The Department of Chemistry
Presents
Dr. Yirong Mo

SEMINAR:
Exploring Chemistry in Silico

Abstract
While it seems that computational chemistry means molecular orbital (MO) theory for many people, there is also valence bond (VB) theory, which is complement to the MO theory and at the ultimate level, both MO and VB theories are essentially identical. The current unpopularity of the VB theory results from the computational complexity. Our objective is to reanimate the VB theory by introducing the advantages of MO theory into VB theory and developing a new hybrid approach, called the block-localized wave function (BLW) method. Two of the successful applications of the BLW method is the elucidation of the ethane rotation barrier and the anomeric effect. We also work on the electron transfer (ET) theory by developing a BLW-based two model. An electron transfer process is typically described by two electron-localized diabetic states and the real ground (adiabatic) state is the superimposition of these two diabetic states and featured as a double-well potential. Using the BLW method, the electron-localized diabetic states can be well defined and subsequently, their coupling interaction can be computed. The second line of research in my lab is the computational biochemistry, which is an interdisciplinary research and one of the most active areas in computational chemistry. Our interests lie in the elucidation of enzymatic catalysis, biological processes and the redesign of proteins in silica.

Monday, October 2nd, 2017
4 pm
Chemistry Building, Room 1220