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 Cances** (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 Nemec** (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 Nemec** (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 l1 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*