

APPOINTMENTS

- 2020 – *present* **Associate Head for Graduate Programs**, Department of Nuclear, Plasma, and Radiological Engineering, University of Illinois at Urbana-Champaign
- 2020 – *present* **Donald Biggar Willett Faculty Scholar**, University of Illinois at Urbana-Champaign
- 2018 – *present* **Associate Professor**, Department of Nuclear, Plasma, and Radiological Engineering, Department of Electrical and Computer and Engineering, Program of Computational Science and Engineering, Illinois Robotics Group, Center for Autonomy, Center for Biophysics and Quantitative Biology, Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign
- 2019 – 2020 Visiting Professor, Department of Materials Science and Engineering, University of California, Berkeley and Lawrence Berkeley National Laboratory
- 2012 – 2018 **Assistant Professor**, Department of Nuclear, Plasma, and Radiological Engineering, University of Illinois at Urbana-Champaign
- 2010 – 2012 **Clifford G. Shull Fellow**, Neutron Sciences Directorate, Oak Ridge National Laboratory

EDUCATION

- Ph.D.** Nuclear Science and Engineering, **Massachusetts Institute of Technology** (MIT), 2010  
Thesis: “*Neutron Scattering Investigations on the Unusual Phase Behavior of Water*”
- B.S.** Electrical Science and Technology, **University of Science and Technology of China** (USTC), 2004

RESEARCH INTERESTS

YZ’s research can be summarized into two words: **Matter and Machine**. On the basic science side, his group synergistically combines and pushes the boundaries of accelerated atomistic simulations, stochastic dynamics theories, and neutron scattering experiments, with the goal of significantly extending our understanding of a wide range of long timescale phenomena, rare events, and far-from-equilibrium properties of materials from the atomic and molecular level. Particular emphasis is given to the physics and chemistry of liquids and complex fluids, especially at interfaces, driven away from equilibrium, or under extreme conditions. On the applied research side, leveraging their expertise in materials and modeling, his group advances the development of soft robots and human-compatible machines, robots in extreme environments, and understandable artificial intelligence and intelligent control, which can lead to immediate societal impact. The common theme between these two research thrusts is complexity and emergence, where the whole is greater than the sum of its parts.

- **Matter**
  - Far-from-equilibrium physics, accelerated atomistic simulations, and stochastic dynamics (long timescale phenomena, rare events)
  - Physics and chemistry of liquids and complex fluids, especially under interfacial/non-equilibrium/extreme conditions (water, metallic liquids, molten salts, ionic liquids, electrolyte solutions)
  - Neutron scattering, sources, and instrumentation
- **Machine**
  - Soft robots and human-compatible machines
  - Robots in extreme environments
  - Understandable artificial intelligence and intelligent control

## PUBLICATIONS

**More than 60 publications (citations > 2,000, h-index = 25)** in book sections and high-impact journals such as *Phys. Rev. Lett.*, *J. Am. Chem. Soc.*, *Angew. Chem.*, *P. Natl. Acad. Sci. USA*, and *Nature Commun.* A full list of publications is appended.

