Zhe Liu

https://zheliu17.github.io

Department of Chemistry, University of Alberta

Edmonton, Canada

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Education

M.Sc. in Chemistry

University of Alberta, Edmonton, 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 Experience (more details available at zheliu17.github.io)

University of Alberta, Canada *(Advisor: Prof. Gabriel Hanna)*   Sept. 2019 – Present

- Energy transport dynamics in an open 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, Canada *(Advisor: Prof. Peter Kusalik)*   July 2018 – Oct. 2018

- Probing hydroxyl radical reactions 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 single metal atom adsorbed TiO_2 (110) surface
- Theoretical studies on the solvated structures and properties of lithium ions in dimethyl carbonate

Research Internships

RWTH Aachen University, Germany, *Visiting Graduate Student*	Sept. 2020 – Dec. 2020
University of Calgary, Canada, *Research Intern (Mitacs Program)*	July 2018 – Oct. 2018
Dalian Institute of Chemical Physics, China, *Visiting Student*	June 2017 – June 2019

Other Experience

Teaching Assistantships

CHEM 10X General Chemistry	Jan. 2020 – Apr. 2020
CHEM 303 Environmental Chemistry	Sep. 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 a car driven by chemical energy, which could safely deliver specified loads at specified stops

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

Research Interests

- theoretical chemistry, computational chemistry, mixed quantum-classical dynamics, open quantum systems, ReaxFF parameterization