CHEMISTRY & BIOCHEMISTRY COLLOQUIUM: Developing Electronic Structure Methods for Metals and Electrons with Finite Temperature

James Shepherd
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Date:
9/17/2021

Time:
1:30 PM- 2:30 PM

Link:
Please contact snsgradstaff@ucmerced.du for the Zoom information.

About the Speaker:

James Shepherd joined the University of Iowa chemistry department as an Assistant Professor in 2017. His research interests are methods development in electronic structure theory with an emphasis on quantum materials modelling. This work is funded through grants from the Department of Energy's Early Career Research Program and the National Science Foundation's CAREER award.

He received his B.A./M.Sci. and PhD. in 2009 and 2013, respectively, from the University of Cambridge, United Kingdom. From 2013 to 2017, he spent two years as a postdoctoral researcher at Rice University and then two more at the Massachusetts Institute of Technology. During this time he was awarded a Research Fellowship of the Royal Commission of 1851 and was a visiting researcher at Imperial College London..

Abstract:

When electronic energy levels become degenerate or when the thermal energy is comparable to their spacing, many interacting quantum states can contribute to electronic properties.

The first part of my talk will address how we are trying to make coupled cluster calculations effective for metals and low-gap solids. Wavefunction theories can struggle to model these materials because of their vanishing band gaps and the need to simulate large numbers of electrons interacting over long ranges. I will show how techniques based around the transition structure factor can be used to make metals as straight-forward to simulate as insulators using coupled cluster theory. I will also show more preliminary results obtained from using simple machine learning techniques.

The second part of my talk will address finite temperature electronic structure theory, which is physically significant in phase transitions in solids and laser-induced catalysis. I will show how we are making progress in this field through simulations of the exact N-body density matrix for small molecules.

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