## AWARDS & HONORS

- 2020.03 **Donald Biggar Willett Faculty Scholar Award**, UIUC  
2020.02 **Dean's Award for Excellence in Research**, Grainger College of Engineering, UIUC  
2017.04 **Landis Young Member Engineering Achievement Award**, American Nuclear Society, "in recognition of his contributions to nuclear and advanced experimental techniques to understand the complex makeup, nature and performance of materials in the far-from-equilibrium state"  
2015.05 **Doctoral New Investigator Award**, American Chemical Society Petroleum Research Fund  
2013.05 Collins Fellow, College of Engineering Academy for Excellence in Engineering Education, UIUC  
2013 – present List of Teachers Ranked as Excellent (Fall 2013, Fall 2014, Spring 2015, Spring 2017, Fall 2017, Spring 2018, Fall 2018, Spring 2019)  
2010.09 **Clifford G. Shull Fellowship**, ORNL  
2010.03 Student Research Showcase, Nuclear Science and Engineering Research Expo, MIT  
2009.10 Best Poster Award, the 15th User's Meeting of National Synchrotron Radiation Research Center, Taiwan, "Water in the Confined Space: Study of Density Anomalies of Supercooled Water"  
2008.05 **Manson Benedict Award**, "in recognition of the outstanding excellence of your academic and research performance" and "for excellence in neutron scattering research, particularly the study of critical behavior of supercooled water", MIT  
2008.05 **Neutron Scattering Society of America Prize** "for cyber development of enhancing the North American neutron community"  
2004.07 Distinguished Graduate of Anhui Province, Distinguished Graduate of USTC  
2003.05 Elected representative of USTC for the Associations of East Asian Research Universities  
2000.11 Best Paper Award on Modern Chinese Society Research  
1999 – 2003 Recipient of five scholarships, including **Guo Moruo Scholarship** (2003), **Samsung Scholarship** (2003), Outstanding Student Scholarship (2001), **Lenovo Scholarship** (2000), Outstanding Freshman Scholarship (1999)  
2002 – 2004 Recipient of nine prizes in international contests in *Mathematical Modeling*, including Interdisciplinary Contest in Modeling (ICM 2003, 2004), Mathematical Contest in Modeling (MCM 2002), INRIA and LIAMA Contests in Scientific Computing Software Scilab (2003)

## EDITORSHIPS

- Associate Editor, *Science and Technology of Advanced Materials*, **IF = 8.090** (2020), 2016 – present
- Associate Editor, *Frontiers in Materials*, Glass Science section, owned by Springer Nature, 2015 – present
- Associate Editor, *Frontiers in Physics* and *Frontiers in Chemistry*, Physical Chemistry and Chemical Physics section, owned by Springer Nature, 2015 – present
- Co-editor, with Rene A. Nome and Pilar Cossio, of the special issue *Integrating timescales from molecules up* in *Frontiers in Chemistry*, 2020
- Guest Editor, *MRS Advances*, Theory, Characterization, and Modeling section, Fall 2015

## INVITED TALKS

**More than 70 invited talks (some as a keynote speaker)** at national and international conferences, workshops, peer universities, national labs, and other organizations.

1. School of Nuclear Engineering Seminar, Purdue University, 2022.01
2. Workshop for the Molten Salt Thermal Properties Working Group, University of South Carolina, 2021.11
3. QENS/WINS 2021, 2021.05
4. Women in Nuclear Student Chapter at UIUC, 2021.04
5. Department of Materials Science and Engineering Colloquium, Rensselaer Polytechnic Institute, 2021.03
6. Solvation Phenomena in Energy Storage Workshop (rescheduled)

