Qiang Zhu, PhD
School of Science
University of Wollongong, Australia
Website: https://csu1505110121.github.io/about/
Tel: (+61)478540518
Email: qiangzhu@uow.edu.au

Professional Experience

28 Jan 2025 – Present.	**Vice-Chancellor Research Fellow** School of Chemistry and Molecular Bioscience University of Wollongong, Australia
1 Oct 2022 – 30 Aug 2024	**Postdoctoral Fellow** Department of Molecular Biology and Biochemistry University of California, Irvine, U.S.A. Supervisor: Prof. Ray Luo
1 Oct 2020 – 30 June 2022	**Postdoctoral Fellow** Institute of Theoretical and Computational Chemistry Nanjing University, China Supervisor: Prof. Jing Ma

Education

Sept 2015 – Jun 2020	**PhD** in Theoretical and Computational Chemistry (conferred: 22.06.2020) Nanjing University, China Supervisors: Prof. Jing Ma and Prof. Hao Dong
Sept 2011 – Jun 2015	**BSc** in Pharmaceutical Engineering Department of Pharmaceutical Engineering Central South University, China

Honors and Awards

2024	Vice-Chancellor Research Fellowship (UOW)
2024	Recipient of Barbara K. Burgess Postdoctoral Fellowship (UC Irvine)
2021	Excellent Poster Awards, The 32nd Chinese Chemical Society Congress
2021	The Second Prize in the Competition of Unpaired Probability Prediction
2021	The Third Prize in the Competition of Deep Modeling Hackathon 2021
2017	The Ph.D. Second Talent Scholarship of Nanjing University
2015, 2016, 2017	The First Prize Scholarship of Nanjing University
2015	Outstanding Graduate of Central South University
2013	BYD Scholarship
2012	The Second Prize Scholarship of Central South University
2011, 2013	The First Prize Scholarship of Central South University
2011, 2012	Excellent Student of Central South University
2011	National Scholarship of Central South University

Service to Professions

2022	Guest Editor, "Deep Learning in Molecular Recognition", *Frontiers of Molecular Biosciences*
2022–	Peer reviewer for *Cell Reports Physical Science, J. Chem. Inf. Model (x2)*, *ACS omega*, *J. Phys. Chem. A/B/C.(x2), J. Comput. Chem.*, *ChemistrySelect, Quantitative Biology, Scientific Data, Journal of Molecular Recognition, Molecules*, *Encyclopepdia*
2019	Co-organizer, Workshop on Computational Statistical Mechanics of Complex Systems, Nanjing, China, 2019

Significant Contributions to Science

AI-enhanced property prediction for drug-like molecules: Determining the properties of drug-like molecules is essential for drug design. While experimental methods offer direct measurements, they

can be significantly time-consuming and costly. Accurately predicting such properties across a wide chemical spectrum remains a formidable challenge. By harnessing the synergistic capabilities of artificial intelligence and molecular dynamics (MD) simulations, I have developed efficient methods for predicting pharmacokinetic properties. It is the first time that both conformations and polarity are implemented into descriptors simultaneously. My method has notably enhanced the accuracy of the predictions. This advancement not only streamlines property determination, but also enriches our understanding of the molecular determinants influencing drug behavior.

Development of enhanced sampling method: MD simulations serve as a powerful tool for investigating complex biological systems by providing insights into their time-dependent motions that are often elusive to experimental probing. However, conventional MD simulation is hampered by the rugged energy landscape of biomolecular systems where conformational transitions can span from microseconds to seconds; this surpassing the capabilities of standard MD approaches. To overcome this limitation and bridge the gap between experimental observations and simulation predictions, I have developed a novel algorithm: the Data-Driven Accelerated (DA2) method. Based on a series of short, parallel conventional MD simulations, this process efficiently distills the principal directions of dominant protein motions by harnessing principal component analysis, thereby enhancing the ability to capture the critical conformational changes of proteins within accessible simulation timeframes.

Mechanistic biophysics: I have utilized multi scale simulations to unravel intricate processes native to biological macromolecules; my primary aim has been the elucidation of their machinations and the exploration of novel therapeutic approaches. For instance, we identified a new allosteric site in SHP2, a potential anti-cancer target, and revealed the possible mechanism by which a small molecule is transported into biological membrane (highlighted by *Chem. Rev.* and *Annu. Rev. Biophys.*). Leveraging my expertise in both method development and complex systems, I have taken on the challenge of studying the liquid-liquid phase separation (LLPS), a process fundamental to the formation of numerous membraneless organelles with essential cellular functions. Aberrant phase transitions can lead to the formation of insoluble protein aggregates, which are pathological hallmarks of neurodegenerative diseases. Our work, based on a model protein system, provides a deeper, thermodynamic understanding of LLPS formation, distinct from most of the works done by phenomenological and experimental observation. This sheds lights on the development of novel bioreactor and primitive artificial cells for synthesizing key chemicals for certain diseases.

