Weiren Zhao

Master of Engineering (M.Eng.)

SiChuan Province
ChengDu city
China
26 August 1999
13980339144
32227015@mail.dlut.edu.cn
zwr0.github.io/
ZWR0

In the convergence of machine learning and chemistry, you bridge the empirical with the abstract. Each hypothesis steps toward truth, each experiment paints knowledge. Forge ahead with courage and curiosity, transforming our universe's understanding.

Education

2022–2025 **Master Degree**, *Dalian university of technology*, Chemical Engineering, *GPA: 3.29*

2018–2022 **Bachelor Degree**, *Qingdao university of science and technology*, Applied Chemistry, *GPA: 3.10*

Master Research Areas

keywords *Machine Learning, Computational Chemistry.*

supervisors Yang Li

description Primarily involved in utilizing machine learning algorithms for catalyst design and reaction prediction, conducting research on the mechanism of transition metal catalysis, characterizing novel aromatic systems, and developing associated parameters.

Experience

Achievement

2022–2025 **University Level**, *Dalian University of Technology Third-Class Scholarship*

2020–2021 **University Level**, *the first semester*, Qingdao university of science and technology Moral Excellence Scholarship

2019–2020 **University Level**, *the second semester*, Qingdao university of science and technology Outstanding Literary and Artistic Scholarship

2019–2020 **University Level**, *the first semester*, Qingdao university of science and technology Third-Class Scholarship

2018–2019 **University Level**, *the second semester*, Qingdao university of science and technology Moral Excellence Scholarship

Languages

License CET-6 *550*

Language 1	Python	*Proficient*
Language 2	Windows Batch	*Moderate*
Language 3	Linux bash	*Moderate*
Language 4	TCL command	*Moderate*
Language 5	Latex	*Moderate*

Computer skills

category 1	Guassian	category 4	OpenBabel
category 2	Multiwfn	category 5	Vasp
category 3	VMD	category 6	Materials Studio

Skill matrix

Skill matrix

■□□□□ basic knowledge
■■□□□ intermediate knowledge with some project experience
■■■□□ extensive project experience
■■■■□ deepened expert knowledge
■■■■■ expert / specialist

	Level	Skill	Years	Comment
Language:	■■■■□	Python	3	*Proficient in using the Python language for data analysis (Pandas, NumPy, SciPy), scientific visualization (Seaborn, Matplotlib, Plotly), chemical description (RDKit, DGL, PyG), and model construction (PyTorch, scikit-learn, TensorFlow) tasks.*
	■■■□□	Windows Batch	2	*Capable of writing scripts that interface with Windows applications (such as Multiwfn, VMD, Gaussian, etc.) to perform batch processing for computational tasks, data analysis, and graphical plotting.*
	■■■□□	Linux	2	*Proficient in common command-line operations, with experience in submitting computational tasks.*
	■■■□□	Latex	2	*Experienced in using LaTeX code to create personal resume PDFs and typesetting mathematical equations.*
Software:	■■■□□	Guassian	3	*Gaussian: Skilled in building models using GView and performing computational tasks with Gaussian on Linux systems, primarily focusing on locating transition state structures for organic reactions.*

■■■□□	Multiwfn	3	*Proficient in computing various electronic and structural parameters for the analysis of molecular electronic and structural properties, and experienced in training neural network models using these computations*
■■■□□	VMD	2	*Skilled in rendering 3D visualizations of molecular structures, capable of customizing graphics and performing batch operations using TCL scripting in conjunction with VMD software.*
■■■□□	OpenBabel	2	*Skilled in batch converting various input and output files for further analysis through other software tools.*
■■□□□	Vasp	2	*Have undergone basic and intermediate training materials for VASP software usage within the group, possessing foundational experience in utilizing VASP.*
■■□□□	Materials Studio	2	*Capable of constructing simple periodic structure models of catalyst systems.*

Expected research direction

- Future plan

Combining ML model simulation with chemical materials experimentation to address design problems of property-oriented and function-oriented related compound materials. Utilizing pre-trained ML models and other generative models to discover and design target materials, followed by conducting relevant experiments myself for theoretical validation. I am enthusiastic about the future research direction, particularly the development and application of machine learning in the field of materials chemistry. I believe that working on future projects in the group will allow me to further deepen my understanding and application in this area.

Interests

hobby 1 Listen to songs and sing songs

hobby 2 Badminton

大连理工大学
DALIAN UNIVERSITY OF TECHNOLOGY