Joint Theory Seminar
European XFEL, CFEL & University of Hamburg

Thursday, 30 September 2021, 16:00

Valentin V. Karasiev

Laboratory for Laser Energetics, University of Rochester
New York, USA

Development of free-energy density functional methods for warm dense matter applications

Ab initio molecular dynamics (AIMD) simulations based on the free-energy density functional theory (DFT) in combination with the Kubo--Greenwood (KG) formulation for transport and optical properties, has proven to be a successful and key tool to understand warm-dense-matter (WDM) and high-energy density (HED) plasmas across different regimes. In this talk I present a novel DFT-based methodology for optical property calculations of warm dense matter to cover a wide range of thermodynamic conditions and photon energies including the entire x-ray range. The methodology was applied to opacity calculations of warm dense silicon plasmas and revealed a very interesting phenomenon of redshift-to-blueshift in K-L (1s → 2p) and K-edge absorptions along both isotherm and isochore, which are absent in most continuum-lowering models of traditional plasma physics.

The potential for predictive DFT calculations of WDM depends crucially upon having an exchange-correlation (XC) free-energy functional accurate across temperature regimes. Furthermore we discuss development of XC density functionals with explicit temperature dependence at the meta generalized gradient approximation (meta-GGA) level of theory providing improved accuracy across the temperature regimes. Thermal meta-GGA functional provides a systematically improved accuracy of WDM simulations, as we show on example of dense Hydrogen and Helium.

Host: Nils Brouwer

Zoom link
https://xfel.zoom.us/j/96004923285?pwd=K0ZvLytIV0NZYmx6eU4vbG03K0J3UT09
Meeting ID: 960 0492 3285
Passcode: 216328