

Zhe Liu

<https://zheliu17.github.io>

University of Alberta, Edmonton, Alberta, Canada

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Education

M.Sc. in Chemistry (Thesis Based)

University of Alberta, Edmonton, Alberta, Canada

Sept. 2019 – Present

B.S. in Applied Chemistry

Dalian University of Technology, Dalian, China

Sept. 2015 – June 2019

Zhang Dayu School of Chemistry (Honors Track)

Research Interests

Theoretical chemistry, Mixed Quantum-Classical Dynamics, Open Quantum System, ReaxFF

Parameterization, Computational Chemistry

Research Experience (Details available at zheliu17.github.io)

University of Alberta, Canada (*Advisor: Prof. Gabriel Hanna*)

Nov. 2019 – Present

- Simulate the Quantum Dynamics of the Excitonic Quantum Battery
- Mixed Quantum-Classical Liouville Dynamics in the Position Basis

RWTH Aachen University, Germany (*Advisor: Prof. Kai Leonhard*)

Sept. 2020 – Dec. 2020

- Reactive Force Field Parameterization for Phosgenation of Alcohols and Amines

University of Calgary, Calgary, Canada (*Advisor: Prof. Peter Kusalik*)

July 2018 – Oct. 2018

- Probing Reactions of the Hydroxyl Radical in Aqueous Environments

Dalian Institute of Chemical Physics, China (*Advisor: Prof. Hongjun Fan*)

June 2017 - June 2019

- Theoretical Studies on the Structures and Properties of TiO₂ Surface Adsorbed by Single Metal Atom
- Theoretical Studies on the Solvated Structures and Properties of Lithium Ions in Dimethyl Carbonate

Other Experience

Teaching Experience *Teaching Assistant*

CHEM 10X General Chemistry Experiments

Jan. 2020 – Apr. 2020

CHEM 303 Environmental Chemistry (*Instructor: Prof. Julianne M Gibbs*)

Sept. 2019 – Dec. 2019

AICHE Chem-E-Car Competition

Team member, (Advisor: Prof. Hongguang Dong and Prof. Qing Mao)

Feb. 2017 – Sept. 2017

- Designed and constructed of a car driven by chemical energy, which could safely deliver specified loads at specified distances and stops

Select Awards and Scholarships

RWTH Aachen – University of Alberta Junior Research Fellowship	2020
Globalink Graduate Fellowship, Mitacs	2019
Outstanding Graduates, Dalian University of Technology	2019
Mitacs - CSC (China Scholarship Council) scholarship	2018
Second Place of China Division in the Chem-E-Car Competition, Chemical Industry and Engineering Society of China	2017
DICP scholarship, Dalian Institute of Chemical Physics	2015 - 2016, 2016 - 2017

Software Skills

Computational Chemistry: AMS, VASP, p4vasp, VESTA, CPMD, VMD, Gaussian

Programming: C++, Python, Bash Shell Script, MATLAB, Fortran