JIACE SUN

email: jsun3@caltech.edu
personal website github page google scholar

EDUCATION

University of Science and Technology of China (USTC) Sep 2015 - Jun 2019
B.S., School of the Gifted Young
Major: Theoretical physics **GPA: 3.96/4.30**

California Institute of Technology (Caltech) Oct 2019 -
Division of Chemistry and Chemical Engineering
Advisor: Prof. Thomas F. Miller III Oct 2019 - Jan 2022
Prof. Austin J. Minnich Feb 2022 -

RESEARCH INTERESTS

- Quantum chemistry (electronic structure & quantum dynamics)
- Quantum computing algorithms and quantum simulation
- Machine learning for quantum chemistry and quantum computing

RESEARCH PROJECTS

Quantum computing and quantum simulation

Stabilizer ground states: theory, algorithms and applications Mar 2023 - Mar 2024

- Introduced the concept of stabilizer ground states to quantum many-body problems
- Presented a theoretical formalism of stabilizer ground states for general Pauli Hamiltonians
- Developed an exact and linear-scaled algorithm to find the stabilizer ground state for 1D local Hamiltonians
- Extended the theoretical formalism and the 1D local algorithm to infinite periodic Hamiltonians
- Numerically verified the scalability and efficiency of different Hamiltonians
- Demonstrated the applications of stabilizer ground states and the corresponding algorithms on improving variational quantum eigenvalues algorithms, qualitative understanding of phase transitions, and cornerstones of more advanced ground state ansatzes

Experimental demonstration of measurement-induced phase transitions (MIPT) Jan 2023 - Mar 2024

- Developed a circuit compression algorithm for Clifford circuit and non-Clifford input
- Applied the circuit compression to the linear cross-entropy benchmarking of MIPT and achieved a clear experimental MIPT signal with up to 22 qubits.

Development of Clifford-based Hamiltonian transformation for variational quantum eigenvalue (VQE) in chemical problems Jan 2023 - Mar 2024

- Derived a scalable method to compute the initial energy gradients of a given quantum circuit ansatz
- Developed a polynomial-scaled and optimization-free approach to appropriately find the Clifford transformation that maximizes the initial gradients given an arbitrary hardware-efficiently ansatz as input
- Verified significant performance improvements on a series of chemical systems
- Achieved chemical accuracy for systems as large as 12 qubits with fewer than 30 two-qubit gates

Implementation of tensor network simulations in *tensorcircuit* Jun 2021 - Dec 2021

- Implemented a matrix-produce-state (MPS) simulator for quantum circuits with just-in-time (JIT) compilation and automatic differentiation support

Electronic structure and quantum dynamics

Study of two-phonon scattering in electron transport of GaAs Jan 2022 - Dec 2022

- Implemented the on-shell two-phonon treatment of electron-phonon interaction and applied to calculation of transport and noise in GaAs
- Developed a semi-analytical model for the full two-phonon contributions to the electron-phonon interaction
- Applied the semi-analytical model to GaAs and analyze the source of difference with experiments
- Estimated the contribution of electron-two-phonon scattering in GaAs and analyzed the relationship with the experimental observations

Theory development of path integral molecular dynamics Oct 2019 - May 2020

- Introduced a generalized class of strongly stable and dimension-free thermostatted ring-polymer molecular dynamics integrators
- Analytically study in terms of integrators based on equilibrium state accuracy and convergence rate
- Derived the superiority of the "BCOCB" and benchmarked by liquid water simulation.

Embedding method for regulation of graphene nanoribbon electronic structure Sep 2017 - Jan 2019

- Developed an embedded density functional theory (DFT) method named dopant central insertion scheme for doped graphene nanoribbon (GNR)
- Revealed oscillation phenomenon of density of states (DOS) modulated by long-range interactions of dopants
- Developed a quantum-based theoretical toy-model for the oscillations
- Developed a proof-of-principle protocol prescribing on-demand GNR-DOS regulation

Machine learning for quantum chemistry

Machine-learned sum-of-products potential energy surfaces (PES) for density matrix renormalization group (DMRG) simulations Jul 2023 - Jan 2024

- Developed a Gaussian Process Regression (GPR) based machine learning algorithm that generates PES in the sum-of-product form
- Designed a novel kernel in GPR to achieve point group symmetry and size consistency of the PES
- Introduced a self-consistent process of DMRG calculations and GPR training to enhance the PES accuracy
- Achieved accurate excitation energies for HONO and accurate vibrational spectrum for water dimer

Development of molecular-orbital-based machine learning (MOB-ML) June 2020 - Dec 2021

- Developed an improved feature design of MOB-ML and achieved great accuracy improvement
- Benchmarked the improved feature design on reactions and molecular interactions
- Developed the alternative black-box matrix-matrix multiplication (AltBBMM) algorithm to scale up the MOB-ML training and achieved 4x speedup without accuracy loss
- Implemented the interface between MOB-ML prediction and quantum dynamics simulation
- Designed a classical algorithm of molecular-orbital classification for comparison with the classification of MOB-ML through unsupervised learning
- Developed a rotational equivariant derivative formalism for MOB-ML to learn response properties
- Benchmarked the learning of response properties and achieved state-of-the-art accuracy on both energy and dipole moment learning
- Developed the additive kernel method for MOB-ML and extended it to open-shell and multireference systems.

