Chong Sun

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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 Research *Apr. 2024 - Present*
- Developing numerical frameworks to solve industrial chemistry problems.

Postdoctoral Researcher, Rice University *May. 2023 - Present*
Supervisor: Dr. Gustavo E. Scuseria
- Developing state-of-the-art quantum chemistry algorithms for strongly correlated systems.

Research Scientist, Zapata Computing Inc. *Nov. 2022 - Jan. 2023*
- Developed quantum algorithms and software for ground-state energy estimation and quantum resource estimation.

Postdoctoral Researcher, University of Toronto *Feb. 2021 - Oct. 2022*
Supervisor: Dr. Alán Aspuru-Guzik
- Conducted interdisciplinary research involving quantum chemistry, quantum computing, and artificial intelligence.

Lecturer, University of Toronto *Jan. 2022 - Jun. 2022*
- CHM427-CHM1480 Statistical Mechanics.

Awards & Honors

- Barbara J. Burger Fellowship *Caltech, 2019*
- CCE Teaching (TA) Award *Caltech, 2018*
- Centennial Fellowship in the Natural Science and Engineering *Princeton University, 2015*
- Chun-Tsung Scholarship *Peking University, 2014*
- Merit Student *Peking University, 2014*
- Pan Gu Fellowship *Peking University, 2013*
- First Prize in the 29th National Undergraduate Physics Contest *Beijing, 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*
- Quantum computing for quantum chemistry. *Peking University, Beijing, 2020*

Publications & Preprints

1. C. Sun, F. Gao and G. E. Scuseria, Selected non-orthogonal configuration interaction with compressed single and double excitations. Pre-print: arXiv:2403.02350. Submitted to *J. Chem. Theory Comput.* (2024)
2. C. Sun, Electron localization in disordered quantum systems at finite temperatures. Pre-print: arXiv:2403.16868 (2024)
3. 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)
4. 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)
5. M. Krenn *et. al.* SELFIES and the future of molecular string representations. *Patterns*, **3**, 100588 (2022)
6. K. Gratsea, C. Sun, P. Johnson. When to Reject a Ground-State Preparation Algorithm. Pre-print: arXiv:2212.09492. Accepted by *Phys. Rev. A*. (2023)
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
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.