# Qiang Zhu

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## Experience

**2022 - present** **Postdoctoral Fellow**
Department of Molecular Biology and Biochemistry, Chemical and Biomolecular Engineering, Materials Science and Engineering, and Biomedical Engineering, University of California, Irvine
Supervisor: Prof. Ray Luo

**2020 - 2022** **Postdoctoral Fellow**
Institute of Theoretical and Computational Chemistry, Key Laboratory of Mesoscopic Chemistry of MOE, School of Chemistry and Chemical Engineering, Nanjing University
Supervisor: Prof. Jing Ma

## Education

**2015 - 2020** **Ph.D.** in Theoretical and Computational Chemistry
Institute of Theoretical and Computational Chemistry, Key Laboratory of Mesoscopic Chemistry of MOE, School of Chemistry and Chemical Engineering, Nanjing University (Supervisor: Prof. Jing Ma & Hao Dong)

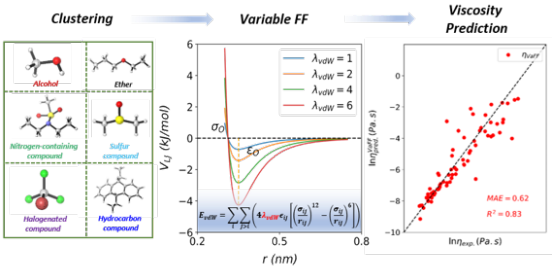
**2011 - 2015** **B.S.** in Department of pharmaceutical engineering
Chemistry and Chemical Engineering, Central South University

## Research Interests

(1) Property Prediction

**Shear Viscosity**

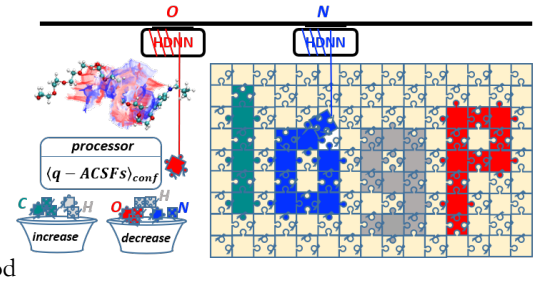
Viscosity of organic liquids is an important physical property in application of printing, pharmaceuticals, oil extracting, engineering, and chemical processes. Experimental measurement is a direct but time-consuming process. Accurate predicting the viscosity with a broad range of chemical diversity is still a great challenge. In this work, a protocol named Variable Force Field (VaFF) combined with the machine learning was implemented to efficiently vary the force field parameters, especially $\lambda_{vdW}$ for the shear viscosity prediction of 75 organic liquid molecules with viscosity ranging from -9 to 0 in their nature logarithm. (***J. Chem. Phys.*, 2021, 154(7): 074502**.)




**Partition Coefficient**

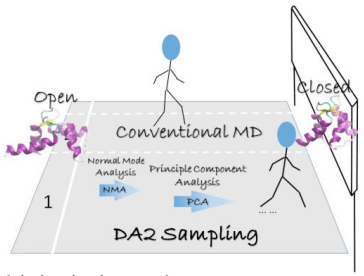
Efficient prediction of the partition coefficient (log *P*) between polar and non-polar phases could shorten the cycle of drug and materials design. In this work, a descriptor, named $\langle q - ACSFs \rangle_{conf}$, is proposed to take the explicit polarization effects in the polar phase and the conformation ensemble of energetic and entropic significance in the non-polar phase into consideration. The polarization effects are involved by embedding the partial charge directly derived from force fields or quantum chemistry calculations into the atom-centered symmetry functions (ACSFs), together with the entropy effects, which are averaged according to the Boltzmann distribution of different conformations taken from the similarity matrix. The model was trained with high-dimensional neural networks (HDNNs) on public datasets. Satisfactory log *P* prediction performance was achieved on three other datasets. The model we presented in this work can be applied to arbitrary sized systems and give a transferable atom-based partition coefficient. (***Phys. Chem. Chem. Phys.*, 2022, 23082-23088. (HOT Article); *J. Chem. Inf. Model,* 2022,**

**62, 4928-4936**)



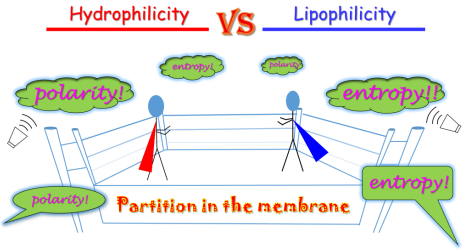

(2) Enhanced sampling method

Molecular dynamics (MD) simulation serves as a robust tool to study large biological systems such as the protein, it could provide time-dependent motions of a protein which is difficult to be probed experimentally. However, suffering from the rough energy landscape of proteins, the time-scale of conformational changes from one state to another state often spans from microseconds to seconds, which exceeds the capacity of conventional MD simulation. To bridge the gap between the experiment and simulations, a new algorithm named data-driven accelerated (DA2) method, which applied a linear dimensional reduction (Principle Component Analysis, PCA) method on short parallel conventional MD simulations to extract the directions of dominant motions, is developed by me. (***Adv. Theory and Simu.,* 2019, 2(4): 1800171.**)