7. Department of Materials Science and Engineering Colloquium, University of California Berkeley (rescheduled)
8. ANS Winter Meeting, 2020.11
9. Computational Approaches to Molten Salts 2020 Workshop, University of South Carolina, 2020.11
10. Materials Science Colloquium, ANL, 2020.10
11. Illinois Ignite 2020, 2020.09
12. ACS Fall Meeting, 2020.08
13. X Development (formerly Google X), Mountain View, CA, 2019.11
14. Neutron Scattering Techniques for Time-Resolved Studies Workshop, ORNL, 2019.10
15. Society of Engineering Science Annual Meeting, St. Louis, MO, 2019.10
16. J-PARC Symposium 2019, Tsukuba, Japan, 2019.09
17. Pacific Northwest National Laboratory (PNNL) Interfacial Dynamics in Radioactive Environments and Materials (IDREAM) Energy Frontier Research Center (EFRC), 2019.09
18. 26th International Symposium of Metastable, Amorphous and Nanostructured Materials, Chennai, India, 2019.07
19. 2019 DOE/BES/MSED Neutron Scattering Program PI Meeting, Gaithersburg, MD, 2019.07
20. Nvidia Corporation, Santa Clara, CA, 2019.06
21. Honda Research Institute, San Jose, CA, 2019.06
22. Roma Tre Congress on Water Under Extreme Conditions, Rome, Italy, 2019.06
23. Department of Mechanical and Energy Engineering, Purdue University, 2019.04
24. Tutorial on modern modeling methods in neutron spectroscopy, ORNL, 2019.04
25. Department of Engineering Physics, Tsinghua University, Beijing, China, 2018.07
26. China Spallation Neutron Source, Dongguan, China, 2018.07
27. Keynote Speaker, QENS/WINS 2018, Hong Kong, 2018.07
28. Telluride Workshop on Water: Grand Challenges for Molecular Science and Engineering, Telluride, CO, 2018.07
29. The 12th International Conference on Bulk Metallic Glasses (BMG XII), Seoul, Korea, 2018.05
30. International Center for Quantum Materials, Peking University, Beijing, China, 2018.05
31. Beckman Institute Director's Seminar, UIUC, 2017.11
32. The 8th International Discussion Meeting on Relaxations in Complex Systems (8IDMRCs), Wilsa, Poland, 2017.07
33. Theoretical and Computational Biophysics Seminar, Beckman Institute, UIUC, 2017.04
34. Department of Materials Science and Engineering Colloquium, University of Florida, 2017.04
35. TMS Annual Meeting, San Diego, CA, 2017.02
36. WPI-AIMR Workshop on Structure and Dynamics of Glasses, Tohoku University, Sendai, Japan, 2017.02
37. 2019 DOE/BES/MSED Neutron Scattering Program PI Meeting, Gaithersburg, MD, 2016.12
38. Department of Chemistry, Physical Chemistry Seminar, UIUC, 2016.11
39. Department of Materials Science and Engineering Colloquium, University of California Berkeley, 2016.10
40. Neutron Electrostatic Levitator (NESL) User Workshop, ORNL, 2016.08
41. American Conference on Neutron Scattering, Long Beach, CA, 2016.07
42. The 11th International Conference on Bulk Metallic Glasses (BMG XI), Washington University in St. Louis, 2016.06
43. Institute of Physics, Chinese Academy of Sciences, Beijing, China, 2016.05
44. 40 Years of Neutron Scattering Symposium, NIST, 2016.02
45. Gordon Research Conference, Neutron Scattering: Effect of Disorder and Disordered Materials, Hong Kong, 2015.06
46. NIST Center for Neutron Research Summer School on Fundamentals of Neutron Scattering, NIST, 2015.06
47. National Synchrotron Light Source II (NSLS-II) and Center for Functional Nanomaterials (CFN) Joint Users' Meeting, BNL, 2015.05
48. Future and Current Use of Neutron Spin-Echo Spectroscopy in Condensed Matter Research Workshop, ORNL, 2015.05
49. US Army Construction Engineering Research Laboratory (CERL), Champaign, IL, 2015.03
50. DOE Workshop on Fundamental Challenges in Our Understanding of the Physics and Chemistry of Water, Houston, TX, 2015.01
51. The Center for High Resolution Neutron Scattering (CHRNS) NSF Review, NIST, 2015.01
52. DOE Grand Challenges in Soft Matter Workshop, University of California Santa Barbara, 2014.05

53. Department of Physics, Condensed Matter Seminar, UIUC, 2014.02
54. Berkeley Mini Stat Mech Meeting breakout session, University of California Berkeley, 2014.01
55. International collaborative online course “Neutrons in Soft Matter Science: Complex Materials on Mesoscopic Scales” invited lecturer, Joint Institute for Neutron Sciences, 2013.11
56. Department of Materials Science and Engineering, Soft Materials Seminar, UIUC, 2013.09
57. School of High Resolution Neutron Scattering to Measure Slow Dynamics, ORNL, 2013.03
58. Petersen Asphalt Research Conference, Laramie, WY, 2012.07
59. Department of Food Science and Engineering, University of Tennessee Knoxville, 2012.02
60. Department of Nuclear, Plasma and Radiological Engineering, UIUC, 2012.02
61. Berkeley Mini Stat Mech Meeting breakout session, University of California Berkeley, 2012.01
62. Departments of Physics and Materials Research Laboratory, University of California Santa Barbara, 2012.01
63. Department of Materials Science and Engineering, University of Tennessee Knoxville, 2011.10
64. Neutron Sciences Seminar, ORNL, 2011.10
65. Center for Molecular Biophysics, ORNL, 2011.09
66. Young Faculty and Research Scientist Seminar, Department of Nuclear Science and Engineering, MIT, 2011.03
67. NIST Center for Neutron Research, NIST, 2011.02
68. Department of Materials Science and Engineering, University of Tennessee Knoxville, 2010.03
69. Clifford G. Shull lecture, ORNL, 2010.03
70. Department of Civil Engineering, MIT, 2008.11

