Zhuoran Qiao, Ph.D.

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Education

California Institute of Technology — Pasadena, CA
Doctor of Philosophy in Chemistry, with a minor in Quantum Science and Engineering — *Oct 2019 – Dec 2022*

Peking University — Beijing, China
Bachelor of Science, College of Chemistry and Molecular Engineering — *Sept 2015 – Jul 2019*

Experience

Entos, Inc — San Diego, CA
Lead Machine Learning Scientist — *Feb 2023 – Present*
Provisioned, designed, and delivered the company's core generative AI technology for computational structure prediction and de novo molecular design (2 U.S. patents filed in 2023). Project lead for building the company's next-generation multi-modal integrated platform for accelerating drug discovery and clinical-stage programs.

Division of Chemistry and Chemical Engineering, Caltech — Pasadena, CA
Graduate student. Advisors: Prof. Thomas F. Miller III and Prof. Anima Anandkumar — *Oct 2019 – Dec 2022*
Ph.D. Thesis: Physics-informed neural approaches for multiscale molecular modeling and design.

Institute of Theoretical and Computational Chemistry, Peking University — Beijing, China
Undergraduate researcher. Advisor: Prof. Yi Qin Gao — *Jan 2017 – Apr 2019*
Senior thesis: Statistical mechanics and anisotropic dynamics in nano-confined soft matters.

Department of Chemistry and Chemical Biology, Harvard University — *Jul 2018 – Sept 2018*
Studies of non-equilibrium mRNA folding-induced codon bias. Advisor: Prof. Eugene I. Shakhnovich.

Biomedical Pioneering Innovation Center (BIOPIC), Peking University — *Dec 2017 – Jan 2019*
Fluorescence Correlation Spectroscopy for non-equilibrium steady states. Advisor: Prof. Xinsheng Zhao.

Selected Publications

1. **Zhuoran Qiao**, Weili Nie, Arash Vahdat, Thomas F. Miller III, Anima Anandkumar. **State-Specific protein-ligand complex structure prediction with a multi-scale deep generative model**. *arXiv preprint* arXiv:2209.15171 (2023). Under review. Appeared at *Machine Learning for Structure Biology workshop at NeurIPS 2022* as a **contributed talk**.
2. **Zhuoran Qiao**, Anders S. Christensen, Frederick R. Manby, Matthew Welborn, Anima Anandkumar, Thomas F. Miller III. **Informing Geometric Deep Learning with Electronic Interactions to Accelerate Quantum Chemistry**. *Proceedings of the National Academy of Sciences (PNAS)* 119.31 (2022): e2205221119.
3. **Zhuoran Qiao**, Feizhi Ding, Matthew Welborn, Peter J. Bygrave, Daniel G. A. Smith, Animashree Anandkumar, Frederick R. Manby and Thomas F. Miller III. **Multi-task learning for electronic structure to predict and explore molecular potential energy surfaces**. *arXiv preprint* arXiv:2011.02680 (2020). Appeared at *Machine Learning for Molecules workshop at NeurIPS 2020* as a **contributed talk**.
4. **Zhuoran Qiao**, Matthew Welborn, Animashree Anandkumar, Frederick R Manby, Thomas F Miller III. **OrbNet: Deep learning for quantum chemistry using symmetry-adapted atomic-orbital features**. *The Journal of Chemical Physics* 153.12 (2020): 124111. (**Editor's Pick**)
5. **Zhuoran Qiao**, Yuheng Zhao, Yi Qin Gao. **Ice nucleation of confined monolayer water conforms to classical nucleation theory**. *The Journal of Physical Chemistry Letters* 10.11 (2019): 3115-3121.

Selected Honors & Awards

Amazon/Caltech AI4Science Fellowship (awarded to 8 Caltech students and postdocs) — *2021-2022*
Excellent Graduate of PKU (top 4%) — *Jul 2019*
Outstanding Research Award (top 6%) — *Oct 2018*

Skills & Interests

Skilled in project management, Linux, C/C++, Python, CUDA, Pytorch, HPC & Cloud Computing.

HTML, JavaScript, and Node.js for Web Development. Designed a conference platform that served 2000+ users.