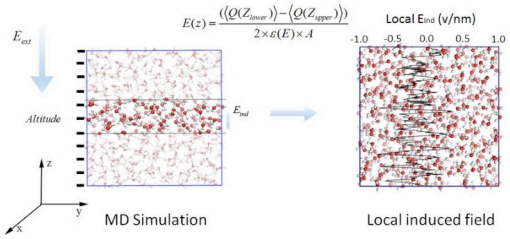

(3) Mechanism of small molecule in biological membranes

Absorption, distribution, metabolism, and elimination (ADME) are four criteria to influence the drug levels and kinetics of drug exposure. The capacity of drug to move across membranes is a prerequisite factor. Molecular dynamics (MD) simulations are utilized by me to unveil how a small molecule penetrates into membrane at atomic level. Machine Learning is also applied to disclose that entropy and polarity play an important role in drugs' potency. (***Sci. Rep.* 2017, 7, 17749.**)




(4) Property of bulk water in external electrical field

The simplicity of continuum electrostatic model makes it popular in accounting for the long-ranged electrostatics interactions in biological and materials. Experimentally, measurement of dielectric constant is usually under some mild conditions, and it is hard under some extreme conditions, such as high pressure and high temperature. Taking these into consideration, using molecular dynamics (MD) simulations is becoming increasingly appealing. A clear profile of dielectric constant under different external electrical field was provided by us with molecular dynamics (MD) simulations, which is helpful for understanding the electrostatic polarization and distribution of local induced electric fields. (***J. Electrochem.* 2017, 23, 391**)




## Publications

(1) "*Polarization Effects on the Cellulose Dissolution in Ionic Liquids: Molecular Dynamics Simulations with Polarization Model and Integrated Tempering Enhanced Sampling Method*"

Z. Kan, **Q. Zhu**, L. Yang, Z. Huang, B. Jin, and J. Ma*. *J. Phys. Chem. B,* **2017**, 121(17): 4319.

(2) "*Electrostatic Interactions of Water in External Electric Field: Molecular Dynamics Simulations*"
**Q. Zhu**, Z. Kan, and J. Ma*. *J. Electrochem.* **2017**, 23, 391.

(3) "*Entropy and Polarity Control the Partition and Transportation of Drug-like Molecules in Biological Membrane*"
**Q. Zhu**, Y. Lu, X. He, T. Liu, H. Chen, F. Wang, D. Zheng, H. Dong*, and J. Ma*. *Sci. Rep.* **2017**, 7, 17749.

(4) "*Tuning the collective switching behavior of azobenzene/Au hybrid materials: flexible versus rigid azobenzene backbones and Au (111) surfaces versus curved Au nanoparticles*"
C. Liu, D. Zheng, W. Hu, **Q. Zhu**, Z. Tian, J. Zhao, Y. Zhu, and J. Ma*. *Nanoscale,* **2017**, 9(43): 16700.

(5) "*On-Demand Electrical Switching of Antibody-Antigen Binding on Surfaces*"
B. S. Gomes, E. Cantini, S. Tommasone, J. S. Gibson, X. Wang, **Q. Zhu**, J. Ma, J. D. McGettrick, T. M. Watson, J. A. Preece, J. C. Krikman-Brown, S. J. Publicover, and P. M. Mendes*. *ACS Appl. Bio Mater.,* **2018**, 1(3): 738.

(6) "*Synergistic steric pairing effects of terfluorenes with ternary side groups on β-conformation transition: experiments and computations*"
X. Yuan, M. Yu, **Q. Zhu**, W. Zhang, L. Xie, W. Huang, and J. Ma*. *J. Mater. Chem. C,* **2018**, 6(6): 1551.

(7) "*Direct Extracellular Electron Transfer of the Geobacter Sulfurreducens Pili Relevant to Inter-aromatic Distances*"
C. Shu[≠], **Q. Zhu**[≠], K. Xiao, Y. Hou, H. B. Ma, J. Ma, X. Sun. *BioMed Research Internatioal* **2019**(2019)(contributed equally)

(8) *"A Data-Driven Accelerated Sampling Method for Searching Functional States of Proteins"*
**Q. Zhu**, Y. Yuan, J. Ma*, and H. Dong*, *Adv. Theory and Simu.,* **2019**, 2(4): 1800171.

(9) "*A Two-ended DAta-Driven Accelerated Sampling Method for Exploring the Transition Pathways between Two Known States of Protein"*
Y. Yuan**, Q. Zhu**, R. Song, J. Ma, H. Dong. *J. Chem. Theory Comput.* **2020**. 16, 4631-4640.

