

# YANQIN ZHAI

Ph.D. Candidate

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## EDUCATION

Ph.D. in Nuclear, Plasma, and Radiological Engineering with Concentration in Computational Science and Engineering (M.S. Granted in 2019 Fall)

University of Illinois at Urbana-Champaign

2017 – 2022 December (Expected) Champaign, Illinois

B.S. in Nuclear Engineering

University of Science and Technology of China

2013 – 2017

Hefei, China

## MAIN PROJECTS

LiquidLib: Computational Package Development

<http://z-laboratory.github.io/LiquidLib/>

2018 – present

- Lead the development of LiquidLib (a comprehensive toolbox written in C++ for analyzing molecular dynamics simulation trajectories)
- Design the framework and lead the implementation of detailed functions
- Optimize OpenMP and implement MPI parallelization for improving performance
- Design the GPU parallelization using CUDA (in progress)
- Maintain the package and solve issues from our users all over the world
- At least two scientific papers are in preparation

Ascent Dynamics: Algorithm Development

2020 – present

- Develop and improve the Ascent Dynamics which is an enhanced sampling algorithm for exploring high-dimensional complex energy landscapes
- Implement the Ascent Dynamics on LAMMPS, a widely used simulation package written in C++
- Utilize the Ascent Dynamics to investigate the relaxation of realistic system in ultra long-time scale

Dimensionality Reduction: Application of Deep Learning

2020 – present

- Write Shell Scripts to perform molecular dynamics simulations using GROMACS to generate high-dimensional potential energy surfaces
- Use persistent homology to analyze the energy surface with the publication being selected as the **Editor's Pick**
- Implement and train the an Autoencoder using TensorFlow to perform dimensionality reduction on obtained high-dimensional energy surfaces to extract appropriate low-dimensional collective variables

## EXPERIENCE

Guest Researcher

National Institute of Standards and Technology

Aug 2019 – Jul 2020 Gaithersburg, Maryland

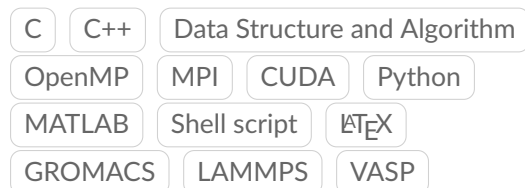
- Perform computer simulations to understand experimental phenomena
- Study the structure and dynamics of glass-forming liquids
- Design and conduct neutron scattering experiments
- Published at least 4 peer-reviewed papers

## PUBLICATIONS

- 10 publications in high-impact scientific journals such as *ACS Appl. Nano Mater.*, *J. Phys. Chem. Lett.*, *J. Chem. Phys.*, and *Phys. Rev. B*
- Several other papers submitted to scientific journals and under review process
- Multiple oral presentations on international academic conferences

A full list of publications can be found on my [Google Scholar](#)

## SKILLS



## RELATIVE COURSES

- CS 473: Algorithm
- CS 483: Applied Parallel Programming
- CS 519: Scientific Visualization
- CS 547: Deep Learning
- CSE 485: Atomic Scale Simulation

## HONORS AND AWARDS

- 2021–2022 Mavis Future Faculty Fellow
- 2015–2017 Scholarship of Institute of Modern Physics, Chinese Academy of Science
- 2014 Scholarship of Outstanding Student