# Dawei Si

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## Education

- **Brown University** — Providence, RI
  *PhD in Chemistry; Advisor: Richard Stratt* — *Sept. 2018 – Present*
- **Brown University** — Providence, RI
  *Master of Science in Computer Science (Computational Biology Pathway); GPA: 4.00/4.00* — *Mar. 2020 – May. 2023*
- **Zhejiang University** — Hangzhou, China
  *Bachelor of Science (Honours) in Chemistry; GPA: 3.53/4.00* — *Sept. 2013 – June 2018*

## Experience

- **Richard M. Stratt's Group, Brown University** — Providence, RI
  *Graduate Research Assistant* — *Sept. 2018 - Present*
  - **Geodesic Theory for Polymer Systems**: Studying the inherent dynamics of polymers by potential energy landscapes and geodesic pathway methods. Trying to apply this knowledge to better understand intrinsically disordered proteins.
- **Brenda M. Rubenstein's Group, Brown University** — Providence, RI
  *Collaborator* — *Sept. 2018 - Feb. 2019*
  - **Visualization for Chemical Multi-Spectral Space**: Designed & developed a visualization approach including chemical fingerprinting, similarity calculations, and graphing techniques for exploring the chemical space with multi-spectral (NMR, IR) data.
- **David van der Spoel's Group, Uppsala University** — Uppsala, Sweden
  *Guest Student* — *Sept. 2016 - Feb. 2017*
  - **RNA Analysis in Gromacs**: Developed a trajectory analysis tool in C++ that can find base pairs in RNA structures for Gromacs.
- **The Julia Language** — Online
  *GSoC Student* — *Apr. 2016 - Aug. 2016*
  - **RandomNumbers.jl, Random123.jl, VSL.jl** : Implemented random number generators for the Julia Language in **Google Summer of Code 2016**. Mentor: Simon Byrne
- **Li, Haoran's Group, Zhejiang University** — Hangzhou, China
  *Undergraduate Research Assistant* — *Sept. 2013 - June 2018*
  - **Quantum Chemistry for New Ionic Liquids**: Studied the structures and electronic properties of several new ionic liquids that contain coordination metal ions by quantum chemistry methods.
  - **MD Force Field Development**: Attempted to develop a new force field or use QM/MD methods to study those ionic liquids in order to understand and predict their properties.

## 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. J. Chem. Inf. Model, 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.jpcb.6b00731*

## Presentations

- **Julia in Practice**: Introduced projects done in GSoC 2016 and the package mirror project at *Julia Meetup @ Beijing 2017*

## Skills Summary

- **Programming Languages**: Highly proficient in **Julia**, **TypeScript**, **Python**, **C/C++**; Familiar with CUDA, Rust, Go, MatLab, Haskell, Lean, C#
- **Tools & Platforms**: TensorFlow, Flux.jl, Git, Docker, NodeJS, Deno, LLVM, AWS, GCP
- **Simulation & Modeling**: Gromacs, PyMol, Gaussian and many homemade tools
- **Web Frameworks**: Vue, Quasar, React, Django, Koa, NestJS
- **Languages**: Mandarin Chinese (Native), English (Professional), Japanese (JLPT N1 qualified)

## Teaching

- **CHEM 0330L Equilibrium, Rate, and Structure Lab**: Fall 2019, Summer 2021, Fall 2022, Spring 2023, Fall 2023. Supervised two 16-student laboratory sections each semester. Graded lab quizzes, reports, and exams.
- **CHEM 1150 Statistical Mechanics and Thermodynamics**: Spring 2020, Spring 2024. Worked as a teaching assistant.

## Projects

- **MosimoBase.jl, MosimoMD.jl, SmartMonteCarlo.jl, GeodesicPathways.jl** : Packages for simulating molecular systems in Julia. Methods include Molecular Dynamics, Smart Monte Carlo, and Geodesic calculations.
- **The Julia Community**: Helping translate the documentation for the Julia Chinese community. Developed scripts for building a mirror site for Julia packages as well as its client PkgMirrors.jl. Maintained the ZJU mirror for Julia. Contributing to many packages such as RandomNumbers.jl, NodeCall.jl, Webviews.jl, AESNI.jl.
- **IDPSequences.jl**: Multiple Sequence Alignment for Intrinsically Disordered Proteins.
- **Xtructure**: Deep learning of X-ray scattering signals to predict molecular structures.
- **Seer.jl**: Discover charge density functionals with artificial neural networks.
- **More**: Please refer to the full table on GitHub (**44** public projects, since **2012**). I am very enthusiastic and also participate in open-source projects created by others. Moreover, there are also a lot of private projects that I have participated in to improve the skills listed above.