

Hands-on Summer School: Electronic Structure Theory for Materials and (Bio)molecules

Monday July 21, 2014

- 8:00 *First Principles - Overview*
- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00–9:30 *Welcome and Opening Remarks*
- 9:30–10:30 **Matthias Scheffler** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Overview: Electronic Structure Theory for the Ground State
- 11:00–12:00 **Kieron Burke** (University of California, Irvine (UCI))
Electronic Structure Beyond the Ground State
- 12:00–1:30 *Lunch (on your own)*
- 1:30–2:30 **Eric Cancès** (École Nationale des Ponts-et-Chaussées)
Mathematical Foundations of DFT
- 2:45–3:45 **John Perdew** (Temple University)
Climbing the Ladder of Density Functional Approximations
- 4:00–5:00 *Poster Parade*
- 5:00–6:30 *Poster Session and Welcome Gathering*
- 7:00–8:30 *Dinner*



Tuesday July 22, 2014

- 8:00 *The Basics of DFT*
- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00–10:00 **Christian Ratsch** (Institute for Pure and Applied Mathematics)
Electronic Structure Theory for Periodic Systems: The Concepts
- 10:15–11:15 **Volker Blum** (Duke University)
Practical Implementations: The Nuts and Bolts of DFT (Part I)
- 11:30–12:30 **Bjoern Lange** (Duke University)
Practical Implementations: The Nuts and Bolts of DFT (Part II)
- 12:30–2:00 *Lunch (on your own)*
- 2:00–2:30 **Lydia Nemeč** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Introduction to Hands-on Exercise 1: Basics of Electronic Structure Theory; Tutorial Leader: Oliver Hofmann
- 2:30–6:00 **Oliver Hofmann** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Hands-on Exercise 1: Basics of Electronic Structure Theory; Tutorial Leader: Oliver Hofmann
- 6:30–8:00 *Dinner*
- 8:00–10:00 *Additional computer time with tutors on hand*

Wednesday July 23, 2014

- 8:00 *Periodic Systems*
- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00–10:00 **Alexandre Tkatchenko** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Van der Waals Interactions in Molecules and Materials
- 10:15–11:15 **Anderson Janotti** (University of California, Santa Barbara (UC Santa Barbara))
The Plane-Wave Pseudopotential Approach
- 11:30–12:30 **David Singh** (Oak Ridge National Laboratory)
The (Linearized) Augmented Plane Wave Method
- 12:30–2:00 *Lunch (on your own)*
- 2:00–2:30 **Lydia Nemeč** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Introduction to Hands-On Exercise 2: Periodic Systems; Tutorial Leader: Bjoern Bieniek
- 2:30–6:00 **Bjoern Bieniek** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Hands-On Exercise 2: Periodic Systems; Tutorial Leader: Bjoern Bieniek
- 6:30–8:00 *Dinner*
- 8:00–10:00 *Additional computer time with tutors on hand*

Thursday July 24, 2014

- 8:00 *Beyond LDA and GGA and Molecular Dynamics*
- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00–10:00 **Ken Jordan** (University of Pittsburgh)
Quantum Chemistry Approaches to the Electron Correlation Problem
- 10:15–11:15 **Adrienn Ruzsinszky** (Temple University)
Beyond Conventional Functionals in DFT
- 11:30–12:30 **Luca Ghiringhelli** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Statistical Mechanics and Molecular Dynamics
- 12:30–2:00 *Lunch (on your own)*
- 2:00–2:30 **Jan Hermann** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Introduction to Hands-On Exercise 3: Van der Waals; Tutorial Leader: Alex Tkatchenko
- 2:30–6:00 **Alexandre Tkatchenko** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Hands-On Exercise 3: Van der Waals; Tutorial Leader: Alex Tkatchenko
- 6:30–8:00 *Dinner*
- 8:00–10:00 *Additional computer time with tutors on hand*

Friday July 25, 2014

- 8:00 *Molecular Dynamics and NQE*
- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00–10:00 **Luca Ghiringhelli** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Search for Minimum Energy Paths: Nudged Elastic Band and Beyond
- 10:15–11:15 **Mauro Maggioni** (Duke University)
Geometric methods for the learning fast simulators of high-dimensional dynamical systems, and global reaction coordinates
- 11:30–12:30 **Mariana Rossi** (University of Oxford)
Quantum nuclei: (ab initio) path integral molecular dynamics for static and dynamic observables
- 12:30–2:00 *Lunch (on your own)*
- 2:00–2:30 **Mariana Rossi** (University of Oxford)
Introduction to Hands-On Exercise 4: Molecular Dynamics; Tutorial Leader: Mariana Rossi and Luca Ghiringhelli
- 2:30–6:00 **Luca Ghiringhelli** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Hands-On Exercise 4: Molecular Dynamics; Tutorial Leader: Mariana Rossi and Luca Ghiringhelli
- 6:30–8:00 *Dinner*
- 8:00–10:00 *Additional computer time with tutors on hand*