Selected Presentations

- "Understanding and Fine Tuning the Propensity of ATP-Driven Liquid-Liquid Phase Separation with Oligolysine", BPS 2024, Philadelphia, Pennsylvania, USA (Poster)
- "PyRESP_GEN: A user-friendly program simplifies the process of electrostatic parameterization", ACS Fall 2023, San Francisco, CA, USA (Poster)
- "Improvements of force fields guided by machine learning methods", The 10th International Conference on Advanced Fibers and Polymer Materials, Shanghai, China, (**Invited Speaker**)
- The 14th National Conference of Quantum Chemistry, Shanghai, China, 2021
- Forum on Material Design and Intelligent Manufacturing, Shanghai, China, 2021
- "Shear Viscosity Prediction using Variable Force Fields", The 32nd Chinese Chemical Society Congress, Zhuhai, China, 2021 (Poster)
- From Free Energy Perturbation to Biomedicine: Bridging Experiment and Computation, Shenzhen, China, 2019
- "A Data-Driven Accelerated Sampling Method for Searching Functional States of Proteins", The Workshop on Computational Statistical Mechanics of Complex Systems, Nanjing, China, 2019 (Poster)
- "A Data-driven Accelerated Sampling Method for Searching Functional States of Proteins", Energy Landscape 2019, Belgrade, Serbia, 2019 (Poster)

- "A Data-driven Accelerated Sampling Method for Searching Functional States of Proteins", Theory and computational biology: From molecule to System, Dongguan, China, 2019 (Poster)
- "A Data-driven Accelerated Sampling Method for Searching Functional States of Proteins", The 4th China-Japan-Korea Workshop on Theoretical & Computational Chemistry, Nanjing, China, 2019 (Poster)
- "Entropy and Polarity Control the Partition and Transportation of Drug-like Molecules in Biological Membrane", The 3rd Chinese Chemical Society Congress, China, 2018 (Poster)
- The 14th National Computational Chemistry, Nanjing, China, 2017
- 2017 Summer School on Machine Learning in the Molecular Sciences, Shanghai, China
- "Molecular mechanism of the partition of 2-aminoethyldiphenylborinate in a fully hydrated lipid bilayer", The 13th Chinese Quantum Chemistry, Dalian, China, 2017 (Poster)
- "Study of the Dynamics of a Membrane-protein-targeted Drug with Molecular Modelling", The 10th National Conference on Soft Matter and Biophysics, Xiamen, China, 2017 (Poster)
- 2016 International Workshop on Frontiers in Molecular Biophysics, Shanghai, China

Teaching Experience

2025 Lectures, "Computational Chemistry" CHEM374/964, University of Wollongong
2015, 2016 Teaching Assistant, "Structural Chemistry", Nanjing University
2015 Teaching Assistant, "Instrumental Analysis", Nanjing University

Research Supervision

UC Irvine, co-supervised with Prof. Ray Luo

Yongxian Wu: PhD student, Publication #2, #6, #8, #11, #13
Cizhang Zhao: Undergraduate, Publication #5, *Full scholarship to attend graduate school at UW Madison*
Tianhong Wang: Undergraduate, *Full scholarship to attend graduate school in Stanford/MIT*

Nanjing University, co-supervised with Prof. Jing Ma and Prof Hao Dong

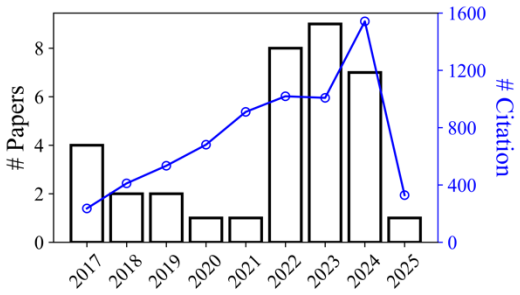
Ziyi Cui: Undergraduate (Berkeley), Publication #18, #20, *Now software engineer at Google*
Ruizhe Shen: PhD student #1
Lulu Fu: PhD student, Publication #14, #16, *Now faculty at TUST*
Yang Ge: PhD student, Publication #12, #24, *Now postdoc at University of Maryland*
Limu Hu: PhD student, Publication #3, #25
Qingqing Jia: PhD student, Publication #18, #20
Mengting Fan: Master student, Publication #18, #20, *Now research scientist at PetroChina*
Chang Cui: Undergraduate, #3, *Now PhD student at Peking University*

