

Navigating Chemical Compound Space for Materials and Bio Design: Tutorials

Tuesday March 15, 2011

- 8:00–8:45 *Check-In/Light Breakfast (Hosted by IPAM)*
- 8:45–9:00 *Welcome and Opening Remarks*
- 9:00–10:00 **Anatole von Lilienfeld** (Argonne National Laboratory)
Introduction
- 10:00–10:30 *Break*
- 10:30–12:00 **Cynthia Phillips** (Sandia National Laboratories)
Introduction to Optimization
- 12:00–12:30 *IPAM Core Orientation*
- 12:30–2:00 *Lunch (on your own)*
- 2:00–3:30 **Kieron Burke** (University of California, Irvine (UCI))
ABC of DFT
- 3:30–4:00 *Break*
- 4:00–4:45 **Jeff Hammond** (Argonne National Laboratory)
High Performance Computing I

Wednesday March 16, 2011

- 8:00–9:00 *Continental Breakfast*
- 9:00–10:15 **Pierre Baldi** (University of California, Irvine (UCI))
Machine Learning I
- 10:15–10:45 *Break*
- 10:45–12:00 **Kendall Houk** (University of California, Los Angeles (UCLA))
DFT and Electronic Structure II
- 12:00–2:00 *Lunch (on your own)*
- 2:00–3:15 **Brian Adams** (Sandia National Laboratories)
Simulation-based Optimization Tutorial
- 3:15–3:45 *Break*
- 3:45–5:00 **Tudor Oprea** (University of New Mexico)
QSPR I



Thursday March 17, 2011

- 8:00–9:00 *Continental Breakfast*
- 9:00–10:15 **Kieron Burke** (University of California, Irvine (UCI))
ABC of TDDFT
- 10:15–10:45 *Break*
- 10:45–12:00 **Tudor Oprea** (University of New Mexico)
QSPR II
- 12:00–1:30 *Lunch (on your own)*
- 1:30–2:15 **Jeff Hammond** (Argonne National Laboratory)
High Performance Computing II
- 2:15–2:45 *Break*
- 2:45–3:45 **Klaus-Robert Müller** (Technische Universität Berlin)
Machine Learning II
- 3:45–4:15 *Break*
- 4:15–5:30 **Mark Tuckerman** (New York University)
Exploring the free energy landscape of biomolecules and crystalline polymorphs

Friday March 18, 2011

- 8:00–9:00 *Continental Breakfast*
- 9:00–10:15 **Cynthia Phillips** (Sandia National Laboratories)
Mathematical programming and combinatorial heuristics
- 10:15–10:45 *Break*
- 10:45–12:00 **Saivenkataraman Jayaraman** (Sandia National Laboratories)
Alchemical changes within molecular dynamics
- 12:00–2:00 *Lunch (on your own)*
- 2:00–3:15 **Mark Tuckerman** (New York University)
Exploring the free energy landscape of biomolecules and crystalline polymorphs
- 3:15–3:45 *Break*
- 3:45–4:15 **Matthias Rupp** (Technische Universität Berlin)
Machine Learning III
- 4:15–4:30 *Break*

(Friday schedule continued on next page)

(Friday schedule continued from previous page)

4:30–5:15 **Denis Andrienko** (Max Planck Institute for Polymer Research)
Hot Topics in Materials Design