#### CONFERENCE ORGANIZATIONS

- Lead organizer, APS March Meeting Focus Session “Physics of Liquids”, 2017, 2018, 2019, 2020, 2021
- Lead organizer, “New Science Opportunities with Time-of-Flight Wide-Angle Neutron Spin-Echo at STS”, 2021.02
- Lead organizer, 2019 MRS Fall Meeting Symposium “Advanced Materials Explorations with Neutrons”, co-organizers: K. Herwig, D. Louca, V. Garcia-Sakai, 2019.11
- Co-organizer, ORNL Joint Nanoscience and Neutron Scattering User meeting, 2017.07
- Co-organizer, ORNL Center for Nanophase Materials Sciences (CNMS) User Meeting, 2016.08
- Member, Advisory Committee, the 11th International Conference on Bulk Metallic Glasses (BMG XI), St. Louis, MO, 2016.06
- Lead organizer, 2015 MRS Fall Meeting Symposium “Liquids and Glassy Soft Materials – Theoretical and Neutron Scattering Studies”, co-organizers: T. Egami, E. L. Liu, H. E. Stanley, 2015.11
- Co-organizer, “Workshop on Topics in Soft Condensed Matter”, MIT, 2015.11
- Co-organizer, ORNL Neutron Sciences User Meeting, 2015.10

#### OTHER SYNERGISTIC ACTIVITIES

- Spokesperson, EXPANDED Angle Neutron Spin Echo (EXPANSE) instrument at ORNL, 2020 – present
- Member, Pennsylvania State University Neutron Science Advisory Council, 2019 – present
- Member, Program of Computational Science and Engineering Steering Committee at UIUC, 2017 – present
- Member, Science Review Committee, Neutron Sciences Directorate at ORNL, 2014 – present
- Member, Proposal Review Committee, Center for Nanophase Materials Sciences (CNMS) at ORNL, 2016 – present
- Faculty and Staff Mental Health Ambassador, UIUC, 2021 – present
- Co-chair, DOE Neutron Scattering PI Meeting, 2021.12
- Member, ORNL Second Target Station (STS) Hiring Committee, 2021
- Reviewer, HFIR/SNS Review of the Instrument Suite for Spectroscopy at ORNL, 2020.09
- Member, COVID-19 Emergency Response Science Review Committee, Neutron Sciences Directorate at ORNL, 2020
- Member, Users Organization Steering Committee, Advanced Photon Source (APS) at ANL, 2017 – 2020
- Member, Program Advisory Committee, Beckman Institute for Advanced Science and Technology, 2017 – 2020
- Chair, Artificial Intelligence/Machine Learning/Data Science Townhall Discussion, Science at the Second Target Station Workshop, ORNL, 2019.12

- Panel Chair, Machine Learning & Data Science Approaches for Neutron Scattering Research, 2019 DOE/BES/MSED Neutron Scattering Program PI Meeting, 2019.07
- Panelist, NSF CHE/DMS Innovation Lab: Learning the Power of Data in Chemistry, 2018.12
- Panelist, Polsky Center Soft Materials Workshop, 2018.06
- Panelist, NSF Strategic Planning Workshop on Progress and Prospects for Neutron Scattering in the Biological Sciences, 2018.02
- Reviewer, HFIR/SNS Review of the Instrument Suite for Inelastic Scattering at ORNL, 2017.11
- Member, NIST Center for Neutron Research (NCNR) Beam Time Allocation Committee, 2017
- Secretary, Users Executive Committee, Center for Nanophase Materials Sciences (CNMS) at ORNL, 2015 – 2017
- Member, Proposal Review Panel, Center for Functional Nanomaterials (CFN) at BNL, 2015 – 2017
- Panelist, Neutron Spin Echo for Slow Dynamics Investigations Workshop, 2016.11
- Member, Executive Committee, Spallation Neutron Source and High-Flux Isotope Reactor User Group (SHUG) at ORNL, 2013 – 2015
- Panelist, Spallation Neutron Source Second Target Station Workshop, ORNL, 2015.10
- Panelist, Neutron Measurements for Materials Design and Characterization Workshop organized by NIST, Potomac, MD, 2014.08
- Panelist, DOE Grand Challenges in Soft Matter Workshop, UCSB, 2014.05
- Panelist, Future Science Impact Meeting, ORNL, 2013.10
- Member, Science Highlights Editorial Committee, Neutron Sciences, ORNL, 2012

