

Si Dawei

BROWN UNIVERSITY

Providence, RI

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Education

Brown University

SC.M. STUDENT IN COMPUTER SCIENCE

- Pursuing with fellowship from the Open Graduate Education Program.
- Taking the pathway in Computational Biology.

Providence, RI

Mar. 2020 - present

Brown University

PH.D. STUDENT IN CHEMISTRY

- Took courses in the first year:
 - Chemistry: Quantum Chemistry
 - Physics: Quantum Mechanics, Theoretical Mechanics, Statistical Mechanics
 - Applied Math: Computational Probability and Statistics, Recent Applications of Probability and Statistics
 - Computer Science: Interdisciplinary Scientific Visualization

Providence, RI

Sept. 2018 - present

Zhejiang University

BACHELOR OF SCIENCE IN CHEMISTRY (HONOURS)

- Got a First-class and a Second-class Scholarship for Elite Students in Basic Science. (2014, 2015)
- Got a Third-class Scholarship for Outstanding Students. (2014)
- GPA: 3.53/4.00
- Took additional courses from other departments such as physics, mathematics and computer science:
 - Methods of Mathematical Physics, Quantum Mechanics, Theoretical Mechanics, Thermodynamics and Statistical Mechanics, Electrodynamics, Computational Physics, Solid State Physics
 - Stochastic Process, Real Analysis, Abstract Algebra
 - Fundamentals of Data Structures, Advanced Data Structure and Algorithm Analysis, Parallel Algorithms, Database System
- Thesis: Parameterization of a New Force Field for Lithium Chelate-Based Ionic Liquids

Hangzhou, China

Sept. 2013 - Jun. 2018

Skills

Programming

Familiar with Julia, Python, Javascript, C/C++, C#, LLVM
Have some knowledge on Haskell, Rust, OpenMP, CUDA

Chemistry Software

Gromacs, PyMol, Gaussian, Amber, OpenBabel

Languages

Chinese (native language), English, Japanese (JLPT N1 qualified)

Tools

Vim, Git, Linux, WSL, JetBrains IDEs, LaTeX

Experience

Richard M. Stratt's Group, Brown University

PHD STUDENT

- Studying the inherent dynamics of polymers by potential energy landscapes and geodesic pathway methods.
- Studying the intrinsically disordered proteins.

Providence, RI

Sept. 2018 - PRESENT

Brenda M. Rubenstein's Group, Brown University

COLLABORATOR

- Developed a visualization approach for multispectral data in chemical space.

Providence, RI

Sept. 2018 - PRESENT

David Van der Spoel's Group, Uppsala University

GUEST STUDENT

- Developed a trajectory analysis tool for RNA structures in Gromacs.

Uppsala, Sweden

Sept. 2016 - Feb. 2017

The Julia Language

GSoC STUDENT

- Developed random number generators for the Julia language in Google Summer of Code 2016. Mentor: Simon Byrne.

Online

Apr. 2016 - Aug. 2016

Li Haoran's Group, Zhejiang University

UNDERGRADUATE RESEARCH ASSISTANT

- Studied the structures and electronic properties of several new ionic liquids that contain coordination metal ions by quantum chemistry methods.
- Attempted to develop a new force field or using QM/MD methods to study those ionic liquids in order to understand and predict their properties.

Hangzhou, China

Sept. 2013 - Jun. 2018

Publications

The Utility of Chemical Space for Molecular Information Storage

Dylan Sam, Xinhao Li, Phyo Phyo Kyaw Zin, Kevin Guo, Dawei Si, Denis Fourches and Brenda M. Rubenstein

The Journal of Chemical Information and Modeling

Preparing Submission

Structures and Electronic Properties of Lithium Chelate-Based Ionic Liquids

Dawei Si, Kexian Chen, Jia Yao and Haoran Li. *J. Phys. Chem. B*, 2016, 120, 3904 DOI: 10.1021/acs.jpcc.6b00731

The Journal of Physical Chemistry B

April 12th, 2016

Teaching

CHEM 1150: Statistical Mechanics and Thermodynamics

TEACHING ASSISTANT

- Did homework grading.

Providence, RI

Spring 2020

CHEM 0330L: Equilibrium, Rate, and Structure Lab, Brown University

TEACHING ASSISTANT

- Supervised two 16-student laboratory classes.
- Graded lab quizzes, reports, and exams.

Providence, RI

Fall 2019

Presentations

Julia in Practice

<https://github.com/JuliaCN/MeetUpMaterials/tree/master/Beijing2018/sunoru>

- Presented in *Julia Meetup @ Beijing*.
- Introduced the project done in GSoC 2016 and also introduced GSoC.
- Released the first version of the mirror server and client for Julia packages.

Beijing, China

July 29th, 2018

Projects

Visualization for Multispectral Chemical Space

<https://github.com/sunoru/VisChemSpace>

- Developing a pipeline to visualize spectral data like NMR and IR of thousands of molecules, to help understand them.

Sept. 2018 - PRESENT

Analysis Tool for RNA Structures

<https://gerrit.gromacs.org/#/c/3618/>

- Developed a tool in *Gromacs* that can analyze RNA PDB structures or RNA MD simulation trajectories.
- Refined the program to run better and more precisely than existing similar ones.
- Open-sourced the code using for generating the RNA database: <https://github.com/sunoru/rnaAnalysis>

Sept. 2016 - PRESENT

Computational Study for New Ionic Liquids

- Explored theoretically the conformations, electronic properties, and interaction energies of four chelate-based ionic liquids [Li(EA)][Tf₂N], [Li(HDA)][Tf₂N], [Li(DEA)][Tf₂N], and [Li(DOBA)][Tf₂N] using quantum mechanics methods.
- Attempted to refine a new force field for the ionic liquids. Failed in the conventional way and attempting QM/MD methods.

2014 - 2018

Contributions to Julia Community

<https://github.com/sunoru>

- Developed the package *RandomNumbers.jl* which includes several kinds of RNG families basically implemented in pure Julia. Will integrate one of the best RNGs to the Julia standard library.
- Developed the package *VSL.jl* which makes use of the Intel Vector Statistics Library to generate random numbers fast in Julia.
- Helping translate the documentations for the Julia Chinese community.
- Developed scripts for building a mirror site for Julia packages as well as its client *PkgMirrors.jl*.
- Maintaining the ZJU mirror for Julia.

2015 - PRESENT

Other Various Open-Source Projects

<https://github.com/sunoru>, <https://bitbucket.org/sunoru>

- Maintaining the website for *Pokemon Only in Shanghai*.
- Participating in open source projects like OpenBabel and SWIG.

2011 - PRESENT