

ZHIXIA LI

☎ 217.979.9686 ✉ zhixia2@illinois.edu

EDUCATION

- University of Illinois at Urbana-Champaign (UIUC)** 08/2016 – present
Ph.D. Candidate in Department of Nuclear, Plasma, and Radiological Engineering (Advisor: Prof. Y Z)
- University of Science and Technology of China (USTC)** 08/2012 – 06/2016
B.S. in School of Nuclear Science and Technology

RESEARCH INTERESTS

- Understanding long time scale phenomenon and rare events; Developing efficient enhanced sampling methods; Classical and ab-initio molecular dynamics (MD) modeling and simulation
- Understanding the characteristics of water at interfaces; Neutron and X-ray scattering experiments

RESEARCH EXPERIENCE

- **Validation of a new advanced sampling method: ascend dynamics simulation** 08/2019 – present
 - Revisited nucleation process of monodisperse lennard jones liquid
 - Recovering kinetics from ascend dynamics trajectory
- **Simulating water at interfaces using ab-initio deep neural network potential** 08/2018–08/2019
 - Perform ab-initio molecular dynamics (AIMD) simulation to generate input datasets
 - Build multidimension neural network potentials (NNPs)
 - Run MD generated NNPs at larger spacial scales and longer time scales
- **Molecular dynamics simulations of nonaqueous electrolytes** 08/2017 – 08/2018
 - Run quantum chemistry calculations to optimize geometry and partial charges
 - Performed MD simulations with updated geometry and partial charges
 - Performed neutron PDF to measure structural quantities and benchmark MD results
- **Study of microheterogeneity in nonaqueous electrolyte solutions** 08/2017 – 08/2018
 - Performed differential scanning calorimetry to quantify bulk phase behavior
 - Performed quasi-elastic neutron scattering (QENS) to study the phase behavior at molecular level
- **Collaborative projects**
 - Studied the dynamical behavior of random heterogeneous polymers by MD simulations and neutron scattering measurements 11/2019 – present
 - Performed quantum chemistry calculations of urea macrorocycles 04/2019 – 08/2019
 - Participation in neutron scattering measurements and data analysis of glass and phase behavior of ionic liquids 06/2017 – 08/2019

HONORS

- **Computational Science Engineering Fellowship**, UIUC 08/2018
- China General Nuclear Power Group Scholarship (2013), Institute of Modern Physics Scholarship (2014), **Guo Morou Scholarship** (2015), Outstanding Student Scholarship (2015), USTC 2013–2015

SKILLS

- Programming Languages: C++/C, Python, Julia, Matlab
- Software: GROMACS, LAMMPS, VASP, CP2K, VMD, Paraview

PUBLICATIONS

1. Lima, T. A., **Li, Z.**, Tyagi, M. & Ribeiro, M. C. C. Spatial and thermal signatures of and relaxations in glassy and glacial aliphatic ionic liquids. *J. Chem. Phys* **150**, 144506 (2019).
2. Robertson, L. A. *et al.* Observation of Microheterogeneity in Highly Concentrated Nonaqueous Electrolyte Solutions. *J. Am. Chem. Soc* **141**, 8041–8046 (2019).