#### REVIEW ACTIVITIES

- Reviewer for neutron and X-ray beam time allocations at SNS/HFIR, NCNR, and SSRL
- Reviewer for National Science Foundation, DOE Basic Energy Science, DOE Advanced Scientific Computing Research, DOE Nuclear Energy, DOE SBIR/STTR, ACS Petroleum Research Fund, Italian Cineca, Austrian Science Fund, Chilean National Science and Technology Commission
- Reviewer for Tenure and Promotion and Performance at Tsinghua University and Chinese Academy of Sciences
- Reviewer for *Nature*, *Nature Chem*, *Nature Commun*, *Phys Rev Lett/X/B/E*, *P Natl Acad Sci USA*, *J Chem Phys*, *J Phys Chem Lett/B/C*, *Soft Matter*, *Phys Chem Chem Phys*, *J Phys-Condens Mat*, *J Comp Chem*, *J Non-Cryst. Solids*, *ACS Macro Lett*, *Biophys J*, *J of Mater Chem B*, *Nano Lett*, *Langmuir*, etc.

#### PROFESSIONAL SOCIETY MEMBERSHIPS

American Physical Society, American Nuclear Society, Institute of Electrical and Electronics Engineers, American Chemical Society, Materials Research Society, Society of Engineering Science, Minerals Metals and Materials Society, American Association for the Advancement of Science, Neutron Scattering Society of America, Society for Science at User Research Facilities

#### TEACHING

The classical and quantum theories of the interaction of radiation (neutrons, photons, and charged particles) with matter are core components of nuclear and materials science and engineering. At UIUC, I teach a sequence of four courses at different progressive levels on this subject:

- Part 1. (Undergraduate, Required) *NPRE-446 Radiation Interaction with Matter I*, covers classical mechanics, classical electrodynamics, and quantum mechanics.
- Part 2. (Undergraduate, Required) *NPRE-447 Radiation Interaction with Matter II*, covers fundamentals of atomic and nuclear physics, and interaction of radiation with matter.
- Part 3. (Graduate, Required) *NPRE-521 Interaction of Radiation with Matter*, covers quantitative treatments of single interaction event in atomic and nuclear physics.
- Part 4. (Graduate, Elective) *NPRE-529/CSE-529 Interaction of Radiation with Matter II: Multiple Events and Computational Methods*, covers thermodynamics, kinetic theory, equilibrium and non-equilibrium statistical mechanics, phase transitions and critical phenomena, liquid theory, and atomistic simulations.

The sequence, in the aggregate, aims to provide the students with solid training concerning essential physical principles, mathematical competence, and computational skills.