Recent Collaborators

Dr. Piotr Cieplak, SBP Medical Discovery Institute, USA (Method Development)
Prof. Yong Duan, University of California, Davis, USA (Method Development)
Prof. Han Li, University of California, Irvine, USA (Synthetic Biology)
Prof. Yitao Long, Nanjing University (Single Molecule Nanopore Sensing, Asso. Editor, Chem. Sci.)
Prof. Junmei Wang, University of Pittsburgh, USA (Method Development)
Prof. Wenqi Wang, University of California, Irvine, USA (Drug Design)
Prof. Yilun Ying, Nanjing University, China (Single Molecule Detection)

Publications

Total published articles: **35**
(co)first author: 18
(co)corresponding author: 3
Q1 journals: 32
Preprints/submitted: **1**
Total Citations: **7264**
h-index: **13**
Google Scholar: **FEzFWA8AAAAJ**



Publications in **high-profile** journals including:
Nature Nanotechnol. (IF=38.3)
Angew Chem Int Ed (IF=16.1)
ACS Nano (IF=17.1)
J. Mater. Chem. A (IF=11.9)
Environ. Sci. Technol. (IF=11.4)
J. Phys. Chem. Lett. (x2, IF=5.7)
J. Chem. Inf. Model (×2, IF=5.6)
J. Chem. Theory Comput. (×6, IF=5.5)

Submitted

(S1) *"Wide-temperature Zn-organic battery with a super-long life"*
Lei Yan, Xiaomeng Yu, Kang Zhou, Yae Qi, **Qiang Zhu**, Zhi Li, Jing Ma, and Yonggang Wang*, **2024**, *Under Revision*

Peer Reviewed

(1) *"Bridging Dimensionality Reduction and Stochastic Sampling: The DA2-MC Algorithm for Protein Dynamics"*
Ruizhe Shen, # **Qiang Zhu**, # Limu Hu, Jing Ma, Wei Wang,* and Hao Dong.* *J. Phys. Chem. Lett.* **2025**, 16, 4788-4795. (**co-first author**)

(2) *"Automated Refinement of Property-Specific Polarizable Gaussian Multipole Water Models Using Bayesian Black-Box Optimization"*
Yongxian Wu, **Qiang Zhu**, Zhen Huang, Piotr Cieplak, Yong Duan,* and Ray Luo.* *J. Chem. Theory Comput.* **2025**, 21(7), 3563-3575.

(3) *"Decoding Hairpin Structure Stability in Lin28-Mediated Repression"*
Qiang Zhu, Limu Hu, Chang Cui, Min Zang, Hao Dong,* and Jing Ma.* *Biochem.* **2025**, 64(6), 1276-1284.

(4) *"Proton coordination chemistry in pyrene-based anodes for ultralong-life aqueous proton batteries"*
Wenhui Yang, # Chensi Zhan, # **Qiang Zhu**, # Lei Liu, Baiming Su, Haoxiang Yu, Liyuan Zhang, Lei Yan,* and Jie Shu*. *Inorg. Chem. Front.*, **2025**, Advance Article (**co-first author**)

(5) *"Targeting SHP2 Cryptic Allosteric Sites for Effective Cancer Therapy"*
Rehman, Ashfaq Ur, # Cizhang Zhao, # Yongxian Wu, **Qiang Zhu**, and Ray Luo*. *Int. J. Mol. Sci.*, **2024**, 25(11), 6201

(6) *"Shifting Redox Reaction Equilibria on Demand Using an Orthogonal Redox Cofactor"*
Derek Aspacio,# Yulai Zhang,# Youtian Cui,# Emma Luu, Edward King, William B. Black, Sean Perea,

Qiang Zhu, Yongxian Wu, Ray Luo, Justin B. Siegel, and Han Li*, *Nat. Chem. Biol.,* **2024**, 1-12

(7) *"Single-Molecule Sensing inside Stereo- and Regio-Defined Hetero-Nanopores"*
Wei Liu,[#] **Qiang Zhu,[#]** Chao-Nan Yang,[#] Ying-Huan Fu, Ji-Chang Zhang, Meng-Yin Li, Zhong-Lin Yang, Kai-Li Xin, Jing Ma, Mathias Winterhalter, Yi-Lun Ying*, Yi-Tao Long, *Nat. Nanotechnol.,* **2024,** 1-9 (**co-first author**)

Deciphered the asymmetric stereo and regio-defined structure under hetero-nanopore and revealed the underlying mechanism for its sensing ability.

