Physical Chemistry Student Seminar Series

Accurate Electronic Structure Predictions via Quantum Monte Carlo

Who? James Shee Reichman/Friesner Group

When? Wednesday, November 14th, 2018 at 5:30 pm

Where? 7th Floor Lounge, 711 Havemeyer

Abstract

This talk will begin with a brief overview of traditional electronic structure methods, including Density Functional Theory and wavefunction approaches. I will then make the case that Quantum Monte Carlo is a promising alternative for chemical systems which exhibit substantial electronic correlation effects, such as transition metal complexes and biradicals, due to 1) the explicit treatment of electron-electron interactions, 2) the fact that the accuracy of the method's predictions can be systematically improved, 3) the algorithm's unprecedented parallel efficiency, and 4) the ability to accelerate calculations using graphical processing units and novel sampling techniques. Recent calculations of redox potentials, bond dissociation energies, non-covalent binding energies, and singlet-triplet gaps agree very well with experimental measurements. In the near future we will be computing aqueous pKas of hexaaqua transition metal complexes, and the quasiparticle and optical gaps of semiconducting materials.

Plenty of pizza will be provided.