

Putting the Theory Back in Density Functional Theory

Monday August 22, 2016

- 8:00–8:45 *Check-In/Light Breakfast (Hosted by IPAM)*
- 8:45–9:00 *Welcome and Opening Remarks*
- 9:00–9:30 **Mel Levy** (Tulane University)
Hohenberg-Kohn theorem and generalizations
- 9:45–10:15 **Carlos Garcia-Cervera** (University of California, Santa Barbara (UCSB))
Mathematical foundations
- 10:30–10:45 *Break*
- 10:45–11:15 **Kieron Burke** (University of California, Irvine (UCI))
Kohn-Sham equations
- 11:30–12:00 **Carlos Garcia-Cervera** (University of California, Santa Barbara (UCSB))
Kohn-Sham models (mathematical)
- 12:00–1:30 *Lunch (on your own)*
- 1:30–2:00 **John Perdew** (Temple University)
Local density approximation (LDA)
- 2:15–2:45 **Mel Levy** (Tulane University)
Exact constraints
- 3:00–3:15 *Break*
- 3:15–3:45 **Kieron Burke** (University of California, Irvine (UCI))
Density matrices and holes
- 4:00–4:30 **John Perdew** (Temple University)
Generalized gradient approximation (GGA)
- 4:30–4:45 *Break*
- 4:45–5:05 **Attila Cangi** (Max Planck Institute of Microstructure Physics)
Participant talk: The potential of Potential Functional Theory
- 5:15–7:00 *Poster Session & Reception (Hosted by IPAM)*
- 7:30–9:00 *Discussion*



Tuesday August 23, 2016

- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00–9:30 **Carlos Garcia-Cervera** (University of California, Santa Barbara (UCSB))
Mathematical spin density functional theory
- 9:45–10:15 **Mel Levy** (Tulane University)
Coordinate Scaling and Adiabatic Connection
- 10:30–10:45 *Break*
- 10:45–11:15 **Weitao Yang** (Duke University)
Optimized-effective-potential method and hybrids
- 11:30–12:00 **Weitao Yang** (Duke University)
Derivative discontinuity and gaps
- 12:00–1:30 *Lunch (on your own)*
- 1:30–2:00 **Jianfeng Lu** (Duke University)
Localization (mathematical)
- 2:15–2:45 **Paola Gori-Giorgi** (Vrije Universiteit)
Exchange-correlation potential
- 3:00–3:15 *Break*
- 3:15–3:45 **Hardy Gross** (Max Planck Institute of Microstructure Physics)
Time-dependent density functional theory
- 4:00–4:30 **Neepta Maitra** (Hunter College, CUNY)
Basics of time-dependent density functional linear response theory
- 4:30–4:45 *Break*
- 4:45–5:05 **Eli Kraisler** (Max Planck Institute for Microstructure Physics)
Participant talk: Addressing long-standing problems in density-functional theory with the ensemble generalization approach
- 5:15–5:35 **Aurora Pribram-Jones** (Lawrence Livermore National Laboratory)
Participant talk: New exchange-correlation free energy approximations from time-dependent density functional theory
- 6:00–7:30 *Dinner (on your own)*
- 8:00–9:30 *Discussion*

Wednesday August 24, 2016

- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00–9:30 **Adam Wasserman** (Purdue University)
Chemical reactivity theory
- 9:45–10:15 **Adrienn Ruzsinszky** (Temple University)
Van-der-Waals interactions
- 10:30–10:45 *Break*
- 10:45–11:15 **Hardy Gross** (Max Planck Institute of Microstructure Physics)
Many-body theory
- 11:30–12:00 **John Perdew** (Temple University)
Meta-generalized gradient approximations (meta-GGAs)
- 12:00–1:30 *Lunch (on your own)*
- 1:30–2:00 **Kieron Burke** (University of California, Irvine (UCI))
Static correlation
- 2:15–2:45 **Hardy Gross** (Max Planck Institute of Microstructure Physics)
Magnetism
- 3:00–3:15 *Break*
- 3:15–3:45 **Paola Gori-Giorgi** (Vrije Universiteit)
The strong-coupling limit of density functional theory
- 4:00–4:30 **Neepa Maitra** (Hunter College, CUNY)
Memory in Time-Dependent Density Functional Theory
- 4:30–4:45 *Break*
- 4:45–5:05 **Chen Li** (Duke University)
Participant talk: Gentlest Ascent Dynamics for Calculating First Excited State and Exploring Energy Landscape of Kohn-Sham Density Functionals
- 5:15–5:35 **Yael Cytter** (The Hebrew University of Jerusalem)
Participant talk: A Stochastic approach to thermal density functional theory
- 6:00–7:30 *Dinner (on your own)*
- 8:00–9:30 *Discussion*

Thursday August 25, 2016

- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00–9:45 **Adrienn Ruzsinszky** (Temple University)
Renormalized perturbation theory for materials science
- 10:00–10:15 *Break*
- 10:15–11:00 **John Perdew** (Temple University)
Physical Interpretation of the Generalized Kohn-Sham Band Gap for a Solid
- 11:15–11:30 *Break*
- 11:30–12:15 **Mel Levy** (Tulane University)
Total energy as a simple sum of augmented orbital energies and Open Mathematical Problems
- 12:30–2:00 *Lunch (on your own)*
- 2:00–2:45 **Paola Gori-Giorgi** (Vrije Universiteit)
Lieb-Oxford bound
- 3:00–3:15 *Break*
- 3:15–4:00 **Neepa Maitra** (Hunter College, CUNY)
Spuriously shifting resonances in TDDFT, and their impact on dynamics
- 4:15–4:30 *Break*
- 4:30–4:50 **Manuel Schoettler** (Universität Rostock)
Participant talk: Miscibility gap of hydrogen-helium mixtures
- 5:00–5:20 **Shree Ram Acharya** (University of Central Florida)
Participant talk: Time-Dependent Density-Functional Theory+ Dynamical Mean-Field Theory for strongly correlated materials: an application to MnO
- 6:30–9:00 *Conference Banquet*

Friday August 26, 2016

- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00–9:45 **Weitao Yang** (Duke University)
- 10:00–10:15 *Break*
- 10:15–11:00 **Adam Wasserman** (Purdue University)
Partition Density Functional Theory
- 11:15–11:30 *Break*

(Friday schedule continued on next page)

(Friday schedule continued from previous page)

- 11:30–12:15 **Jianfeng Lu** (Duke University)
Frozen Gaussian approximation with surface hopping
- 12:30–2:00 *Lunch (on your own)*
- 2:00–2:45 **Carlos Garcia-Cervera** (University of California, Santa Barbara (UCSB))
Hartree-Fock with self-generated magnetic fields
- 3:00–3:15 *Break*
- 3:15–4:00 **Hardy Gross** (Max Planck Institute of Microstructure Physics)
- 4:15–4:30 *Break*
- 4:30–5:15 **Kieron Burke** (University of California, Irvine (UCI))
Recent development in density functional theory
- 5:30 *Conclusion*

