Qi (Jennifer) Qiao

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Education:

Doctor of Philosophy, Chemical Engineering   09/2016 –05/2020
University of Oklahoma (OU), USA.   GPA: 3.67/4.0
Dr. Liangliang Huang's Group

Master of Science, Chemical Engineering   09/2013 – 05/2016
Rutgers University, New Brunswick, USA.   GPA: 3.67/4.0
Dr. Yee Chiew's Group

Bachelor of Science, Chemistry   09/2009 – 05/2013
The Northeast Forestry University, China.   GPA: 86/100

Skill:

Machine Learning, Deep Learning, Data Visualization, Database Structures & Algorithms, Statistical Analysis, Molecular Simulations.

Programming:

Python, Pytorch, Scikit-learn, R, Fortran, XGBoost.

Research Experience:

Bioinformatics Analyst, Dr. David Fardo, University of Kentucky:
Single cell ATCT-seq data analysis, including differentially accessible regions analysis and myeloid cell trajectory analysis using ArchR. (01/2023-Present)
Deep learning for the reoccurrence of breast cancer based on EHR data. (01/2023-Present)
Machine learning using FTIR images for Microcrack. (01/2023-Present)

Post-doctoral Research Scholar, Dr. Jin Chen, University of Kentucky:
Deep learning for the reoccurrence of breast cancer based on EHR data. (01/2022 –12/2022)

- Conduct large data processing and analysis via Python and R programming.
- Extract information from large-scale and sparse data.
- Develop the temporal model (Long short-term memory) in handling time series data.
- Analyze the performance between the stationary model, temporal model and transduction model for time series prediction.

Machine learning using FTIR images for Microcrack. (08/2021 – 12/2022)

- Conduct extensive data analysis via R programming.
- Develop classical machine learning models to predict the crack density and length of bonds with infrared spectroscopic, histomorphometric, and patient-related parameters.

Pangenomic study of Komagataeibacter. (08/2021 – 12/2022)

- Develop automated data quality control and Bioinformatics analysis pipeline for Komagataeibacter.
- Accomplish multiple Bioinformatics analysis including DNA-Seq, whole genome alignment, prokaryotic genome annotation and calculates the pan genome.
- Perform phylogenetic analysis to investigate the loss of cellulose production in Komagataeibacter.

MicroRNA sequence analysis for rat's exosomes. (08/2021 – 12/2022)

- Perform differential gene expression analysis to discover quantitative changes in expression levels between experimental groups.

Machine learning for protein design. (01/2022 – 12/2022)

- Perform statistical analysis of the simulation data using self-developed Python codes.

Post-doctoral Research Scholar, Dr. Qing Shao, University of Kentucky:
Computational molecular design. (08/2020 – 06/2022)
- Design deep eutectic solvents for lignin pretreatment
- Design deep eutectic solvents for biocatalysis.

Computational protein & peptide design. (08/2020 – 06/2022)
- Design zwitterionic peptides to protect therapeutic proteins
- Investigate the effect of mutation on conformation and dynamics of cancer relevant proteins.

Research Assistant, Dr. Liangliang Huang, University of Oklahoma.
Atomistic Computational Studies of Cellulose: Structure, Property and Process. (09/2019 – 05/2020)
- Outlined the state-of-the-art understanding of cellulose structures, interactions, dissolutions and decompositions using computational simulations.
- Summarized the cellulose characterizations methods.

Reactive Molecular Dynamics Simulation of Cellulose and Its Property Evolution Under Pyrolysis Conditions. (05/2018 – 05/2020)
- Mimic the cellulose structure under pyrolysis process.
- Conduct constructed extensive data analysis methods of cellulose properties using self-developed Python codes.

Collaboration of Natural Gas Dew Point Predictions Project with Petroleum & Geological Engineering. (11/2017 – 06/2018)
- Proficient in using PVTsim for natural gas components simulations.
- Investigate Fluent for CFD calculations of heat transfer and familiar with thermodynamics.

Multiscale Modeling of Graphene Oxide and Its Applications. (09/2016 – 05/2020)
- Develop the graphene oxide model using molecular dynamics simulation.
- Conducted extensive data analysis via Python, R, Fortran and Matlab.

Exchange Research Assistant, Dr. Wei Gao, North Carolina State University.
Synthesis of Graphene Oxide and Janus Graphene Oxide and Its Characterizations. (05/2017 – 08/2017)
- Proficient in both simulated and experimental of physicochemical analysis such as FTIR and XRD, trained lab skills.

Research Assistant, Dr. Yee Chiew, Rutgers University, The State University of New Jersey.
Structure and Clustering of Colloidal Dimers on A Surface, (09/2013 – 05/2016)
- Proficient in using Gromacs for polymers and drug delivery system simulations.
- Performed statistical analysis on data sets using Matlab.

Undergraduate Researcher, The Northeast Forestry University, China.
National Undergraduate Innovative Experiments: Photocatalysis and Its Application to Remove Dye from Water & Flame-Retardant Chemistry, (01/2012-12/2013)
- Proficient in the synthesis and characterizations of inorganic chemicals, trained lab skills.

