

Yuanheng Wang

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EDUCATION

Stanford University

June 2019 - Present

Ph.D. Candidate in Theoretical Chemistry

Cumulative GPA: 4.23/4.00

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

- Improvement of *Ab Initio* interactive molecular dynamics
- Implementation of QM/MM with polarizable force field
- Implementation of Gaussian integrals under periodic boundary condition
- Profiling and optimization of a GPU-accelerated electronic structure package
- System administrator for a 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

PUBLICATIONS

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

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

HONORS

Worth H. Rodebush Scholarship, UIUC August 2018 - June 2019

Peter Beak Scholarship for Undergraduate Research, UIUC May 2018 - August 2018

Fudan University Excellent Undergraduate Students Scholarship, Fudan University September 2015 - June 2016