Physical Chemistry Student Seminar Series

Machine Learning in Quantum Chemical Calculation

Who? Guangqi Li, Friesner Group

When? Wednesday, October 2nd, 2019, 5:00-6:00 pm

Where? Miller Room, 328 Havemeyer

Abstract Machine learning (ML) is a method of data analysis, with the powerful ability to independently adapt and learn from previous computations.
Due to the self-interaction term (electron interacts with itself in mathematical equation), DFT is well-known for its error. The hypothesis of Localized Orbital Correction (via adding extra operators to remove the error) had been proposed to the numerical as atomic energies, ionization potential, and the 3d electron in transition metals. With the LOC correction, we show high accuracy when compared to the experiment or benchmark quantum chemical calculations.

Plenty of pizza will be provided.