Saturday July 26, 2014

- 9:00–2:00 *Tutorial Session*
- 2:00–8:00 *Conference Social*

Sunday July 27, 2014

- 10:00–4:00 *Tutorial Session*

Monday July 28, 2014

- 8:00 *Frontier Methods for Ground States and Excited States*
- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00–10:00 **Patrick Rinke** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Excited-state properties
- 10:15–11:15 **Xinguo Ren** (University of Science and Technology of China)
Making GW, the Random Phase Approximation and Beyond Work with Localized Orbitals
- 11:30–12:30 **Steven G. Louie** (University of California, Berkeley (UC Berkeley))
Neutral Excitations and the Bethe-Salpeter Approach
- 12:30–2:00 *Lunch (on your own)*
- 2:00–2:30 **Arvid Ihrig** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Introduction to Hands-On Exercise 5: Theoretical Spectroscopy; Tutorial Leader: Patrick Rinke
- 2:30–6:00 **Patrick Rinke** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Hands-On Exercise 5: Theoretical Spectroscopy; Tutorial Leader: Patrick Rinke
- 6:30–8:00 *Dinner*
- 8:00–10:00 *Additional computer time with tutors on hand*

Tuesday July 29, 2014

- 8:00 *Spectroscopies and Transport*
- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00–10:00 **Ferdinand Evers** (Karlsruhe Institute of Technology (KIT))
Molecular Transport
- 10:15–11:15 **John Rehr** (University of Washington)
Theory and Interpretation of Core-level Spectroscopies
- 11:30–12:30 **Christian Carbogno** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Phonons and Thermal Transport
- 12:30–2:00 *Lunch (on your own)*
- 2:00–2:30 **Christian Carbogno** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Introduction to Hands-On Exercise 6: Phonons, Lattice Expansion, and Band-gap Renormalization; Tutorial Leader: Christian Carbogno
- 2:30–6:00 **Christian Carbogno** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Hands-On Exercise 6: Phonons, Lattice Expansion, and Band-gap Renormalization; Tutorial Leader: Christian Carbogno
- 6:30–8:00 *Dinner*
- 8:00–10:00 *Additional computer time with tutors on hand*

Wednesday July 30, 2014

- 8:00 *Kinetics*
- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00–10:00 **Peter Kratzer** (Universität Duisburg-Essen)
Kinetic Monte Carlo Modelling of Semiconductor Growth
- 10:15–11:15 **Daniel Berger** (Technical University Munich (TUM))
Embedded-Cluster Calculations in a Numeric Atomic Orbital Density-Functional Theory Framework
- 11:30–12:30 **Baron Peters** (University of California, Santa Barbara (UC Santa Barbara))
Transition path sampling and quantitative mechanistic hypothesis testing
- 12:30–2:00 *Lunch (on your own)*
- 2:00–2:30 **Noa Marom** (Tulane University)
Introduction to Hands-On Exercise 7: Structure search and excited states in clusters; Tutorial Leader: Noa Marom
- 2:30–6:00 **Noa Marom** (Tulane University)
Hands-On Exercise 7: Structure search and excited states in clusters; Tutorial Leader: Noa Marom
- 6:30–8:00 *Dinner*
- 8:00–10:00 *Additional computer time with tutors on hand*

Thursday July 31, 2014

- 8:00 *Multiscale & Big Data*
- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00–10:00 **Stan Osher** (University of California, Los Angeles (UCLA))
What Sparsity and l_1 Optimization Can Do For You
- 10:15–11:15 **Gus Hart** (Brigham Young University)
Multiscale modeling with cluster expansion
- 11:30–12:30 **Matthias Rupp** (Universität Basel)
Machine Learning Models
- 12:30–2:00 *Lunch (on your own)*
- 2:00–2:30 **Gus Hart** (Brigham Young University)
Introduction to Hands-On Exercise 8: Multiscale Models; Tutorial Leader: Gus Hart
- 2:30–6:00 **Gus Hart** (Brigham Young University)
Hands-On Exercise 8: Multiscale Models; Tutorial Leader: Gus Hart
- 6:30–8:00 *Dinner*
- 8:00–10:00 *Additional computer time with tutors on hand*

Friday August 1, 2014

- 8:00 *Multiscale & Big Data*
- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00–10:00 **Carlos Garcia-Cervera** (University of California, Santa Barbara (UC Santa Barbara))
Multiscale Modeling
- 10:15–11:15 **Sadasivan Shankar** (Intel Corporation)
DFT for Materials Design – Back to the Future
- 11:30–12:30 **Rampi Ramprasad** (University of Connecticut)
The Materials Genome

