UC MERCED | CHEMISTRY & BIOCHEMISTRY

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CHEMISTRY & BIOCHEMISTRY SEMINAR SERIES:

The interplay of temperature, density, and interaction strength in density functional theories

Aurora Pribram-Jones

Assistant Professor of Chemistry and Biochemistry
UC Merced

Abstract:

Adiabatic connection approaches have a long history in ground-state density functional theory, and their use within the finite-temperature formalism provides similar insights about both exact and approximate exchange-correlation functionals. In particular, geometric and analytical interpretation of these expressions can provide new strategies around the added complications of exchange-correlation entropy and orderings of limits. In this talk, I will introduce the generalized thermal adiabatic connection (GTAC) approach and my group's work on establishing a finite-temperature strictly correlated electron (FT SCE) formalism. In addition, I will discuss how these two perspectives can be used for developing thermal density functional theory, whether as separate approaches or when paired for generating new approximations.

About the Speaker:

Aurora Pribram-Jones is an Assistant Professor in the Department of Chemistry and Biochemistry at University of California, Merced. The PJ Group at UC Merced develops finite-temperature and ensemble electronic structure methods for use in materials science, quantum chemistry, and warm dense matter theory. Pribram-Jones is also the lead theorist in a collaboration with researchers at Harvey Mudd College and University of New South Wales, in which undergraduate researchers from both US institutions use density functional theory(-molecular dynamics) to simulate ordered and disordered compositionally complex alloys. After completing a PhD in Chemistry from UC Irvine, where they studied with Kieron Burke as a DOE Computational Science Graduate Fellow, Pribram-Jones completed Lawrence and UC President's Postdoctoral Fellowships at LLNL and UC Berkeley. Before receiving a BS in Chemistry from Harvey Mudd College, Pribram-Jones completed AS degrees in Biology, Chemistry, and Mathematics from Foothill College. As a 2022 Cottrell Scholar, Pribram-Jones is interested in reframing the way thermal ensembles of strongly interacting electrons are treated theoretically and improving the treatment of students as they develop vivid scholarly identities.

For more info, contact: Liang Shi lshi4@ucmerced.edu