

Workshop IV: Computational Challenges in Warm Dense Matter

Monday May 21, 2012

- 8:00–9:00 *Check-In/Light Breakfast (Hosted by IPAM)*
- 9:00–9:10 *Long Program Overview: Frank Graziani*
- 9:10–10:00 **Michael Desjarlais** (Sandia National Laboratories)
An Introduction to Warm Dense Matter Research
- 10:10–10:25 *Break*
- 10:25–11:15 **Samuel Trickey** (University of Florida)
The Quantum Theory Landscape for Warm Dense Matter
- 11:25–11:40 *Break*
- 11:40–12:30 **Ronald Redmer** (Universität Rostock)
Warm dense matter and the interior of giant planets
- 12:40–2:00 *Lunch (on your own)*
- 2:00–2:50 **Dario Alfe** (University College London)
Complementary approaches to high temperature-high pressure crystal structure stability and melting
- 3:00–3:15 *Break*
- 3:15–4:05 **Stephane Mazevet** (Observatoire de Paris)
X-ray near edge spectroscopy (XANES) as a probe of warm dense matter
- 4:15–4:30 *Break*
- 4:30–5:20 **Carsten Fortmann** (University of California, Los Angeles (UCLA))
Dynamical Structure Factor in Warm Dense Matter and Applications to X-Ray Thomson Scattering
- 5:30–7:00 *Poster Session & Reception (Hosted by IPAM)*

Tuesday May 22, 2012

- 8:00–9:00 *Breakfast (Hosted by IPAM)*
- 9:00–9:50 **Walter Johnson** (University of Notre Dame)
Xray Scattering from WDM: Thomson Scattering in the Average-Atom Approximation
- 10:00–10:15 *Break*

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- 10:15–11:05 **Brian Wilson** (Lawrence Livermore National Laboratory)
Multi-Center Electronic Structure Calculations For Plasma Equation of State
- 11:15–11:30 *Break*
- 11:30–12:20 **Didier Saumon** (Los Alamos National Laboratory)
A model of warm dense matter for small computers
- 12:30–2:00 *Lunch (on your own)*
- 2:00–2:50 **Jerome Daligault** (Los Alamos National Laboratory)
Time-Dependent Thomas-Fermi Molecular Dynamics Simulations of Dense Plasmas
- 3:00–3:15 *Break*
- 3:15–4:05 **James Dufty** (University of Florida)
Effective Forces for Application of Classical Methods to Quantum Systems
- 4:15–4:30 *Break*
- 4:30–5:20 **Luke Shulenburger** (Sandia National Laboratories)
Perspectives on plasma simulation techniques from the IPAM quantum simulation working group

Wednesday May 23, 2012

- 8:00–9:00 *Breakfast (Hosted by IPAM)*
- 9:00–9:50 **Eberhard Gross** (Max Planck Institute of Microstructure Physics)
- 10:00–10:15 *Break*
- 10:15–11:05 **Kieron Burke** (University of California, Irvine (UCI))
The relationship between density functional theory and semiclassical approximations
- 11:15–11:30 *Break*
- 11:30–12:20 **Andreas Goerling** (Friedrich-Alexander-Universität Erlangen-Nürnberg)
Density-functional methods for electronic systems at finite temperatures
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Patrick Rinke** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Towards a unified description of ground and excited state properties
- 3:30–4:00 *Break*
- 4:00–4:50 **David Ceperley** (University of Illinois at Urbana-Champaign)
Quantum Monte Carlo Methods for Warm Dense Matter

Thursday May 24, 2012

- 8:00–9:00 *Breakfast (Hosted by IPAM)*
- 9:00–9:50 **Stefano Pittalis** (University of California, Irvine (UCI))
Exact Conditions in Finite-Temperature Density-Functional Theory
- 10:00–10:15 *Break*
- 10:15–11:05 **Travis Sjoström** (University of Florida)
Finite-Temperature Hartree-Fock Exchange and Exchange-Correlation Free Energy Functionals
- 11:15–11:30 *Break*
- 11:30–12:20 **Ann Mattsson** (Sandia National Laboratories)
Improving the Predictive Power of Calculations for the Warm Dense Matter Region
- 12:30–2:00 *Lunch (on your own)*
- 2:00–2:50 **Carsten Ullrich** (University of Missouri-Columbia)
TDDFT for matter under extreme conditions
- 3:00–3:15 *Break*
- 3:15–4:05 **Normand Modine** (Sandia National Laboratories)
Time-Dependent Density Functional Theory with Moving Ions
- 4:15–4:30 *Break*
- 4:30–5:20 **Volker Blum** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
All electron ab initio molecular simulations - status, successes, and some computational challenges

Friday May 25, 2012

- 8:00–9:00 *Breakfast (Hosted by IPAM)*
- 9:00–9:50 **Paul Grabowski** (Los Alamos National Laboratory)
Simulating Quantum High Energy Density Plasmas: Approximations According to the Time-Dependent Variational Principle
- 10:00–10:15 *Break*
- 10:15–11:05 **Flavien Lambert** (Commissariat à l'Énergie Atomique (CEA))
Plastic ablator in the hydrodynamic-instability regime: a first-principle set of microscopic coefficients
- 11:15–11:30 *Break*
- 11:30–12:20 **Joel Kress** (Los Alamos National Laboratory)
Mass Transport in the Warm, Dense Matter and High-Energy Density Regimes
- 12:30–12:45 *Closing Remarks*