PUBLICATIONS

1. (preparing) **Sun, J.**, Ren, J, etc. (2024). Machine-learned sum-of-products potential energy surfaces for density matrix renormalization group simulations of molecular quantum dynamics.
2. **Sun, J.**, Cheng, L. & Zhang, S.-X. (2024). Stabilizer ground states: theory, algorithms and applications. arXiv preprint arXiv:2403.08441. (Note: First author and corresponding author) [link]
3. Kamakari, H., **Sun, J.**, Li, Y., Thio, J. J., Gujarati, T. P., Fisher, M., Motta, M. & Minnich, A. J. (2024). Experimental demonstration of scalable cross-entropy benchmarking to detect measurement-induced phase transitions on a superconducting quantum processor. arXiv preprint arXiv:2403.00938. [link]
4. **Sun, J.**, Cheng, L. & Li, W. (2024). Towards chemical accuracy with shallow quantum circuits: A Clifford-based Hamiltonian engineering approach. Journal of Chemical Theory and Computation. [link]
5. **Sun, J.** & Minnich, A. J. (2023). Transport and noise of hot electrons in GaAs using a semi-analytical model of two-phonon polar optical phonon scattering. Physical Review B 107, 205201. [link]
6. Zhang, S.X., Allcock, J., Wan, Z.Q., Liu, S., **Sun, J.**, Yu, H., Yang, X.H., Qiu, J., Ye, Z., Chen, Y.Q. & Lee, C.K. (2023). TensorCircuit: a quantum software framework for the NISQ era. Quantum, 7, 912. [link]
7. Cheng, L., **Sun, J.**, Emiliano Deustua, J., Bhethanabotla, V. C. & Miller III, T. F. (2022). Molecular-orbital-based machine learning for open-shell and multi-reference systems with kernel addition Gaussian process regression. The Journal of Chemical Physics, 157, 154105. [link]
8. **Sun, J.**, Cheng, L., & Miller III, T. F. (2022). Molecular dipole moment learning via rotationally equivariant Gaussian process regression with derivatives in molecular-orbital-based machine learning. The Journal of Chemical Physics, 157, 104109. [link]
9. Cheng, L., **Sun, J.** & Miller III, T.F. (2022). Accurate molecular-orbital-based machine learning energies via unsupervised clustering of chemical space. Journal of Chemical Theory and Computation, 18, 8, 4826–4835. [link]
10. Lu, F., Cheng, L., DiRisio, R.J., Finney, J.M., Boyer, M.A., Moonkaen, P., **Sun, J.**, Lee, S.J., Deustua, J.E., Miller III, T.F. & McCoy, A.B. (2022). Fast near ab initio potential energy surfaces using machine learning. The Journal of Physical Chemistry A, 126(25), 4013-4024. [link]
11. Cheng, P. S., **Sun, J.**, Sun, S. N., Choi, A. Y., & Minnich, A. J. (2022). High-field transport and hot electron noise in GaAs from first principles: role of two-phonon scattering. Physical Review B, 106, 245201. [link]

12. Gui, X., Fan, W., **Sun, J.**, & Li, Y. (2022). New stable and fast ring-polymer molecular dynamics for calculating bimolecular rate coefficients with example of OH+CH4. Journal of Chemical Theory and Computation, 18, 9, 5203–5212. [link]
13. **Sun, J.**, Cheng, L., & Miller III, T. F. (2021). Molecular energy learning using alternative blackbox matrix-matrix multiplication algorithm for exact Gaussian process. NeurIPS 2021 AI for Science Workshop. [link]
14. Husch, T., **Sun, J.**, Cheng, L., Lee, S. J., & Miller III, T. F. (2021). Improved accuracy and transferability of molecular-orbital-based machine learning: Organics, transition-metal complexes, non-covalent interactions, and transition states. The Journal of Chemical Physics, 154, 064108. [link]
15. Rosa-Raíces, J. L.*, **Sun, J.***, Bou-Rabee, N., & Miller III, T. F. (2021). A generalized class of strongly stable and dimension-free T-RPMD integrators. The Journal of chemical physics, 154, 024106. [link]
16. **Sun, J.***, Feng, S.*, Wang, X., Zhang, G., Luo, Y., & Jiang, J. (2020). Regulation of electronic structure of graphene nanoribbon by tuning long-range dopant–dopant coupling at distance of tens of nanometers. The Journal of Physical Chemistry Letters, 11(16), 6907-6913. [link]

SOFTWARE DEVELOPMENT

- *Chronus Quantum*: High-performance computational chemistry software with a strong emphasis on explicitly time-dependent and post-SCF quantum mechanical methods

  My contribution: Realtime dynamics of polarizable continuum model
- *Q-Chem*: A general-purpose electronic structure software

  My contribution: Electron affinity algebraic diagrammatic construction (EA-ADC) theory
- *TensorCircuit*: Next generation of quantum circuit simulators

  My contribution: Matrix-product-state (MPS) simulator
- *MathTranslate* (owner & key developer): Efficient translator of latex document & web server to directly translate arxiv papers. **Currently got 900+ stars on github**.

HONOR&AWARDS

- **Hongyan Scholarship**, **$45000 in 4 years** (29 scholarships awarded in USTC that year) 2019
- **National Second Prize**, China Undergraduate Mathematical Contest in Modeling 2017
- **First Place**, qualification of China Undergraduate Physics Tournament (CUPT) in USTC 2017
- **National Scholarship**, (**Top 1%, Highest honor for sophomore**) 2016

INVITED TALKS

1. "Towards chemical accuracy with shallow quantum circuits: A Clifford-based Hamiltonian engineering approach"; University of Science and Technology of China; Invited by Jun Jiang; Mar 12, 2024
2. "Enhancing quantum system simulation with Clifford-based hybrid quantum algorithms"; Shanghai Jiao Tong University; Invited by Lei Zhang; Mar 19, 2024