Zhuoran Qiao

+1(626)372-3150 | zqiao@caltech.edu | github.com/zrqiao

Education

California Institute of Technology — Pasadena, CA
Ph.D. Student, Division of Chemistry and Chemical Engineering — *Oct 2019 – Present*

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

Experience

Division of Chemistry and Chemical Engineering, Caltech — Pasadena, CA
Advisors: Prof. Thomas F. Miller III and Prof. Anima Anandkumar — *Oct 2019 – Present*
Working on physics-based machine learning for molecular electronic structure and dynamics

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

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

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

Selected Publications

1. **Zhuoran Qiao**, Anders S. Christensen, Frederick R. Manby, Matthew Welborn, Anima Anandkumar, Thomas F. Miller III. **UNiTE: Unitary N-body Tensor Equivariant Network with Applications to Quantum Chemistry**. *arXiv preprint* arXiv:2105.14655 (submitted).
2. **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**.
3. **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**)
4. **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.
5. **Zhuoran Qiao**, Wen Jun Xie, Xiaoxia Cai, and Yi Qin Gao. **Interlayer Hopping Dynamics of Bilayer Water Confined in Graphene Nano-capillaries**. *Chemical Physics Letters* 722 (2019):153-159.

Honors & Awards

Amazon/Caltech AI4Science Fellowship (awarded to 8 students/postdocs in Caltech)	*2020-2021*
Excellent Graduate of PKU (top 5%)	*Jul 2019*
Outstanding Research Award (top 8%)	*Oct 2018*
Wei Lin Scholarship	*Oct 2017*
Merit Student of PKU (top 5%)	*Oct 2017*
Beida Pioneer Scholarship	*Oct 2016*

Skills & Interests

Proficient in Linux, C/C++, Python, CUDA, LaTeX, Pytorch, Tensorflow, Mathematica.

Skilled in HTML, JavaScript, and Node.js for Web Development. Designed a conference platform that served 2000+ users: *github.com/Utenaq/pkunmun_conference*.