Zhikun Cai

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Education

University of Illinois at Urbana-Champaign (UIUC) 08/2013 - present
Ph.D. student in Nuclear Engineering GPA: 3.98/4.00

University of Science and Technology of China (USTC) 09/2009 - 05/2013
B.S. in Applied Physics

Certificate

Graduate Specialization in Computational Science and Engineering, UIUC, 2016

Honors

- **Beckman Fellowship**, Beckman Institute for Advance Science and Technology, UIUC 2017
- Conference travel award for graduate students, NPRE, UIUC 2015
- Membership of Alpha Nu Sigma Honor Society for Nuclear Science and Engineering 2015
- **National Scholarship**, China 2012
- Outstanding Freshman Scholarship (Grade 1), USTC 2009

Research Interests

Statistical mechanics of liquids and soft matter; Neutron/X-ray scattering; Atomistic simulation

Research Experience & Projects

- **Ph.D. Research: Statistical Mechanics of Liquids with Application to Neutron Scattering Data Analysis** 2014 - present
  - Developed a ***Relaxation-Excitation Mode Analysis (REMA)*** from kinetic theory to extract the energy landscape statistics of liquid-like matter from inelastic scattering experiments
  - Implemented *REMA* using regularized regression and quadratic programming to invert data represented by linear integral equations (e.g. Laplace transform)
  - Applied *REMA* to analyze multiple systems including confined proteins

- **Soft Matter Physics Studied via Molecular Dynamics Simulations** 2013 - present
  - Compared the dynamics of hydrated proteins in bulk environment and confined in silica nanopores
  - Verified the negative correlation between porosity and flexibility in edge-specific molecular cages
  - Mapped the validity boundaries of the Stokes-Einstein relation in the phase diagram of water
  - Analyzed the relaxational dynamics of a binary Lennard-Jones liquid upon supercooling

- **Development of Research Tools**
  - Co-developed *LiquidLib*, a comprehensive C++ package for analyzing molecular dynamics simulations of liquids with application to neutron scattering experiments (07-08/2015)
  - Implemented *GroPy*, a Python module to process a common atomic structural format (.gro) (05/2016)

- **Participation in Neutron Scattering Experiments**
  - On ionic liquids at NOMAD (12/2013) and BASIS (05/2014), Spallation Neutron Source (SNS), Oak Ridge National Laboratory (ORNL);
  - On ionic liquids and n-alkanes at DCS/HFBS (06/2014), NIST Center for Neutron Research (NCNR), National Institute of Standards and Technology (NIST).
  - On a surfactant conducted at Neutron Spin Echo instrument (06/2015) in the "Summer School on Methods and Applications of Neutron Spectroscopy", NCNR, NIST

Publications

[1] **Z. Cai**, et al., "Energy landscape statistics and coarsening in liquids and liquid-like matter: a relaxtion-excitaion mode analysis", to be submitted *J. Chem. Phys.*.

[2] **Z. Cai**, A. Jaiswal, N. P. Walter, Y. Zhang*, Validity boundary of Stokes-Einstein relation in water, to be submitted.

[3] T. P. Moneypenny II, N. P. Walter, **Z. Cai**, Y.-R. Miao, D. L. Gray, J. J. Hinman, S. Lee, Y. Zhang*, and J. S. Moore*, "Impact of Shape Persistence on the Porosity of Molecular Cages", *J. Am. Chem. Soc.* 139 (8), 3259-3264 (2017).

[4] K. Yang, **Z. Cai**, A. Jaiswal, M. Tyagi, J. S. Moore, Y. Zhang*, "Dynamic Odd-even Effect in Liquid n-Alkanes near Melting Points", *Angew. Chem. Int. Ed.* 128, 14296 (2016).

[5] K. Yang, **Z. Cai**, M. Tyagi, M. Feygenson, J. C. Neuefeind, J. S. Moore*, Y. Zhang*, "Odd-even Structural Sensitivity on Dynamics in Network-forming Ionic Liquids", *Chem. Mater.* 28(9), 3227 (2016).

Presentations

- NPRE Graduate Seminar, UIUC, Illinois, "*Relaxation-Excitation Mode Analysis of the Energy Landscape Statistics in Liquids*" 04/2017
- APS march meeting, New Orleans, Louisiana, "*Relaxation-Excitation Mode Analysis of the Energy Landscape Statistics in Liquids*" 03/2017
- ACNS, Long Beach, California, "*Neutron Scattering Experimental Characterization of Energy Landscape Statistics: a Relaxation-Excitation Mode Analysis*" 07/2016
- APS march meeting, Baltimore, Maryland, "*Quantifying Energy Landscape Statistics in Liquids and Proteins: a Relaxation-Excitation Mode Analysis*" 03/2016
- American Physical Society (APS) march meeting, San Antonio, Texas, "*Energy Landscape Statistics and Coarsening in Liquids: a Relaxation Mode Analysis*" 03/2015
- American Conference on Neutron Scattering (ACNS), Knoxville, Tennessee, "*Quantifying the Dynamic Heterogeneity Of Glassy Matter From Relaxation Time Spectrum*" (Poster) 06/2014

Appointments

- Research Assistant, Prof. Yang Zhang's research group, NPRE, UIUC 01/2014 - present
- Teaching Assistant, NPRE 521 *"Interaction of Radiation with Matter"*, UIUC 01/2015 - 05/2015
- Teaching Assistant, NPRE 446 *"Radiation Interaction with Matter I"*, UIUC 08/2013 - 12/2013

Skills

- Technical: C++, Python, Linux, SQL, Git, Matlab, Mathematica, LaTeX
- Analytical: Algorithms and Data Structures, Statistical Learning