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Density Functional Theory calculations for high-temperature carbon plasmas

Monday 21 February 2022 15:40 (30 minutes)

Accurately modeling dense plasmas over wide ranging conditions of pressures and temperatures is a grand challenge problem critically important to our understanding of inertial confinement fusion (ICF), stellar physics, exoplanets, and planetary formation. Over the last few years planewave- based Kohn-Sham Density Functional Theory Molecular Dynamics (DFT-MD) has proven highly successful in describing the properties of many materials in the condensed and warm dense matter regimes from first principles. However, the tractable number of particles is rather limited due to the method's O(N^3) scaling and it becomes challenging to employ at high temperatures, where the number of partially occupied states increases significantly. Both problems are addressed with the novel SQDFT code [1], which is a large-scale implementation of the Spectral Quadrature (SQ) method for O(N) Kohn-Sham DFT calculations [2,3].
This talk discusses the new capabilities of SQDFT by comparing to the widely-used planewave Kohn-Sham DFT codes as well as other methods such as Path Integral Monte Carlo. Extensive benchmark calculations for the thermodynamic and structural properties of carbon are presented. In particular, the Hugoniot curve for carbon was calculated for conditions spanning the condensed matter regime, the warm dense matter regime and the plasma regime with temperatures up to 10 million Kelvin all within the framework of many particles full Kohn-Sham DFT-MD [4].

REFERENCES
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