

Chong Sun

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EDUCATION

California Institute of Technology (Caltech)

Ph. D. in Theoretical Chemistry

Advisor: Garnet Kin-Lic Chan

Thesis: Finite temperature simulations of strongly correlated systems.

Pasadena, CA

Jul. 2016 - Dec. 2020

Peking University

B. S. in Chemistry with honor

Thesis advisor: Wenjian Liu

Thesis: Density matrix embedding theory in terms of localized molecular orbitals.

Beijing, China

Sep. 2011 - Jul. 2015

Princeton University

Centennial Fellowship graduate Student

Princeton, NJ

Sep. 2015 - Jun. 2016

Massachusetts Institute of Technology (MIT)

Exchange undergraduate Student

Cambridge, MA

Sep. 2013 - Dec. 2013

RESEARCH & WORK EXPERIENCE

Postdoctoral Researcher, Rice University

Supervisor: Prof. Gustavo Scuseria

- Developing state-of-the-art quantum chemistry algorithms for strongly correlated systems.

May. 2023 - Present

Research Scientist, Zapata Computing Inc.

Supervisor: Dr. Peter Johnson

- Developed quantum algorithms and software for ground-state energy estimation and quantum resource estimation.

Nov. 2022 - Jan. 2023

Postdoctoral Researcher, University of Toronto

Supervisor: Prof. Alán Aspuru-Guzik

- Neural quantum states and AI for science.
- Quantum algorithms for physical and chemical systems.

Feb. 2021 - Oct. 2022

Graduate Research Assistant, Caltech

Supervisor: Prof. Garnet Kin-Lic Chan

- Finite-temperature simulation of strongly correlated systems.
- Quantum algorithms for chemical systems.

Jul. 2016 - Dec. 2020

Undergraduate Research Assistant, Peking University

Supervisor: Prof. Wenjian Liu

- Implemented localized molecular orbitals with the Foster-Boys localization method in the density matrix embedding theory (DMET) method to study molecular systems.

Jan. 2015 - Jun. 2015

Undergraduate research assistant, Peking University

Supervisor: Prof. Hong Jiang

- Density functional theory (DFT) for spin-crossover systems.

Jul. 2014 - Nov. 2014

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

- Studying strongly correlated materials with density matrix embedding theory. *ICT-HPCC22, 2022*
- Density matrix embedding theory and quantum imaginary time evolution. *ByteDance, 2021*
- Quantum imaginary time evolution. *QIP, 2020*
- Quantum computing for quantum chemistry. *Peking University, 2020*

TEACHING EXPERIENCE

University of Toronto

- CHM427H1S Statistical Mechanics - Lecturer. *Spring 2021-2022*

Californian Institute of Technology

- CH125a Quantum Mechanics (A) - Recitation instructor. *Fall 2016-2017*
- CH21b Physical Chemistry (B) - Recitation instructor. *Winter 2016-2017*
- CH125b The Elements of Quantum Chemistry - Recitation instructor. *Winter 2017-2018*

PUBLICATIONS&PREPRINTS

- 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)
- 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)
- 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)
- M. Krenn *et. al.* SELFIES and the future of molecular string representations. *Patterns*, **3**, 100588 (2022)
- K. Gratsea, C. Sun, P. Johnson. When to Reject a Ground-State Preparation Algorithm. Pre-print: arXiv:2212.09492. Submitted to *Phys. Rev. A.* (2023)
- 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)
- 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 Submitted to ICML 2023.
- C. Sun, Finite Temperature Simulations of Strongly Correlated Systems. *Dissertation (Ph.D.), California Institute of Technology.* doi:10.7907/dchn-p020 (2021)
- C. Sun, U. Ray, Z.-H. Cui, M. Stoudenmire, M. Ferrero and G. K. Chan. Finite temperature density

[†] equal contribution.

- matrix embedding theory. *Phys. Rev. B*, **101**, 075131 (2020)
- 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)
 - 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)
 - 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)