(8) *"Understanding and Fine Tuning the Propensity of ATP-Driven Liquid-Liquid Phase Separation with Oligolysine"*
Qiang Zhu, Yongxian Wu, Ray Luo*, *Phys Chem Chem Phys*, **2024**, 26, 10568-10578 (**HOT Article**)

Revealed the underlying mechanism of LLPS and propose new strategies for tuning their formation propensities.

(9) *"Prediction of Free Radical Reactions toward Organic Compounds with Easily Accessible Molecular Descriptors"*
Guoyang Zhang,[#] **Qiang Zhu**,[#] Hongcen Zheng, Shujuan Zhang,* Jing Ma.*, *Chemosphere*, **2024**, 346, 140660. (**co-first author**)

(10) *"AmberTools"*
David A. Case, Hasan Metin Aktulga, Kellon Belfon, David S. Cerutti, Gerardo Andres Cisneros, Vinicius Wilian D. Cruzeiro, Negin Forouzesh, Timothy J. Giese, Andreas W. Gotz, Holger Gohlke, Saeed Izadi, Koushik Kasavajhala, Mehmet C. Kaymak, Edward King, Tom Kurtzman, Tai-Sung Lee, Pengfei Li, Jian Liu, Tyler Luchko, Ray Luo, Madushanka Manathunga, Matias R. Machado, Hai Minh Nguyen, Kurt A. O'Hearn, Alexey Onufriev, Feng Pan, Sergio Pantano, Ruxi Qi, Ali Rahnamoun, Ali Risheh, Stephan Schott-Verdugo, Akhil Shajan, Jason Swails, Junmei Wang, Haixin Wei, Xiongwu Wu, Yongxian Wu, Shi Zhang, Shiji Zhao, **Qiang Zhu**, Thomas E. Cheatham, III, Daniel R. Roe, Adrian Roitberg, Carlos Simmerling, Darrin M. York, Maria C. Nagan, and Kenneth M. Merz, Jr. *J. Chem. Inf. Model,* **2023**, 63(20), 6183-6191.

Contribution to the prestigious molecular dynamics simulation engine, AMBER. Strong connections with its developer community.

(11) *"Grid-robust Efficient Neural Interface Model for Universal Molecule Surface Construction from Point Clouds"*
Yongxian Wu, Haixin Wei, **Qiang Zhu,*** Ray Luo.* *J. Phys. Chem. Lett.* **2023**, 14, 9034-9041.

Developed infrastructure for accurate predicting molecule surface with artificial intelligence and deployed it onto GPU platform for efficiency.

(12) *"Machine Learning-Guided Adaptive Parameterization for Coupling Terms in a Mixed United-atom/Coarse-Grained Model for Diphenylalanine Self-assembly in Aqueous Ionic Liquids"*
Yang Ge, Xueping Wang, **Qiang Zhu,** Yuqing Yang, Hao Dong, Jing Ma.* *J. Chem. Theory Comput.* **2023**, 19(19), 6718-6732.

(13) *"Streamlining and Optimizing Strategies of Electrostatic Parameterization"*
Qiang Zhu, Yongxian Wu, Shiji Zhao, Piotr Cieplak, Yong Duan,* Ray Luo.* *J. Chem. Theory Comput.* **2023,** 19(18), 6353-6365.

Comprehensive evaluation of the quality of ESPs among different QM methods and proposed strategies for streamlining electrostatic parameterization.

(14) *"Planar Chirality for Acid/Base Responsive Macrocyclic Pillararenes Induced by Amino Acid Derivatives: Molecular Dynamics Simulations and Machine Learning"*

Lulu Fu,[#] Ranran Wang,[#] **Qiang Zhu,[#]** Yuming Gu, Li-Feng Zheng, Yuan Chen, Juli Jiang,* Jing Ma.* *J. Chem. Theory Comput.* **2023,** 19(14), 4364-4376. (**co-first author**)

(15) *"Treating Polarization Effects in Charged and Polar Bio-Molecules Through Variable Electrostatic Parameters"*
Qiang Zhu, Yang Ge, Wei Li,* Jing Ma.* *J. Chem. Theory Comput*. **2023**, 19, 396-411. (**Invited Review & highlighted by Editor-in-Chief**)

Invited review on the challenges, opportunities, and our contribution on handling the polarization effects.

