

Graduate Research Assistant Openings in YZ's Group at UIUC

(updated: October 3, 2019)

Motivated and ambitious graduate research assistants (GRA) are invited to join [Prof. Yang Zhang](#)'s research group at University of Illinois at Urbana-Champaign.

The research of YZ's group can be summarized in three words: **Molecules, Materials, and Machines**. On the *basic science* side, we synergistically combine and push the boundaries of theoretical and computational molecular science and neutron and X-ray scattering experiments. We develop accelerated molecular simulation methods that can effectively model a wide range of long timescale phenomena and rare events, with the goal of significantly extending our understanding of the equilibrium and non-equilibrium properties of natural and synthetic materials from the molecular and electronic level and providing accurate predictions and rational guidance to the design, synthesis, fabrication, and utilization of novel materials. Particular emphasis is given to the physics and chemistry of liquids, especially at interfaces, driven away from equilibrium, or under extreme conditions. On the *applied research* side, leveraging our expertise in novel soft materials, we advance soft robotics, human-compatible machines, intelligent control, and understandable artificial intelligence that can lead to immediate societal impact.

Immediately, we have several GRA positions to work on the following projects:

1. **NSF Harnessing the Data Revolution (HDR) Institute Project:** *Apply Topological Data Analysis (TDA), which combines algebraic topology with computational methods to extract new knowledge by characterizing the global shape of data, to understand intensive and complex data sets that represent the high-dimensional energy landscapes of chemical and materials systems. [See NSF's HDR big idea: www.nsf.gov/cise/harnessingdata]*
2. **DOE NEUP Project:** *Study of the fundamental physics and chemistry of molten salts that are relevant to Molten Salt Reactors (MSRs) with first-principles accuracy using Molecular Dynamics (MD) simulations driven by Machine-Learned (ML) high-dimensional Neural Network Potentials (NNPs) combined with neutron/X-ray scattering and thermodynamic experimental validations.*
3. **DOE Joint Center for Energy Storage Research (JCESR) Energy Innovation Hub Project:** *Obtain molecular-level understanding of the structure (solvation, aggregation, ion pairing) and dynamics (diffusion, transport, viscoelasticity, conductivity, mobility) of electrolyte and redoxmer solutions, especially at high concentrations and at interfaces. [See www.jcesr.org]*
4. **DOE BES Project:** *Study of the collective density fluctuations in liquids (metallic, water, ionic) and liquid-like matter, at and away from equilibrium, using neutron scattering experiments. The work also includes parallel development of new kinetic and molecular hydrodynamic theories and accelerated molecular simulation methods along with the scattering experiments.*
5. **Soft Robotics and Intelligent control Project:** *Design and build soft robotic devices and human-compatible machines. Develop intelligent control methods/theories for the manipulation and motion planning of soft devices. Develop understandable AI.*

The scattering experiments are usually performed at the neutron and X-ray user facilities around the world. Solid background in theories and programming are essential. All majors are also welcome.

For more information, please contact (with CV, transcript, and code samples):

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