University of Minnesota
Driven to Discover℠

Department of Chemistry

Seminar

9:45 a.m. Tuesday, January 27, 2015 • 331 Smith Hall

Post-Doctoral Research Fellow

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Density Functional Theory Embedding for Correlated Wavefunctions

Abstract

I describe the development of new quantum embedding methods that provide a formally exact approach to performing electronic structure calculations. This framework allows systems to be divided into smaller subsystems that can be treated at different levels of theory, with the intersubsystem potential calculated using embedded density functional theory (DFT). I then use this framework to develop robust wavefunction embedding methods. This allows for wavefunction calculations to be used in regions of large systems where DFT is known to perform poorly, such as van der Waals interactions and strongly correlated electrons. Through a systematic analysis of embedding errors, I determine the largest source of error from wavefunction-in-DFT embedding to be the evaluation of the approximate non-additive exchange-correlation functional. I suggest new algorithms to systematically reduce these errors.

These improvements allow for accurate and efficient electronic structure calculations on large complex chemical systems. Using this method, I first demonstrate its accuracy on a series of simple chemical reactions. Then, I study spin states in FeNi hydrogenase and intramolecular proton transfer for hydrogen evolution in cobalt catalysts. The results suggest promising new design principles for hydrogen evolution catalysts. The development of these new methodologies is crucial for elucidating the fundamental principles that govern large systems, which has broad applications for catalysts, enzymes, condensed phase systems, and solids.

Host: Laura Gagliardi
Refreshments will be served prior to the seminar.