Chong Sun

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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
Advisor: Gustavo E. Scuseria

Research Scientist, Zapata Computing Inc. 2022-2023

Lecturer, University of Toronto 2022

Postdoctoral Researcher, University of Toronto 2021-2022
Advisor: Alán Aspuru-Guzik

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, 2022
Lecture notes can be found on my website.

Teaching Assistant, CH125b The Elements of Quantum Chemistry, Caltech, 2018
Won the 2018 CCE Teaching Award.

Teaching Assistant, CH21b Physical Chemistry (B), Caltech, 2017

Teaching Assistant, CH125a Quantum Mechanics (A), Caltech, 2016

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] L. Thiede†, **C. Sun**† (**co-first and corresponding author**) and A. Aspuru-Guzik. Waveflow: boundary-conditioned normalizing flows applied to fermionic wavefunctions. *APL Mach. Learn.* **2**, 4, 046106 (2024). *Featured article.*

[3] K. Gratsea, **C. Sun**, and P. Johnson. When to reject a ground-state preparation algorithm. *Phys. Rev. A* **109** (4), 042425 (2024). *This work was conducted during K. Gratsea's internship under my supervision.*

[4] 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).

[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] 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). *Selected to the themed collection of "Most popular 2023 physical and theoretical chemistry articles".*

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

[8] **C. Sun**. Finite-temperature simulations of strongly correlated systems. *Dissertation (Ph.D.), California Institute of Technology.* doi:10.7907/dchn-p020 (2021).

[9] **C. Sun** (**co-corresponding author**), 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).

[10] 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). *I presented this work on behalf of my collaborators at the 23rd Annual Conference on Quantum Information Processing (QIP) in 2020.*.

[11] 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).

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

[13] 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).

Patents

[1] **C. Sun**, A. Mills, A. Efimovskaya, H. Liu, and N. Baker. Similarity-driven conditional generation of molecules based on chemical properties. *Patent pending.*

[2] **C. Sun**, Y. Yang, D. Tom, A. Mills, A. Efimovskaya, A. Damboianu, H. Liu, S. Chong, and N. Baker. Novel molecule for two-phase immersion cooling. *Patent pending.*

[3] A. Cheng, **C. Sun**, A. Mills, and H. Liu. 3D molecule generation via diffusion autoregression ML. *Submitted to the Microsoft CELA Team for review.*

Preprints

[1] **C. Sun**. Electron localization in disordered quantum systems at finite temperatures. Preprint: arXiv:2403.16868 (2024). **Independent work**. *Submitted to Phys. Rev. B, under review.*

In Preparation

[1] A. Aldossary, M. Bagherimehrab, J. Kottmann, L. Mantilla, P. Schleich, **C. Sun** (**alphabetical order**), and A. Aspuru-Guzik. Recent developments in quantum computing for chemistry. Invited Review for *ACS In Focus*. *Under review.*

[2] Y. Yang, **C. Sun**(**corresponding author**), J. Unsleber, and H. Liu, A computational study of atmospheric reactivity for organic molecules with automated reaction network exploration. *Collaborative work with Microsoft Quantum on the green chemistry endeavor. Draft ready.*

Talks

[1] "Designing Quantum Chemistry Methods with and Beyond Chemical Intuition." Invited Talk at Rutgers University, January. 2025

[2] "Designing Quantum Chemistry Methods with and Beyond Chemical Intuition." Invited Talk at SUNY Binghamton, December. 2024

[3] "Designing Quantum Chemistry Methods with and Beyond Chemical Intuition." Invited Talk at the University of Oklahoma, December. 2024

[4] "Designing Quantum Chemistry Methods with and Beyond Chemical Intuition." Invited Talk at the University of Rhode Island, Nov. 2024

[5] "Designing Computational Methods for Strongly Correlated Electrons." Rice Quantum Initiative (RQI) Seminar, Nov. 2024.

[6] "How to Design Quantum Chemistry Methods." Invited Talk at the Texas A&M University, Oct. 2024.

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

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

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

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

[11] "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.

[12] "Designing Classical and Quantum Algorithms for Strongly Correlated Materials." Invited Talk at Google Quantum, Nov. 2021.

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

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

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

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

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

[18] "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.