
- 3:15–3:45 *Break*
- 3:45–5:00 **John Bell** (Lawrence Berkeley Laboratory)
Between Kinetic Theory and Navier Stokes - Modeling Fluids at the Mesoscale

Thursday September 12, 2013

- 8:00–9:00 *Continental Breakfast*
- 9:00–10:15 **Graeme Henkelman** (University of Texas at Austin)
Calculations of rare events of atomic scale processes in materials
- 10:15–10:45 *Break*
- 10:45–12:00 **Kieron Burke** (University of California, Irvine (UCI))
THE XYZ of DFT - Part 2
- 12:00–2:00 *Lunch (on your own)*
- 2:00–3:15 **Richard Hennig** (Cornell University)
Introduction to Solid State electron transport 1
- 3:15–3:45 *Break*
- 3:45–5:00 **Ivana Savic** (Tyndall National Institute, University College Cork)
Introduction to phonon transport (heat transport)

Friday September 13, 2013

- 8:00–9:00 *Continental Breakfast*
- 9:00–10:15 **Carlos Garcia-Cervera** (University of California, Santa Barbara (UC Santa Barbara))
Mathematical Foundations of DFT 2
- 10:15–10:45 *Break*

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- 10:45–12:00 **Richard Hennig** (Cornell University)
Introduction to Solid State electron transport 2
- 12:00–2:00 *Lunch (on your own)*
- 2:00–3:30 **Felix Brockherde** (Technische Universität Berlin)
Introduction to Machine Learning
- 3:30–4:00 *Break*
- 4:00–5:00 **Keith Promislow** (Michigan State University)
Continuum Level Transport and Morphology 3