### STUDENTS' AWARDS & HONORS

- 2021.05 Yanqin Zhai, Mavis Future Faculty Fellow
- 2021.05 Shao-Chun Lee, Block Grant Fellowship
- 2021.05 Ganesh Arunachalam, Albert Zhao, and David Null, Promoting Undergraduate Research in Engineering (PURE) Best Poster Award (Audience Choice)
- 2021.05 Sara Alabbadi, Parth Anjaria, and Kevin Wandke, Promoting Undergraduate Research in Engineering (PURE) Best Poster Award (Judge Choice)
- 2020.05 Zhixia Li, Mavis Future Faculty Fellow
- 2020.05 Zhixia Li, Block Grant Fellowship
- 2020.01 Kevin Wandke, Harold L. Olesen Undergraduate Teaching Award
- 2018.08 Zhixia Li, CSE Fellowship
- 2017.04 Zhikun Cai, Beckman Fellowship
- 2017.04 Nathan Walter, Roy A. Axford Fellowship
- 2015.08 Abhishek Jaiswal, CSE Fellowship
- 2015.05 Abhishek Jaiswal, Block Grant Fellowship
- 2014.04 Pawel Piotrowicz, NPRES Outstanding Undergraduate Research Award
- 2014.02 Nathan Walter, Computational Physics Student Summer Workshop Fellowship at LANL
- 2014.01 Nathan Walter, NRC Fellowship
- 2013.08 Ke Yang, Best Group Presentation Award at ANL/ORNL NX Summer School
- 2013.06 Abhishek Jaiswal, Best Group Presentation Award at NCNR Summer School

### PATENTS

- [1] **Y. Zhang**, L. Zhou, "Vasoconstriction-like soft micro pinch valve for localized control", US Nonprovisional Patent Application No. 16/807,490 (2020)

### PUBLICATIONS

- [1] Z. Cai, **Y Z\***, "A viscoelastic hydrodynamic theory of the transverse acoustic excitations in liquids", *Phys. Rev. E* (submitted)
- [2] P. Luo, Y. Zhai, Z. Cai, M. Kofu, K. Nakajima, A. Faraone, **Y Z\***, "de Gennes narrowing modulation and inverse temperature dependence of fast collective relaxation dynamics in fragile glass formers", *Phys. Rev. Lett.* (submitted)
- [3] P. Luo, Y. Zhai, P. Falus, V. Garcia-Sakai, M. Hartl, M. Kofu, K. Nakajima, A. Faraone, **Y Z\***, "Q-dependent collective relaxation dynamics of glass-forming liquid  $\text{Ca}_{0.4}\text{K}_{0.6}(\text{NO}_3)_{1.4}$  investigated by wide-angle neutron spin-echo", *Nature Commun.* (under revision)
- [4] Y. Zhai, P. Luo, J. Waller, J. L. Self, L. W. Harriger, **Y Z\***, A. Faraone, "Dynamics of molecular associates in methanol/water mixtures", *Phys. Chem. Chem. Phys.* (under revision)
- [5] X. Liu, S.-C. Lee, L. Cheng, **Y Z\***, T. Li, "Insight into the nanostructure of "water-in-salt" electrolytes: a small-angle X-ray scattering (SAXS) study on imide-based lithium salts aqueous solutions", *Energy Storage Mater.* (under revision)
- [6] K. Wandke, **Y Z\***, "MOOSE-based finite element hyperelastic modeling for soft robot simulations", *IEEE Access* 9, 139627 (2021)
- [7] S.-C. Lee, Y. Zhai, Z. Li, N. P. Walter, M. Rose, B. J. Heuser, **Y Z\***, "Comparative studies of the structural and transport properties of molten salt FLiNaK using machine-learned neural network and reparametrized classical forcefields", *J. Phys. Chem. B* 125(37), 10562 (2021)
  - **Featured as the journal cover art of *J. Phys. Chem. B***
  - **"Pass the salt: machine learning accelerates molten salt simulations for nuclear power applications", Beckman Institute news, UIUC College of Engineering news, AAAS EurekAlert, Opera News, scienmag, etc.**

