UNIVERSITY OF CALIFORNIA
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First-Principles Modeling of Warm Dense Matter

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Abstract

Understanding high energy density (HED) phenomena generated on pulsed power facilities (Z machine) and at coherent light sources (European XFEL, LCLS) requires interpreting complex diagnostic signals such as fluorescence emission and x-ray scattering emission. Predicting their evolution requires adequate models of transport properties in extreme (and extremely non-equilibrium) states of matter. Furthermore, the persistence of electron correlation in HED materials arising from Coulomb interactions and the Pauli exclusion principle is one of the greatest challenges for accurate numerical modeling and has hitherto impeded our ability to model HED phenomena across multiple length and time scales at sufficient accuracy.

I will give an overview of my research activities on the modeling of HED matter. In anticipation of future experiments, I will assess the ability of time-dependent density functional theory (TDDFT) to reproduce these results and compare its utility with other state-of-the-art approaches such as the Kubo-Greenwood formalism and average-atom models in terms of accuracy, computational cost, and self-consistency.
I will conclude with an outlook on our future research activities on developing a multiscale simulation framework which uses high-fidelity electronic structure data at the microscale and leverages machine learning and high-performance molecular dynamics techniques to capture the kinetics of phase transitions at the mesoscale.

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