

Yuanheng Wang

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EDUCATION

Stanford University

June 2019 - Present

Ph.D. Candidate in Theoretical Chemistry

Cumulative GPA: 4.19/4.00

University of Illinois, Urbana-Champaign (UIUC)

January 2017 - May 2019

B.S. in Chemistry

GPA: 4.00/4.00

Fudan University

September 2015 - January 2017

Major in Chemistry

GPA: 3.67/4.00

RESEARCH EXPERIENCES

Stanford University, Martinez Group

Graduate Researcher

June 2019 - Present

- Development of *Ab Initio* interactive molecular dynamics on VR devices
- Implementation of high-performance Gaussian integrals with high angular momentums
- Implementation of Gaussian integrals under periodic boundary condition
- Implementation of QM/MM with polarizable force field
- Profiling and optimization of a GPU-accelerated electronic structure package
- Maintenance and administration of a large electronic structure codebase, management and extension of its continuous integration pipeline
- Setup, maintenance and administration of a large GPU-based HPC cluster

University of Illinois, Urbana-Champaign, van der Veen Group

Undergraduate Researcher

January 2018 - June 2019

- Simulation and analysis of ultrafast X-ray absorption spectra of quantum dots
- Modeling of the thermal and optical properties of quantum dots

University of Illinois, Urbana-Champaign, van der Donk Group

Undergraduate Researcher

May 2017 - December 2017

- Lantipeptide synthesis, purification and characterization

Technical Skills

Programming Languages: C, C++, CUDA, Python, Unity (C#)

Cluster Administration Skill: docker, network (DHCP, DNS) setup, file server setup, environment module setup, Slurm queue setup, automatic OS installation, hardware inspection through BMC, hardware installation

Knowledge: Parallel programming, metaprogramming, Linux operating system, compilation, computer network, computer graphics, numerical linear algebra, digital circuit (FPGA)

PUBLICATIONS

- Cruzeiro, V. W. D.; **Wang, Y.**; Pieri, E.; Hohenstein, E. G.; Martínez, T. J., TeraChem protocol buffers (TCPB): Accelerating QM and QM/MM simulations with a client–server model. *The Journal of Chemical Physics* 2023, 158 (4), 044801.
- Wang, Y.**; Seritan, S.; Lahana, D.; Ford, J. E.; Valentini, A.; Hohenstein, E. G.; Martínez, T. J., InteraChem: Exploring Excited States in Virtual Reality with Ab Initio Interactive Molecular Dynamics. *Journal of Chemical Theory and Computation* 2022, 18 (6), 3308-3317.
- Seritan, S.; **Wang, Y.**; Ford, J. E.; Valentini, A.; Gold, T.; Martínez, T. J., InteraChem: Virtual Reality Visualizer for Reactive Interactive Molecular Dynamics. *Journal of Chemical Education* 2021, 98 (11), 3486-3492.
- Fales, B. S.; Curtis, E. R.; Johnson, K. G.; Lahana, D.; Seritan, S.; **Wang, Y.**; Weir, H.; Martínez, T. J.; Hohenstein, E. G., Performance of Coupled-Cluster Singles and Doubles on Modern Stream Processing Architectures. *Journal of Chemical Theory and Computation* 2020, 16 (7), 4021-4028.
- Gentle, C. M.; **Wang, Y.**; Haddock, T. N.; Dykstra, C. P.; van der Veen, R. M., Internal Atomic-Scale Structure Determination and Band Alignment of II–VI Quantum Dot Heterostructures. *The Journal of Physical Chemistry C* 2020, 124 (6), 3895-3904.

PRESENTATIONS

- InteraChem: Exploring Excited States with Ab Initio Interactive Molecular Dynamics. American Conference on Theoretical Chemistry (ACTC). July 2022. (Poster)
- Internal structure, band alignment and charge transfer dynamics of ZnTe/CdSe core/shell quantum dots. 3rd Annual ECI ACS Undergraduate Research Conference, UIUC. November 2018. (Oral)

TEACHING EXPERIENCE

Stanford University

Teaching Assistant

- Spectroscopy Laboratory January 2021 - March 2021
- Structure and Reactivity of Organic Molecules September 2020 - December 2020
- Spectroscopy Laboratory January 2020 - March 2020
- Chemical Principles: From Molecules to Solids September 2019 - December 2019

Outreach Opportunities

- Stanford Splash - Learning Chemistry with Virtual Reality December 2022
- Stanford Splash - Learning Chemistry with Virtual Reality May 2022
- Stanford Splash - Learning Chemistry with Virtual Reality November 2019