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CHEMISTRY SEMINAR 291

Interaction Strength and Temperature in Density Functional Theory

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Location: **COB 267**

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ABSTRACT

Electronic structure is at the root of chemical reactions, molecular structure, material properties, and biological function. Density functional theory is one of the most successful ways to balance accuracy and computational cost, but approximations used in the method generally ignore explicit temperature dependence. Simulations using these incomplete approximations impact x-ray free electron laser experiments, simulations of complex alloys, and experimental design and analysis of projects at the National Ignition Facility and other flagship facilities around the world.

The finite-temperature adiabatic connection formula, which gives interaction free energies in terms of the potential energy alone, is recast as a temperature integral to relate correlation components in terms of temperature and the strength of the electron-electron interaction. Using a new linear response proof for thermal ensembles, these thermal connection formulas and the fluctuation-dissipation theorem are combined, producing a method to generate entirely new exchange-correlation free energy approximations. These approximations are crucial for proper modeling of planetary interiors, magnetic transitions, and high-electronic-temperature laser-matter interactions, particularly as molecular bonds form and break. To complement this work, the advantages to using strictly correlated electrons as a reference point for finite-temperature approximations and a new ensemble approach to calculating atomic excitation energies will be introduced.

BIO:

Aurora Pribram-Jones is a Lawrence Postdoctoral Fellow at Lawrence Livermore National Laboratory and a UC President's Postdoctoral Fellow in the Chemistry Department at UC Berkeley. A recent Frederick A. Howes Scholar in Computational Science, she received her PhD in Chemistry from UC Irvine, where she studied with Kieron Burke as a DOE Computational Science Graduate Fellow. Dr. Pribram-Jones develops finite-temperature and ensemble electronic structure methods for use in materials science, quantum chemistry, and warm dense matter theory. Her recent publications focus on extracting accurate atomic excitation energies at low computational cost, linear response theory for thermal ensembles, and mathematical conditions on finite-temperature exchange-correlation functionals. Dr. Pribram-Jones also collaborates with researchers at Harvey Mudd College, using high-performance computing to simulate ordered and disordered complex alloys, and was a coordinator of this year's LLNL Computational Chemistry and Materials Science Summer Institute.