- [8] I. F. T. de Souza, V. H. Paschoal, K. Bernardino, T. A. Lima, L. L. Daemen, **Y Z**, M. C. C. Ribeiro, “Vibrational spectroscopy and molecular dynamics simulation of choline oxyanions salts”, *J. Mol. Liq.* 340(15), 117100 (2021)
- [9] P. Luo, A. Jaiswal, Y. Zhai, Z. Cai, N. P. Walter, L. Zhou, M. Liu, R. Mills, A. Podlesynak, G. Ehlers, A. Faraone, H. Bai, W. Wang, **Y Z\***, “Atomic dynamics of metallic glass melts  $\text{La}_{50}\text{Ni}_{15}\text{Al}_{35}$  and  $\text{Ce}_{69}\text{Cu}_{20}\text{Al}_{10}\text{Nb}_1$  studied by quasi-elastic neutron scattering”, *Phys. Rev. B* 103, 224104 (2021)
- [10] I. A. Shkrob, L. A. Robertson, Y. Zhou, A. Rajeev, L. Cheng, L. Zhang, E. Sarnello, X. Liu, T. Li, A. P. Kaur, T. Suduwella, S. Odom, Y. Wang, R. Ewoldt, H. Farag, **Y Z**, “Crowded electrolytes containing redoxmers in different states of charge: solution structure, properties, and fundamental limits on power density”, *J. Mol. Liq.* 334(15), 116533 (2021)
- [11] R. Nome, Pilar Cossio, **Y Z**, “Editorial: Integrating Timescales from Molecules Up”, *Front. Chem.* 9, 680533 (2021)
- [12] Y. Zhai, N. S. Martys, W. L. George, J. Nayem, **Y Z**, Y. Liu, “Intermediate scattering functions of a rigid body monoclonal antibody protein in solution studied by dissipative particle dynamic simulations”, *Struc. Dyn.* 8, 024102 (2021)
- [13] Y. Zhai, P. Luo, M. Nagao, K. Nakajima, T. Kukuchi, Y. Kawakita, P. Kienzle, **Y Z\***, A. Faraone, “Relevance of hydrogen bonded associates to the transport properties and nanoscale dynamics of liquid and supercooled 2-propanol”, *Phys. Chem. Chem. Phys.* 23, 7220 (2021)
- [14] J. Mirth, Y. Zhai, J. Bush, E. G. Alvarado, H. Jordan, M. Heim, B. Krishnamoorthy, M. Pflaum, A. Clark, **Y Z\***, H. Adams, “Representations of energy landscapes by sublevelset persistent homology: an example with n-alkanes”, *J. Chem. Phys.* 154, 114114 (2021)
- **J. Chem. Phys. Editor’s Pick**
- [15] Y. Zhai, P. Luo, **Y Z\***, “Role of phonon softening induced by anisotropic fluctuations in the enhanced mobility at free glassy surfaces”, *Phys. Rev. B* 103, 085424 (2021)
- [16] Y. Yang, H. Ying, Z. Li, J. Wang, Y. Chen, B. Luo, D. Gray, Q. Chen, A. Ferguson, **Y Z**, J. Cheng, “Near quantitative synthesis of urea macrocycles enabled by bulky N-substituent”, *Nature Commun.* 12, 1572 (2021)
- [17] P. Luo, Y. Zhai, J. Leao, M. Kofu, K. Nakajima, A. Faraone, **Y Z\***, “Neutron spin echo studies of the structural relaxation of liquid  $\text{ZnCl}_2$  at the structure factor primary peak and pre-peak”, *J. Phys. Chem. Lett.* 12(1), 392 (2021)
- [18] P. Luo, C. Jaramillo, A. M. Wallum, Z. Liu, R. Zhao, L. Shen, Y. Zhai, J. C. Spear, D. Curreli, J. W. Lyding, M. Gruebele, W. Wang, J. P. Allain, **Y Z\***, “Coherent atomic-scale ripples on metallic glasses patterned by low-energy ion irradiation for large-area surface structuring”, *ACS Appl. Nano Mater.* 3(12), 12025 (2020)
- [19] Y. Zhao, E. Sarnello, L. A. Robertson, J. Zhang, Z. Shi, Z. Yu, S. R. Bheemireddy, **Y Z**, T. Li, R. S. Assary, L. Cheng, Z. Zhang, L. Zhang, I. A. Shkrob, “Competitive pi-stacking and H-bond piling increase solubility of heterocyclic redoxmers”, *J. Phys. Chem. B* 124(46), 10409 (2020)
- [20] I. A. Shkrob, T. Li, E. Sarnello, L. A. Robertson, Y. Zhao, H. Farag, Z. Yu, J. Zhang, S. R. Bheemireddy, **Y Z**, R. Assary, R. Ewoldt, L. Cheng, L. Zhang, “Self-assembled solute networks in crowded electrolyte solutions and nanoconfinement of charged redoxmer molecules”, *J. Phys. Chem. B* 124(45), 10226 (2020)
- [21] P. Luo, Y. Zhai, E. Senses, E. Mamontov, G. Xu, **Y Z\***, A. Faraone, “Influence of kosmotrope and chaotrope salts on water structural relaxation”, *J. Phys. Chem. Lett.* 11(21), 8970 (2020)
- [22] Y. Zhao, Z. Yu, L. A. Robertson, J. Zhang, Z. Shi, S. R. Bheemireddy, I. A. Shkrob, **Y Z**, T. Li, Z. Zhang, L. Cheng, L. Zhang, “Unexpected electrochemical behavior of an anolyte redoxmer in flow battery electrolytes: solvating cations help to fight against the thermodynamic-kinetic dilemma”, *J. Mater. Chem. A* 8, 13470 (2020)

