



Accurate Quantum Chemistry of Transition Metal Compounds using Auxiliary-Field Quantum Monte Carlo

Who? Benjamin Rudshiteyn, Friesner Group

When? Wednesday, October 30, 2019, 5:00-6:00 pm

Where? Miller Room, 328 Havemeyer

Abstract We demonstrate the accuracy of GPU-enabled phaseless auxiliary-field quantum Monte Carlo (ph-AFQMC) combined with a correlated sampling technique to reliably predict thermochemical properties. These properties include the bond dissociation energies of transition metal diatomics and complexes. Such predictions, as validated by comparison to experiment, will allow the development of large thermochemical databases for cases without experimental measurements for the development of more approximate methods able to simulate the properties of large enzymatic structures such as Cytochrome P450 responsible for drug metabolism in the liver.

Plenty of pizza will be provided.