(16) *"Machine Learning Assisted Prediction of Properties of Charge Transfer Excitations in Fullerene and Non-fullerene Donor/Acceptor Heterojunctions"*
Lulu Fu, Haixia Hu, **Qiang Zhu,** Yuming Gu, Yaping Wen, Haibo Ma, Hang Yin[*], and Jing Ma[*]. *Nano Res.*, **2023,** 3588-3596.

(17) *"Towards High-Performance Aqueous Zinc Batteries via a Semi-Conductive Bipolar-Type Polymer Cathode"*
Lei Yan*, **Qiang Zhu**, Yae Qi, Jie Xu, Yu Peng, Jie Shu, Jing Ma, Yonggang Wang.* *Angew. Chem. Int. Ed.*, **2022**, 61(42), e202211107.

*(18) *"Fast Prediction of Lipophilicity of Organofluorine Molecules: Deep Learning Derived Polarity Characters and Experimental Tests"*
Qingqing Jia, Yifan Ni, Ziteng Liu, Xu Gu, Ziyi Cui, Mengting Fan, **QiangZhu,**[*] Yi Wang,[*] and Jing Ma[*]. *J. Chem. Inf. Model* **2022**, 62, 4928-4936**.**

Co-corresponding author. Proposed that a combination of polarity descriptors outperforms other in the partition coefficient prediction of F-contained molecules.

(19) *"Nitrogen Reduction Reaction Energy and Pathway in Metal-zeolites: Deep Learning and Explainable Machine Learning with Local Acidity and Hydrogen Bonding Features"*
Yuming Gu,[#] Qin Zhu,[#] Ziteng Liu,[#] Cheng Fu, Jiayue Wu, **Qiang Zhu**, Qingqing Jia, and Jing Ma[*]. *J. Mater. Chem. A* **2022,** 10, 14976-14988.

(20) *"Molecular Partition Coefficient from Machine Learning with Polarization and Entropy Embedded Atom-Centered Symmetry Functions"*
Qiang Zhu, Qingqing Jia, Ziteng Liu, Yang Ge, Xu Gu, Ziyi Cui, Mengting Fan, and Jing Ma[*]. *Phys. Chem. Chem. Phys.,* **2022**, 24, 23082-23088. (**HOT Article**)

For the first time, both entropy and polarity were incorporated into the prediction of the partition coefficient using state-of-the-art artificial intelligence.

(21) *"Batch-Scale Synthesis of Nanoparticle-Agminated 3D Porous Cu@Cu_2O Microspheres for Highly-Selective Electrocatalysis of Nitrate to Ammonia"*
Minghang Jiang,[#] **Qiang Zhu**,[#] Xinmei Song, Yuming Gu, Pengbo Zhang, Zuoxiu Tie[*], Changqing Li, Jianxun Cui, Jing Ma, and Zhong Jin.[*] *Environ. Sci. Technol*. **2022**, 56, 10299-10307. (**co-first author**)

(22) *"Identification of Single-Molecule Catecholamine Enantiomers Using a Programmable Nanopore"*
Wendong Jia, ChengZhu Hu, Yuqin Wang, Yao Liu, Liying Wang, Shanyu Zhang, **Qiang Zhu**, Yuming Gu, Panke Zhang, Jing Ma, Hong-Yuan Chen, and Shuo Huang*, *ACS Nano*, **2022**, 16, 6615-6624

(23) *"Surface Stability and Morphology of Calcium Phosphate Tuned by pH Values and Lactic Acid Additives: Theoretical and Experimental Study"*
Hongwei Chen[#], Changchang Lv[#], Lin Guo,* Ming Ma, Xiangfeng Li, Zhengyi Lan, Jun Huo, Hao

Dong, Xiangdong Zhu, **Qiang Zhu**, Yuming Gu, Ziteng Liu, Jianjun Liu, Hangrong Chen, Xuefeng Guo,* Jing Ma*, *ACS Appl. Mater. Interfaces*, **2022**, 14, 4836-4851

