JIACE SUN

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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 computing
Computer sciences: AI for science
Software developments

RESEARCH EXPERIENCE

University of Science and Technology of China (Undergraduate) Sep 2017 - Jan 2019
Prof. Jun Jiang's group: Embedded DFT method for materials
- Developed the dopant central insertion scheme (DCIS) method and studied the regulation of electronic structure of graphene nanoribbon. Related publication: [pdf].

University of Washington (Visiting student) Jul 2018 - Sep 2018
Prof. Xiaosong Li's group: Solvation model
- Implemented real-time dynamics of polarizable continuum model in the *Chronus Quantum* software

Heidelberg University (Visiting student) Feb 2019 - Apr 2019
Prof. Andreas Dreuw's group: Many-body electronic structure theory
- Implemented electron affinity-algebraic diagrammatic construction (EA-ADC) theory in the *Q-Chem* software

California Institute of Technology (PhD student) Oct 2019 -

Prof. Thomas F. Miller III's group: Quantum dynamics & ML for electronic structure

- Developed and analyzed a generalized class of strongly stable and dimension-free thermostatted ring-polymer molecular dynamics (T-RPMD) integrators. Related publication: [pdf].
- Developed an improved feature design of molecular orbital-based machine learning (MOB-ML). Related publication: [pdf].
- Developed the alternative blackbox matrix-matrix multiplication (AltBBMM) algorithm to scale up the MOB-ML training. Related publication: [pdf].
- Developed a rotational-equivariant derivative kernel for MOB-ML to learn response properties. Related publication: [pdf]
- Developed the additive kernel methods for MOB-ML and extend it to open-shell and multi-reference systems. Related publication: [pdf].

Prof. Austin J. Minnich's group: Transport in semiconductors

- Implemented the on-shell two-phonon treatment of electron-phonon interaction and applied to calculation of transport and noise in GaAs. Related publication: [pdf].
- Developed a semi-analytical model for the full two-phonon contributions to the electron-phonon interaction and analyzed the disagreement with experiments. Related publication: will be on arXiv soon.

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. [pdf] 104109.
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. [pdf]
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. [pdf]
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. [pdf]

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. [pdf]

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. [pdf]

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. [pdf]

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. [pdf]

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. [pdf]

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. [pdf]

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. [pdf]

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