Chong Sun

chong.sun@rice.edu +1 (609) 955-8164
v-chongsun@microsoft.com https://sunchong137.github.io

Education

Ph.D., California Institute of Technology 2016-2021
Advisor: Garnet Kin-Lic Chan (*Division of Chemistry and Chemical Engineering*)
Dissertation: *Finite-temperature simulations of strongly correlated systems.*

B.S. in Chemistry, Peking University 2011-2015
Graduated with honors.
Thesis: *Density Matrix Embedding Theory in Terms of Localized Orbitals*

Graduate Fellow, Princeton University 2015-2016
Recipient of Centennial Fellowship.

Special Student, Massachusetts Institute of Technology 2013
Sponsored by Peking University, 2/152.

Research & Work Experience

Research Scientist, Microsoft Quantum 2024 - Present
Postdoctoral Researcher, Rice University 2023 - Present
Research Scientist, Zapata Computing Inc. 2022-2023
Lecturer, University of Toronto 2022
Postdoctoral Researcher, University of Toronto 2021-2022

Honors & Awards

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

Teaching Experience

Lecturer, CHM427H1S Statistical Mechanics, University of Toronto (Spring 2021-2022)
Lecture notes can be found via this link.

Teaching Assistant, CH125b The Elements of Quantum Chemistry, Caltech (Winter 2017-2018)
Won the 2018 CCE Teaching Award.

Teaching Assistant, CH21b Physical Chemistry (B), Caltech (Winter 2016-2017)

Teaching Assistant, CH125a Quantum Mechanics (A), Caltech (Fall 2016-2017)

Mentoring

Alikaterini Gratsea (Zapata Computing Inc., 2022-2023), Romi Lifshitz (University of Toronto, 2021-2022), Shu Fay Ung (Caltech, 2018-2019), Sherry Liang (Caltech WMW, 2016-2017)

Professional Services

Journal Reviewer

Nature Physics, Physical Review A, Physical Review B, Physical Review Research, PRX Quantum, Quantum, Journal of Physical Chemistry Letter, Quantum Science and Technology

Conference Volunteer

Session Chair for APS March Meeting (2024), Student Volunteer for NSF Enabling Quantum Leap Workshop (2019), Session Chair for Caltech CGSC Summar Seminar (2017), Session Chair for Caltech SURF Seminar (2016)

Publications

[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**, and P. Johnson. When to Reject a Ground-State Preparation Algorithm. *Phys. Rev. A* **109** (4), 042425 (2024)

[3] H. Zhai, H. R. Larsson, S. Lee, Z.-H. Cui, T. Zhu, **C. Sun**, L. Peng, R. Peng, K. Liao, J. Tölle, J. Yang, S. Li, and G. K. Chan. 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] 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)

[6] M. Krenn *et. al.* (alphabetical order) SELFIES and the future of molecular string representations. *Patterns*, **3**, 100588 (2022)

[7] **C. Sun**. Finite Temperature Simulations of Strongly Correlated Systems. *Dissertation (Ph.D.), California Institute of Technology.* doi:10.7907/dchn-p020 (2021)

[8] **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)

[9] M. Motta, **C. Sun**, A. T. K. Tan, M. J. O' Rourke, E. Ye, A. J. Minnich, F. G. S. L. Brandao and G. K. Chan. Determining eigenstates and thermal states on a quantum computer using quantum imaginary time evolution. *Nature Physics*, **16**, 205 (2020) *Presented in the 23rd Annual Conference on Quantum Information Processing (QIP), 2020*.

[10] Z.-H. Cui, **C. Sun**, U. Ray, B.-X. Zheng, Q. Sun and 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)

[11] Q. Sun *et. al.* Recent developments in the PySCF program package. *J. Chem. Phys.* **153**, 024109 (2020)

[12] H.-Z. Ye†, **C. Sun**† (**co-first author**) 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)

Preprints

[1] L. Thiede†, **C. Sun**† (**co-first author**) and A. Aspuru-Guzik. Waveflow: boundary-conditioned normalizing flows applied to fermionic wavefunctions. Pre-print: arXiv:2211.14839 (2024) *Invited submission to APL Machine Learning, under review*

[2] **C. Sun**. Electron localization in disordered quantum systems at finite temperatures. Pre-print: arXiv:2403.16868 (2024) *Submitted to Phys. Rev. B, under review*

Talks

[1] "Neural networks as a quantum chemistry ansatz: a chemist's view", Invited Talk at the University of Washington, Aug. 2024

[2] "Study of many-body localization with complex polarization", Contributed Talk at APS March Meeting, Mar. 2024

[3] "A Chemist's View of Quantum Computing", Invited Talk at Tulane University, Nov. 2023

[4] "Numerical Solutions to Large Eigenvalue Problems in Chemistry", Invited Talk at Lawrence Berkeley National Laboratory (LBNL), Mar. 2023

[5] "Study of strongly correlated materials with density matrix embedding theory." Invited Talk at the 15th International Conference on Theoretical and High-Performance Computational Chemistry (ICT-HPCC22), Jul. 2022

[6] "Density matrix embedding theory and quantum imaginary time evolution." Invited Talk at ByteDance, Aug. 2021

[7] "Solving Chemistry Problems with Quantum Computers", Student Talk at Caltech CCE Seminar Day, Nov. 2020

[8] Quantum algorithms for quantum chemistry simulations. Invited Talk at Peking University, Jan. 2020

[9] "Quantum imaginary time evolution." Contributed Talk at the 23rd Annual Conference on Quantum Information Processing (QIP), Jan. 2020

[10] "Finite-Temperature Density Matrix Embedding Theory", Invited Student Talk at Simons Many-Electron Collaboration Summer School, Jun. 2019

[11] "Finite-Temperature Density Matrix Embedding Theory", Contributed Talk at APS March Meeting, Mar. 2017

Open-Source Scientific Packages

[1] SNOCISD (Author): https://github.com/sunchong137/snocisd
Non-orthogonal configuration interaction (NOCI) with single and double excitations, with GPU compatibility.

[2] Waveflow (Co-Author): https://github.com/aspuru-guzik-group/waveflow
Normalizing flows for fermionic wavefunctions, with GPU compatibility.

[3] PySCF (Contributor): https://github.com/pyscf/pyscf
One of the most popular quantum chemistry packages.

[4] Block2 (Contributor) : https://github.com/block-hczhai/block2-preview
Density matrix renormalization group (DMRG) for both spin an fermionic systems.

[5] libdmet (Contributor): https://github.com/gkclab/libdmet_preview
Density matrix embedding theory (DMET) that can handle periodic *ab initio* systems.