(24) *"An Electrostatic-variable Coarse-Grained Model for Predicting Enthalpy of Vaporization, Surface Tension, Diffusivity, Conductivity, and Dielectric Constant of Aqueous Ionic Liquid"*
Yang Ge[≠], **Qiang Zhu**[≠], Yunzhi Li, Hao Dong*, Jing Ma*, *J. Mol. Liq.*, **2022**, 346, 118230. (**co-first author**)

(25) *"Shear viscosity prediction of alcohols, hydrocarbons, halogenated, carbonyl, nitrogen-containing, and sulfur compounds using the variable force fields"*
Qiang Zhu, [≠] Yuming Gu, [≠] Limu Hu, [≠] Theophile Gaudin, Mengting Fan, and Jing Ma*, *J. Chem. Phys*, **2021**, 154, 074502.

(26) "*A two-ended data-Driven accelerated sampling method for exploring the transition pathways between two known states of protein"*
Yigao Yuan**, Qiang Zhu**, Ruiheng Song, Jing Ma, Hao Dong.* *J. Chem. Theory Comput*. **2020**. 16, 4631-4640. (**Supplementary Cover**)

(27) *"A Data-Driven Accelerated Sampling Method for Searching Functional States of Proteins"*
Qiang Zhu, Yigao Yuan, Jing Ma*, and Hao Dong*, *Adv. Theory and Simu.,* **2019**, 2(4): 1800171.

Proposed a novel enhance-sampling method free of target, collective variables, and external biases.

(28) "*Direct Extracellular Electron Transfer of the Geobacter Sulfurreducens Pili Relevant to Inter-aromatic Distances*"
Chuanjun Shu[≠]**, Qiang Zhu**[≠], Ke Xiao, Yue Hou, Haibo Ma,* Jing Ma, Xiao Sun.* *BioMed Research International* **2019**, 6151587 (**co-first author**)

(29) "*Synergistic steric pairing effects of terfluorenes with ternary side groups on β-conformation transition: experiments and computations*"
Xiang-Ai Yuan, Meng-Na Yu, **Qiang Zhu**, Wan-Wan Zhang, Ling-Hai Xie, Wei Huang, and Jing Ma*. *J. Mater. Chem. C,* **2018**, 6(6): 1551.

(30) "*On-Demand Electrical Switching of Antibody-Antigen Binding on Surfaces*"
Barbara Santos Gomes, Eleonora Cantini, Stefano Tommasone, Joshua S. Gibson, Xingyong Wang, **Qiang Zhu**, Jing Ma, James D. McGettrick, Trystan M. Watson, Jon A. Preece, Jackson C. Krikman-Brown, Stephen J. Publicover, and Paula M. Mendes*. *ACS Appl. Bio Mater.,* **2018**, 1(3): 738.

(31) "*Tuning the collective switching behavior of azobenzene/Au hybrid materials: flexible versus rigid azobenzene backbones and Au (111) surfaces versus curved Au nanoparticles*"
Chunyan Liu, Dong Zheng, Weigang Hu, **Qiang Zhu**, Ziqi Tian, Jun Zhao, Yan Zhu, and Jing Ma*. *Nanoscale,* **2017**, 9(43): 16700.

(32) "*Entropy and Polarity Control the Partition and Transportation of Drug-like Molecules in Biological Membrane*"
Qiang Zhu, Yilin Lu, Xibing He, Tao Liu, Hongwei Chen, Fang Wang, Dong Zheng, Hao Dong*, and Jing Ma*. *Sci. Rep.* **2017**, 7, 17749.

Provided a clear mechanism on transporting small molecule from water phase into biological membrane at the atomic level.

(33) "*Electrostatic Interactions of Water in External Electric Field: Molecular Dynamics Simulations*"
Qiang Zhu, Zigui Kan, and Jing Ma*. *J. Electrochem.* **2017**, 23, 391.

(34) "*Polarization Effects on the Cellulose Dissolution in Ionic Liquids: Molecular Dynamics Simulations with Polarization Model and Integrated Tempering Enhanced Sampling Method*"
Zigui Kan, **Qiang Zhu**, Lijiang Yang, Zhixiong Huang, Biaobing Jin, and Jing Ma*. *J. Phys. Chem. B,* **2017**, 121(17): 4319.

Editorials

(E1) *"Recent Advances in Biomolecular Recognition"*
Qiang Zhu*, Ray Luo*, *Int. J. Mol. Sci.*, **2023**, 24(9): 8310.