Juncheng (Harry) Zhang

zhar@stanford.edu
orcid.org/0000-0002-2790-8567
Google Scholar

EDUCATION

Stanford University (09/2023 –)
Theoretical Chemistry, Ph.D.

- Research Assistant at **Todd Martinez Group** (09/2023 –)
  Theoretical, physical, and computational chemistry

Indiana University Bloomington (08/2018 – 05/2022)
Chemistry, B.S.
Minors: Computational Linguistics, Math, Physics

- Undergraduate Researcher at **Srinivasan Iyengar Group** (05/2019 – 05/2022)
  Theoretical, physical, and computational chemistry
  - Created and maintained the group's molecular fragmentation calculation toolkit
  - Molecular fragmentation for electronic structure calculation
    - Studying the effect of higher order interactions
    - Exploring the method's applications in electronic structure calculation
- Undergraduate Researcher at **Francis Tyers Group** (02/2019 – 11/2019)
  Computational linguistics
  - Build a text-to-speech model for low-resource language (with < 2 hours speech data)
    - Adpated DeepSpeech for RNN transfer learning training

WORK

SLAC National Accelerator Laboratory (06/2022 - 04/2023)
Stanford PULSE Institute

- Intern Student / Research Assistant at **Todd Martínez Group** (06/2022 – 04/2023)
  Theoretical, physical, and computational chemistry
  - Tree tensor network quantum simulator
    - Developed interface to Qiskit for applications, such as variantional quantum eigensolver (VQE)
  - Major contributor to TeraChem, a commercial GPU-accelerated electronic structure software
    - Reformulated and accerlerated two-electron integrals implementation
    - Maintained continuous integration and benchmark suite
  - Molecular fragmentation for electronic structure calculation

PUBLICATION

- **J. H. Zhang** and S. S. Iyengar.
  Graph-$|Q\rangle\langle C|$: A Graph-based Quantum-classical algorithm for efficient electronic structure on hybrid quantum/classical hardware systems: Improved quantum circuit depth performance
  Journal of Chemical Theory and Computation (2022)
  doi: 10.1021/acs.jctc.1c01303

  Summary: Propose a way to apply the graph-theoretic molecular fragmentation method to electronic structure calculation on quantum circuit.

- **J. H. Zhang**, T. C. Ricard, C. Haycraft and S. S. Iyengar.
  Weighted Graph-theoretic methods for many-body corrections within ONIOM: smooth AIMD and the role of high order many-body terms
  Journal of Chemical Theory and Computation (2021)
  doi: 10.1021/acs.jctc.0c01287

  Summary: Study the effect of higher order interactions in the graph-theoretic molecular fragmentation method, and propose a way to apply the fragmentation method to do molecular dynamics simulation.

SKILLS

- Languages: Mandarin (native), English (fluent), Cantonese (fluent)
- Programming languages: Python, Go, Rust, C++
- Data analysis (NumPy, SciPy, Pandas, Matplotlib, Seaborn)