Teaching Assistant, University of Oklahoma:
- Teaching Assistant, Design Laboratory. (09/2019- Present)
- Teaching Assistant, Unit Operations Laboratory. (01/2019-05/2019)
- Grader, Chemical Engineering Thermodynamics. (06/2016-12/2016)
- Grader, Structure and Properties of Materials. (01/2017-05/2017)

Awards & Activities:
- Dolese Teaching Fellowship, (09/2019)
- Chevron Scholarship, University of Oklahoma, Norman, OK. (2019)
- Chevron Scholarship, University of Oklahoma, Norman, OK. (2017)

- Scholarship for master study, Rutgers University, The State University of New Jersey. (2015)
- Scholarships for undergraduate study, The Northeast Forestry University, China. (2010-2012)
- President of Social Practice, The Northeast Forestry University, China. (2011)
- Outstanding Social Practice Award, The Northeast Forestry University, China. (2011)
- First prize in the Debate Competition, The Northeast Forestry University, China. (2010)
- Sixth prize of women's High Jump in the College Student's Sports Game, The Northeast Forestry University, China. (2010)

Presentation:
- Oral Presentation at AIChE Annual Meeting, Hyatt Regency, Orlando, FL. (11/2019)
- Oral Presentation, 64th Annual ACS Pentasectional Meeting, Norman, OK. (04/2019)
- Oral Presentation at AIChE Annual Meeting, David L. Lawrence Convention Center, Pittsburgh, PA. (11/2018)
- Poster Competition at the 2nd Annual Chemical and biochemical Engineering Graduate Research Symposium, Rutgers University, The State University of New Jersey. (2015)

Publications:
1. McMullen, Patrick; Qi, Qiao; Luozhong, Sijin; Cai, Lirong; Fang, Liang; Shao, Qing; Jiang, Shaoyi, Motif-based zwitterionic peptides impact their structure and immunogenicity. *Chemical Science*. 2022. doi.org/10.1039/D2SC03519G
2. Zhang, Z.; Cheng, L.; Li, J.; Qiao, Q.; Karki, A.; Allison, D. B.; Shaker, N.; Li, K.; Utturkar, S. M.; Atallah Lanman, N. M., Targeting Plk1 sensitizes pancreatic cancer to immune checkpoint therapy. *Cancer Research*. CAN-22-0018.
3. McMullen, P.; Fang, L.; Qiao, Q.; Shao, Q.; Jiang, S., Impacts of a Zwitterionic Peptide on its Fusion Protein. Bioconjugate Chemistry 2022.
4. Qiao Q, Cai L, Shao Q. Molecular simulations of zwitterlation-induced conformation and dynamics variation of glucagon-like peptide-1 and insulin. *Journal of Materials Chemistry B*. 2022, 10, 2490-2496
5. Qiao Q, Shi J, Shao Q. The multiscale solvation effect on the reactivity of β-O-4 of lignin dimers in deep eutectic solvents. *Physical Chemistry Chemical Physics*. 2021;23(45):25699-25705.
6. Qiao Q, Shi J, Shao Q. Effects of water on the solvation and structure of lipase in deep eutectic solvents containing a protein destabilizer and stabilizer. *Physical Chemistry Chemical Physics*. 2021;23(40):23372-23379.
7. Abbas UL, Qiao Q, Nguyen MT, Shi J, Shao Q. Molecular dynamics simulations of heterogeneous hydrogen bond environment in hydrophobic deep eutectic solvents. *AIChE Journal*. 2022;68(1): e17382.
8. Abbas UL, Qiao Q, Nguyen MT, Shi J, Shao Q. Structure and hydrogen bonds of hydrophobic deep eutectic solvent-aqueous liquid–liquid interfaces. *AIChE Journal*. 2021;67(12): e17427.
9. Ding, J.; Xu, N.; Nguyen, M. T.; Qiao, Q.; Shi, Y.; He, Y.; Shao, Q., Machine learning for molecular thermodynamics. Chinese Journal of Chemical Engineering 2021, 31, 227-239.
10. Qiao, Q.; Li, X.; Huang, L., Crystalline Cellulose under Pyrolysis Conditions: The Structure–Property Evolution via Reactive Molecular Dynamics Simulations. *Journal of Chemical & Engineering Data* 2020. **65**(2): p. 360-372.
11. Cao, Y.; Zhou, G.; Chen, X.; Qiao, Q.; Zhao, C.; Sun, X.; Zhong, X.; Zhuang, G.; Deng, S.; Wei, Z.; Yao, Z.; Huang, L.; Wang, J., Hydrogen peroxide synthesis on porous graphitic carbon nitride using water as a hydrogen source. *Journal of Materials Chemistry A* **2020,** *8* (1), 124-137.
12. Li Li, Guobing Zhou, Zhen Yang, Fang Fang, Qi Qiao, Na Hu, Liangliang Huang, Xiangshu Chen, "Molecular-Level Understanding of Translational and Rotational Motions of C2H6, C3H8, n-C4H10 and Their Binary Mixtures with CO2 in ZIF-10", *Journal of Chemical & Engineering Data*, 2019, *64* (2), 484-496.

13. Qiao, Q.; Liu, C.; Gao, W.; Huang, L., Graphene oxide model with desirable structural and chemical properties. *Carbon*, 2019, 143, 566-577.
14. Li Li, Deshuai Yang, Trevor R. Fisher, Qi Qiao, Zhen Yang, Na Hu, Xiangshu Chen and Liangliang Huang, "Molecular Dynamics Simulations for Loading-Dependent Diffusion of CO2, SO2, CH4, and Their Binary Mixtures in ZIF-10: The Role of Hydrogen Bond", *Langmuir*, 2017, *33* (42), 11543-11553.