

## 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*

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- 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*

