Chong Sun

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EDUCATION

California Institute of Technology (Caltech) **Pasadena, CA**
Ph. D. in Theoretical Chemistry, GPA: 4.1/4.0 *Jul. 2016 - Dec. 2020*
Advisor: Garnet Kin-Lic Chan
Thesis: Finite temperature simulations of strongly correlated systems.

Peking University **Beijing, China**
B. S. in Chemistry with honor, GPA: 3.74/4.0 *Sep. 2011 - Jul. 2015*
Thesis advisor: Wenjian Liu
Thesis: Density matrix embedding theory in terms of localized molecular orbitals.

Princeton University **Princeton, NJ**
Centennial Fellowship graduate Student, GPA: 3.8/4.0 *Sep. 2015 - Jun. 2016*

Massachusetts Institute of Technology (MIT) **Cambridge, MA**
Exchange undergraduate Student, GPA: 5.0/5.0 *Sep. 2013 - Dec. 2013*

SKILLS

Research Topics: quantum chemistry, numerical simulation, quantum computing, machine learning.
Coding & Software: Python, C/C++, PySCF, OpenFermion, PyTorch, JAX.

RESEARCH & WORK EXPERIENCE

Research scientist, Zapata Computing Inc. *May. 2022 - Jan. 2023*
Supervisor: Dr. Peter Johnson (URL for website)
- Developed quantum algorithms and software for ground-state energy estimation and quantum resource estimation.

Postdoctoral fellow, University of Toronto *Feb. 2021 - Oct. 2022*
Supervisor: Prof. Alán Aspuru-Guzik (URL for website)
- Extended normalizing flows to be able to preserve the anti-symmetric feature of fermionic wavefunctions, which provided an alternative view to encoding antisymmetry with the Slater determinant.
- Co-developed quantum iterative power algorithm (QIPA) to accelerate solving large number factorization and ground-state energy estimation.

Graduate research assistant, Caltech *Jul. 2016 - Dec. 2020*
Supervisor: Prof. Garnet Kin-Lic Chan (URL for website)
- Developed the finite-temperature density matrix embedding theory (FT-DMET) algorithm for strongly-correlated systems.
- Implemented the finite temperature extension of existing numerical algorithms, including exact diagonalization, Lanczos algorithm, density matrix renormalization group (DMRG), and spin-symmetry restored coupled cluster (CC).
- Developed quantum imaginary time evolution (QITE) algorithm and quantum minimally entangled typical thermal states (QMETTS) algorithm.

Undergraduate research assistant, Peking University *Jan. 2015 - Jun. 2015*
Supervisor: Prof. Wenjian Liu (URL for website)
- Implemented localized molecular orbitals with the Foster-Boys localization method in the density matrix embedding theory (DMET) method to study molecular systems.

Undergraduate research assistant, Peking University *Jul. 2014 - Nov. 2014*

Supervisor: Prof. Hong Jiang (URL for website)

- Studied the low-spin to high-spin (LS-HS) phase transition of $[Fe(pz)Pt(CN)_4]\cdot 2H_2O$ with Monte Carlo and density functional theory (DFT).

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

- 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 - course instructor. — *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*

SELECTED PUBLICATIONS

- 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.
- K. Gratsea, **C. Sun**, P. Johnson. When to Reject a Ground-State Preparation Algorithm. Pre-print: arXiv:2212.09492.
- **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)
- 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)
- **C. Sun**, Finite Temperature Simulations of Strongly Correlated Systems. *Dissertation (Ph.D.), California Institute of Technology.* doi:10.7907/dchn-p020 (2021)

- 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)