SPECIAL CORE-CM/SATE SEMINAR
Michigan State University

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Modeling Real-Time Electron-Ion Dynamics Using Time-Dependent Density Functional Theory

The calculation of the ground state properties of many-electron systems using density functional theory (DFT) has become standard practice in many fields, ranging from geophysics to complex materials to fusion science. In recent years, the time-dependent extension of DFT (TDDFT) has become an increasingly useful tool for going beyond the ground state to study excited and non-equilibrium properties of this same breadth of systems. In this talk, I will discuss the development and application of TDDFT methods to the study of warm dense matter - a region of thermodynamic phase space typified as being intermediate between a condensed phase and a plasma. These methods give us access to a wide variety of properties, including optical/x-ray spectra, stopping powers, and electron-ion equilibration rates, which are being probed in the warm dense regime at experimental facilities such as Rochester's OMEGA laser, SLAC's LCLS, and Sandia's Z-Machine. While the extreme thermodynamic conditions of the warm dense state present one theoretical challenge for TDDFT, recent ultrafast experiments on materials with exotic orderings being driven out of equilibrium present an array of new theoretical challenges that we will also discuss. Many of the open problems in these seemingly disparate conditions are more related than one may expect, and I will discuss some of the synergies that may exist between the two fields.

Bio:

Andrew Baczewski received his Ph.D. in Electrical Engineering and Physics at Michigan State University in 2013. From 2013-2014 he was a postdoc in the multiscale science group at Sandia National Laboratories. In late 2014, he became technical staff at the Center for Computing Research at Sandia National Laboratories, where he works in the space between electronic structure and quantum information theory.

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