- [23] T. A. Lima, V. H. Paschoal, R. S. Freitas, L. F. O. Faria, Z. Li, M. Tyagi, **Y Z**, M. C. C. Ribeiro, “An inelastic neutron scattering, Raman, far-infrared, and molecular dynamics study of the intermolecular dynamics of two ionic liquids”, *Phys. Chem. Chem. Phys.* 22, 9074 (2020)
- [24] Z. Li, L. A. Robertson, I. A. Shkrob, K. C. Smith, L. Cheng, L. Zhang, J. S. Moore, and **Y Z\***, “Realistic ion dynamics through charge renormalization in nonaqueous electrolytes”, *J. Phys. Chem. B* 124(15), 3214 (2020)
- [25] Z. Yu, L. A. Curtiss, R. E. Winans, **Y Z**, T. Li, L. Cheng, “Asymmetric composition of ionic aggregates and the origin of high correlated transference number in water-in-salt electrolytes”, *J. Phys. Chem. Lett.* 11(4), 1276 (2020)
- [26] L. A. Robertson, Z. Li, Y. Cao, I. A. Shkrob, M. Tyagi, K. C. Smith, L. Zhang, J. S. Moore, and **Y Z\***, “Observation of microheterogeneity in highly concentrated nonaqueous electrolyte solutions”, *J. Am. Chem. Soc.* 141(20), 8041 (2019)
- **“Stability and microheterogeneity in concentrated nonaqueous electrolyte solutions”, 2020 Accomplishments and Opportunities, NIST Center for Neutron Research (2020)**
- [27] T. A. Lima, Z. Li, M. Tyagi, M. C.C. Ribeiro, **Y Z\***, “Spatial and thermal signatures of  $\alpha$  and  $\beta$  relaxations in glassy and glacial aliphatic ionic liquids”, *J. Chem. Phys.* 150, 144506 (2019)
- [28] R. Ashkar, H. Bilheux, H. Bordallo, R. Briber, D. Callaway, X. Cheng, X.-Q. Chu, J. Curtis, M. Dadmun, P. Fenimore, D. Fushman, F. Gabel, K. Gupta, F. Herberle, F. Heinrich, L. Hong, J. Katsaras, Z. Kelman, E. Kharlampieva, G. Kneller, A. Kovalevskyi, S. Krueger, P. Langan, R. Lieberman, Y. Liu, M. Losche, E. Lyman, Y. Mao, J. Marino, C. Mattos, F. Meilleurz, P. Moody, J. D. Nickels, W. O'Dell, H. O'Neill, U. Perez-Salas, J. Peters, L. Petridis, A. Sokolov, C. Stanley, N. Wagner, M. Weinrich, K. Weiss, T. Wymore, **Y. Zhang**, J. C. Smith, “Neutron scattering in the biological sciences: progress and prospects”, *Acta Cryst.* D74, 1129 (2018).
- [29] T. P. Moneypenny II, A. Yang, N. P. Walter, T. J. Woods, D. L. Gray, **Y. Zhang**, J. S. Moore, “Product distribution from precursor bite angle variation in multitopic alkyne metathesis: evidence for a putative kinetic bottleneck”, *J. Am. Chem. Soc.* 140(17), 5825 (2018)
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