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 sciences: Quantum chemistry (electronic structure & quantum dynamics)
Quantum simulation
Computer sciences: AI for science
Software developments

RESEARCH PROJECTS

Method development for regulation of graphene nanoribbon electronic structure
University of Science and Technology of China Sep 2017 - Jan 2019
Advisor: Prof. Jun Jiang

- Developed an embedded density functional theory (DFT) method named dopant central insertion scheme for dopped graphene nanoribbon (GNR)
- Revealed wave-like oscillations 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

Development of many-body electronic structure method
Heidelberg University Feb 2019 - Apr 2019
Advisor: Prof. Andreas Dreuw

- Implemented electron affinity-algebraic diagrammatic construction (EA-ADC) theory in the *Q-Chem* software
- Benchmarked the theory on a set of molecules

Theory development of path integral molecular dynamics

California Institute of Technology Oct 2019 - May 2020

Advisor: Prof. Thomas F. Miller III

- Developed a generalized class of strongly stable and dimension-free thermostatted ring-polymer molecular dynamics (T-RPMD) integrators
- Analyzed the integrators on the basis of convergence to equilibrium and efficiency at evaluating equilibrium expectation values
- Confirmed that the BCOCB-type integrator is superior over all other integrators

Development of molecular-orbital-based machine learning (MOB-ML)

California Institute of Technology June 2020 - Dec 2021

Advisor: Prof. Thomas F. Miller III

- Developed an improved feature design of MOB-ML and achieved great accuracy improvement
- Benchmarked the improved feature design on machine learn reactions and molecular interactions
- Developed the alternative blackbox matrix-matrix multiplication (AltBBMM) algorithm to scale up the MOB-ML training
- Benchmarked the AltBBMM algorithm and achieved 4x speedup compared with the original algorithm 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
- Implemented the local MP2 dipole moment calculation for label generation of response properties.
- Benchmarked the learning of response properties and achieve the 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.

Study of two-phonon scattering in electron transport of GaAs

California Institute of Technology Jan 2022 - Dec 2022

Advisor: Prof. Austin J. Minnich

- Implemented the on-shell two-phonon treatment of electron-phonon interaction and apply 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

PUBLICATIONS

1. (Will be on arXiv soon) **Sun, J.**, Minnich, A. J. (2022). Transport and noise of of hot electrons in GaAs using an ab-initio-based analytical model of two-phonon polar optical phonon scattering.
2. 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]
3. **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]
4. 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]
5. 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]
6. 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]
7. 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]
8. 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. (2022). TensorCircuit: a quantum software framework for the NISQ era. arXiv preprint arXiv:2205.10091. [link]
9. **Sun, J.**, Cheng, L., & Miller III, T. F. (2021). Molecular energy learning using alternative blackbox matrix-matrix multiplication algorithm for exact Gaussian process. arXiv preprint arXiv:2109.09817. [link]
10. 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]

11. 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]
12. **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* (key developer): Next generation of quantum circuit simulators

  My contribution: Matrix-product-state (MPS) simulator

HONOR&AWARDS

- **Hongyan Scholarship**, **$45000 in 4 years** (29 scholarships awarded in USTC that year) 2019
- **Honorable Mention**, The Interdisciplinary Contest in Modeling 2017
- **National Second Prize**, China Undergraduate Mathematical Contest in Modeling 2017
- **Grade 1**, Outstanding Student Scholarship (**Top 5%**) 2017
- **First Place**, qualification of China Undergraduate Physics Tournament (CUPT) in USTC 2017
- **National Scholarship**, (**Top 1%, Highest honor for sophomore**) 2016