Chong Sun

Mobile: +1 (609) 955-8164
Email: chong.sun@rice.edu
Homepage Google Scholar Github

Education

Peking University **Beijing, China**
B.S. in Chemistry *2011 - 2015*
Thesis: Density matrix embedding theory in terms of localized molecular orbitals.

Princeton University **Princeton, NJ**
Centennial Fellowship Graduate Student *2015 - 2016*

California Institute of Technology **Pasadena, CA**
Ph.D. in Theoretical Chemistry *2016 - 2021*
Advisor: Garnet Kin-Lic Chan
Thesis: Finite-temperature simulations of strongly correlated systems.

Appointments

- Visiting Researcher, Microsoft Azure Quantum — Apr. 2024 - Now
- Postdoctoral Researcher, Rice University — May. 2023 - Now
- Research Scientist, Zapata Computing Inc. — Nov. 2022 - Jan. 2023
- Postdoctoral Researcher, University of Toronto — Feb. 2021 - Oct. 2022
- Lecturer, University of Toronto — Jan. 2022 - Jun. 2022

Awards & Honors

- Chair's Poster Award, American Conference on Theoretical Chemistry (ACTC), 2024
- Barbara J. Burger Fellowship, 2019
- CCE Teaching (TA) Award, Caltech, 2018
- Centennial Fellowship in the Natural Science and Engineering, 2015
- Chun-Tsung Scholarship, 2014
- Merit Student, Peking University 2014
- Pan Gu Fellowship, 2013
- First Prize in the 29th National Undergraduate Physics Contest, 2012

Invited Talks

- Study of strongly correlated materials with density matrix embedding theory. *ICT-HPCC22, Beijing 2022*
- Density matrix embedding theory and quantum imaginary time evolution. *ByteDance, Beijing, 2021*
- Quantum imaginary time evolution. *QIP, Shenzhen, 2020*

Services

- Peer reviewer for Nature Physics, Physical Review A, Physical Review B, Physical Review Research, PRX Quantum, Quantum, and the Journal of Physical Chemistry Letter.
- Active contributor to the open-source quantum chemistry packages PySCF and Block2.

Publications & Preprints

1. C. Sun, F. Gao and G. E. Scuseria, Selected non-orthogonal configuration interaction with compressed single and double excitations. *J. Chem. Theory Comput.* **20**, 9, 3741–3748 (2024)
2. K. Gratsea, C. Sun, P. Johnson. When to Reject a Ground-State Preparation Algorithm. *Phys. Rev. A* **109** (4), 042425 (2024)
3. C. Sun, Electron localization in disordered quantum systems at finite temperatures. Pre-print: arXiv:2403.16868 (2024)
4. H. Zhai, H. R. Larsson, S. Lee, Z.-H. Cui, T. Zhu, C. Sun, et. al., Block2: A comprehensive open source framework to develop and apply state-of-the-art DMRG algorithms in electronic structure and beyond. *J. Chem. Phys.* **159**, 234801 (2023)
5. T. H. Kyaw, M. B. Soley, B. Allen, P. Bergold, C. Sun, V. S. Batista and A. Aspuru-Guzik, Boosting quantum amplitude exponentially in variational quantum algorithms. *Quantum Sci. Technol.* **9** 01LT01 (2023)
6. M. Krenn *et. al.* SELFIES and the future of molecular string representations. *Patterns*, **3**, 100588 (2022)
7. F. Ren *et. al.* AlphaFold accelerates artificial intelligence powered drug discovery: efficient discovery of a novel CDK20 small molecule inhibitor. *Chem. Sci.*, **14**, 1443 (2023)
8. L. Thiede[†], C. Sun[†], A. Aspuru-Guzik. Waveflow: Enforcing boundary conditions in smooth normalizing flows with application to fermionic wave functions. Pre-print: arXiv:2211.14839 (2022)
9. C. Sun, Finite Temperature Simulations of Strongly Correlated Systems. *Dissertation* (*Ph.D.*), *California Institute of Technology.* doi:10.7907/dchn-p020 (2021)
10. C. Sun, U. Ray, Z.-H. Cui, M. Stoudenmire, M. Ferrero and G. K. Chan. Finite temperature density matrix embedding theory. *Phys. Rev. B*, **101**, 075131 (2020)
11. M. Motta, C. Sun, A. T. K. Tan, M. J. O' Rourke, E. Ye, A. J. Minnich, F. G. S. L. Brandao, G. K. Chan. Determining eigenstates and thermal states on a quantum computer using quantum imaginary time evolution. *Nature Physics*, **16**, 205 (2020)
12. Z.-H. Cui, C. Sun, U. Ray, B.-X. Zheng, Q. Sun, G. K. Chan, Ground-state phase diagram of the three-band Hubbard model in various parametrizations from density matrix embedding theory. *Phys. Rev. Research*, **2**, 043259 (2020)
13. Q. Sun *et. al.*, Recent developments in the PySCF program package. *J. Chem. Phys.* **153**, 024109 (2020)
14. H.-Z. Ye[†], C. Sun[†] and H. Jiang. Monte-Carlo Simulation of Spin-Crossover Phenomena Based on a Vibronic Ising-like Model with Realistic Parameters. *Phys. Chem. Chem. Phys.*, **17**, 6801 (2015)

[†] equal contribution.