(10) *"Shear Viscosity prediction of alcohols, hydrocarbons, halogenated, carbonyl, nitrogen-containing, and sulfur compounds using the variable force fields"*
**Q. Zhu**,[≠] Y. Gu,[≠] L. Hu,[≠] T. Gaudin, M. Fan, and J. Ma*, *J. Chem. Phys*, **2021**, 154, 074502.

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

(12) *"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

(13) *"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

(14) *"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. (contributed equally)

(15) *"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**)

(16) *"Nitrogen Rduction 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.

(17) *"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**.**

(18) *"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.*, **2022,** 1-9.

(19) *"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.

(20) *"Prediction of Free Radical Reactions toward Organic Compounds with Easily Accessible Molecular Descriptors"*
Guoyang Zhang,[#] **Qiang Zhu**,[#] Hongcen Zheng, Shujuan Zhang,* Jing Ma.* **In Revision**, **2022**. (contributed equally)

(21) *"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.

(22) *"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. (contributed equally)

(23) *"Streamlining and Optimizing Strategies of Electrostatic Parameterization"*
**Qiang Zhu,** Yongxian Wu, Shiji Zhao, Piotr Cieplak, Yong Duan,* Ray Luo.* *J. Chem. Theory Comput.* **2023,** DOI: 10.1021/acs.jctc.3c00659.

(24) *"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**, DOI: 10.1021/acs.jctc.3c00809.

(25) *"Grid-robust Efficient Neural Interface Model for Universal Molecule Surface Construction from Point Clouds"*
Yongxian Wu, Haixin Wei, **Qiang Zhu,*** Ray Luo.* **2023**, ***In Revision***.

(26) *"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**, **Accept**.

## Awards

2011-2012 National Scholarship of Central South University
2011-2013 Excellent Student of Central South University, (**Two times**)
2011-2012, 2013-2014 The First Prize Scholarship of Central South University
2012-2013 The Second Prize Scholarship of Central South University
2013-2014 BYD Scholarship
2015 Outstanding graduate of Central South University
2015-2018 The First Prize Scholarship of Nanjing University, (**Three times**)
2017-2018 The Ph.D. Second Talent Scholarship of Nanjing University

## Academic Workshops and Conferences

- 2016 International Workshop on Frontiers in Molecular Biophysics, Shanghai, China, 2016/07/23~07/25
- The 10th National Conference on Soft Matter and Biophysics, Xiamen, China, 2017/03/24~03/27 (Poster)
- The 13th Chinese Quantum Chemistry, Dalian, China, 2017/06/08~06/11 (Poster)
- 2017 Summer School on Machine Learning in the Molecular Sciences, Shanghai, China, 2017/06/12~06/16
- The 14th National Computational Chemistry, Nanjing, China, 2017/11/17~11/20
- The 3th Chinese Chemical Society Congress, Hangzhou, China, 2018/05/05~05/08 (Poster)
- The 4th China-Japan-Korea Workshop on Theoretical & Computational Chemistry, Nanjing, China, 2019/01/09~01/12 (Poster)
- Theory and computational biology: From molecule to System, Dongguan, China, 2019/08/01~08/04 (Poster)
- Energy Landscape 2019, Belgrade, Serbia, 2019/08/26~08/30 (Poster)
- 2019 The Workshop on Computational Statistical Mechanics of Complex Systems, Nanjing, China, 2019/10/26~10/28 (Poster)
- From Free Energy Perturbation to Biomedicine: Bridging Experiment and Computation, Shenzhen, China, 2019/11/09~11/13

- The 32nd Chinese Chemical Society Congress, Zhuhai, China, 2021/04/19-04/22 (Poster, **Excellent Poster Awards**)
- Forum on Material Design and Intelligent Manufacturing, Shanghai, China, 2021/09/17-09/19
- The 14th National Conference of Quantum Chemistry, Shanghai, China, 2021/10/09-10/12
- The 10th International Conference on Advanced Fibers and Polymer Materials (ICAFPM 2021), Shanghai, China, 2021/10/17-20 (**invited lecture**)
- ACS Fall 2023, San Francisco, CA, USA, 2023/08/12-17 (Poster)

## Technical Skills

I could perform molecular dynamics simulation with **NAMD**, **GROMACS**, **AMBER** package suite, and analyze the output such as trajectories and log file with homemade Tool Command Language (**TCL** script) embedded in **VMD**, and present these data with **Gnuplot**. In addition, **Python** script is also utilized to perform some tasks such as **Machine Learning** (ML) and **Windows**, **Mac**, and **Linux OS** are frequently used.

## References

Prof. **Jing Ma** (Advisor)
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Prof. **Hao Dong** (Cooperative Advisor)
*Kuang Yaming Honors School, Nanjing University, Nanjing*, 210023, P. R. China
Email: donghao@nju.edu.cn