Improving Ab-Initio Methods for Warm Dense Matter Simulations

Attila Cangi¹, Aurora Pribram-Jones²

1) Max Planck Institute of Microstructure Physics
2) Department of Chemistry, University of California, Irvine

Corresponding author: Attila Cangi (acangi@mpi-halle.mpg.de)

Warm dense matter (WDM) is a highly energetic phase of matter with characteristics of solids, liquids, gases and plasmas. Many pending and fundamental questions rely on our understanding of WDM, such as the physics behind the formation of planets, the nature of chemistry under extreme conditions, and the possibility to control nuclear fusion. Simulation of WDM requires computational methods that capture both quantum and classical behavior efficiently under high-temperature and high-density conditions. Currently, molecular dynamics in conjunction with Kohn-Sham density functional theory (KS-DFT) is used successfully to model electrons and ions. But this method suffers from two fundamental drawbacks:

(i) the computational cost skyrockets as temperatures and densities increase;
(ii) temperature effects complicate exchange-correlation approximations.

In my talk I introduce an alternative approach – finite-temperature potential functional theory – which avoids the bottleneck of KS-DFT. The underlying premise is that leading corrections to local approximations (such as Thomas-Fermi theory)

(1) are universal functionals of the potential;
(2) can be derived under WDM conditions;
(3) dramatically improve upon efficiency and accuracy.

I demonstrate this for a model system and give a perspective on future developments.