Orbital-free approach for high energy density physics

September 5, 2012 to September 7, 2012

Location : La Maison des Mines et des Ponts et Chaussées, Paris

Details Participants Program Abstracts

Day 1 - September, 5th 2012

- 09:00 to 09:30 - Welcome and Introduction
- 09:30 to 10:30 - **Lee A. Collins**
  Equilibrium and Non-equilibrium Orbital-Free Molecular Dynamics Simulations at Extreme Conditions
- 10:30 to 10:45 - Coffee Break
- 10:45 to 11:45 - **James Dufty**
  Finite Temperature Scaling in Density Functional Theory
- 11:45 to 13:45 - Lunch Break
- 13:45 to 14:45 - **Junchao Xia**
  Orbital-Free Density Functional Theory of Molecules and Semiconductors
- 14:45 to 15:00 - Coffee Break
- 15:00 to 16:00 - **Samuel B. Trickey**
  Design Criteria for Constraint-based Single-Point Orbital-free Density Functional Approximations
- 16:00 to 16:15 - Coffee Break
- 16:15 to 17:15 - **David Garcia Aldea**
  Nonlocal terms for Kinetic Energy Density Functionals based on the Thomas-Fermi and von Weizsäcker functionals
- 17:15 to 18:30 - **S. Pittalis**
  Orbital-free approaches to equilibrium and non-equilibrium properties of many-electron systems: recent development of exact and approximate methods

Day 2 - September, 6th 2012

- 09:00 to 10:00 - **Vikram Gavini**
  Electronic structure calculations at macroscopic scales using orbital-free density functional theory
- 10:00 to 10:15 - Coffee Break
- 10:15 to 11:15 - **V. Karassev**
  Finite temperature GGA orbital-free density functionals: development and application to warm dense hydrogen
- 11:15 to 11:30 - Coffee Break
- 11:30 to 12:30 - **Daniel Neuhauser**
  Time dependent Orbital Free DFT (TD-OFDFT) with Correct Dynamical Susceptibility
- 12:30 to 13:30 - Lunch Break
- 13:30 to 14:30 - **Luis Enrique Gonzalez**
  Structural and dynamical properties of liquid alkaline-earth metals
- 14:30 to 14:45 - Coffee Break
- 14:45 to 15:45 - **T. Sjostrom**
  Exchange-correlation free energy functionals
- 15:45 to 16:00 - Coffee Break
- 16:00 to 17:00 - **Ann Mattsson**
  Creating Orbital Free Functionals using the Subsystem Functional Scheme
- 18:30 to 22:30 - Social Dinner

Day 3 - September, 7th 2012

- 09:00 to 10:00 - **Tomasz Wesolowski**
  Orbital-free approximations for the bifunctional for the non-additive kinetic energy
- 10:00 to 10:15 - Coffee Break
- 10:15 to 11:15 - **Jérôme Daligault**
  Time-Dependent Orbital-Free Molecular Dynamics Simulations of Dense Plasmas
- 11:15 to 11:30 - Coffee Break
- 11:30 to 12:30 - **L. Kazandjian**

Computation of the self-diffusion coefficient and viscosity by orbital-free molecular dynamics

- 12:30 to 14:00 - General Discussion and Conclusion

CECAM - Centre Européen de Calcul Atomique et Moléculaire
Ecole Polytechnique Fédérale de Lausanne, Batochime (BCH), 1015 Lausanne, Switzerland