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UNIVERSITY OF WISCONSIN-MADISON

Graduate Student Positions Available in the Theoretical Chemistry Institute at UW-Madison

The theoretical chemistry institute (TCI) at UW-Madison's chemistry department consists of five labs with a broad range of research interest, including electronic structure, statistical mechanics, computer simulation, artificial intelligence, polymer physics, quantum dynamics, computational materials science, biophysics, and drug discovery. All the chemistry labs in the TCI are on the same floor of the chemistry building, which creates a collaborative environment among research groups. **For Fall 2022**, there are **5-8 Ph.D student positions available** (fully funded) in the TCI groups (see below for a description of individual labs). Interested candidates are **strongly encouraged to contact the PIs and/or directly apply through https://chem.wisc.edu/how-to-apply-to-the-ph-d-program-in-chemistry/**. The application **deadline** is **Dec 1, 2021,** and please contact the PIs of your interest for the **application fee waiver.**

 **Openings**: 2/year xhuang@chem.wisc.edu	**Xuhui Huang (*Hirschfelder Chair in Theoretical Chemistry*):** Prof. Huang joined UW-Madison in Fall 2021 as the Director of TCI. The Huang group's research is at the interface of computational chemistry and biophysics. A few areas that the Huang group are currently working on include: (a) methodological development of the Markov State Models and Generalized Master Equation Models for bimolecular dynamics; (b) elucidation of functional conformational changes of RNA Polymerases, molecular recognition and self-assembly; (c) development of new integral equation theories for solvation; (d) development of deep-learning algorithms to predict novel inhibitors against desired protein targets; (e) and elucidation of structural ensemble from heterogeneity Cryo-EM datasets. Group website: https://huang.chem.wisc.edu/
 **Openings**:1-2/year yethiraj@wisc.edu	**Arun Yethiraj (*V.W. Meloche-Bascom Professor of Chemistry*)**: Professor Yethiraj's research focuses on computational and theoretical studies of soft condensed matter. While it is clear that the short-range structure of complex fluids plays an important role in determining the physical and chemical properties, the complexity of these systems makes modeling them on an atomistic level computationally challenging. A judicious choice of coarse-grained models that hopefully capture the essential features without incorporating much of the detail is therefore a crucial step in the theoretical study of these systems. His group is involved in constructing such models, and then employing liquid state theory, computer simulation, and machine learning to investigate their properties, with the final aim of predicting experimental observables. Group website: https://yethiraj.chem.wisc.edu
 **Openings**:1-2/year schmidt@chem.wisc.edu	**JR Schmidt (*Professor, Senior editor of the Journal of Physical Chemistry*)**: Research in the Schmidt group encompasses a wide range of topics under the broad umbrella of computational materials chemistry and heterogeneous catalysis/electrocatalysis. We use and combine approaches from statistical mechanics and electronic structure theory, both developing new computational methods and applying existing approaches, to expand the envelope of materials systems that can be modeled. The group is currently focusing on challenges including simulating the nucleation and growth of weak electrolytes, including metal-organic framework materials and oxide materials; and modeling the selective electrocatalytic reduction of molecules ranging from O_2 to biomass. Group website: https://schmidt.chem.wisc.edu/

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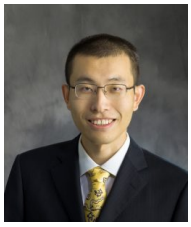 **Openings**:1-2/year yyang222@wisc.edu	**Yang Yang (*Assistant Professor*):** The Yang group develops theoretical methods to include nuclear quantum effects in quantum chemistry calculations and try to apply the methods to practical chemical, materials, and biological systems. In addition, the Yang group is interested in a variety of excited states phenomena and develops methods to describe them. Group website: https://yang.chem.wisc.edu
 **Openings**: none at present elsibert@wisc.edu	**Edwin Sibert (*Professor*):** We are a theoretical chemistry research group with an interest in dynamics of highly excited polyatomic molecules in the gas and liquid phase. We work closely with molecular spectroscopists to reveal and interpret the information content of vibrational spectra of systems where anharmonic effects are large and the normal mode approximation fails. Group website: https://sibert.chem.wisc.edu/