

Shu Fay Ung

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Education

- **Columbia University** **New York, NY**
Ph.D. Chemical Physics *August 2026*
 - Advisor: David Reichman
 - Dissertation: *Correlated electronic states in moiré heterostructures: insights from quantum chemistry*
- **Columbia University** **New York, NY**
MPhil. Chemical Physics *February 2025*
- **California Institute of Technology** **Pasadena, CA**
B.Sc. Physics *June 2021*
 - Advisor: Garnet Chan

Research Experience

- **Graduate Researcher, Columbia University** **New York, NY**
Advisor: David Reichman *August 2021 – August 2026*
 - Studied strongly correlated electronic states in moiré materials, particularly in twisted bilayer transition metal dichalcogenides and rhombohedral pentalayer graphene.
- **Research Fellow, Harvard University** **Cambridge, MA**
Advisor: Joonho Lee *July 2024 – September 2024*
 - Studied topological phases in rhombohedral pentalayer graphene in collaboration with Ashvin Vishwanath's group.
- **Undergraduate Researcher, Caltech** **Pasadena, CA**
Advisor: Garnet Chan *October 2019 – August 2021*
 - Developed a spin-projected perturbation theory (MP2) method for electronic structure calculations.
- **Undergraduate Researcher, Caltech** **Pasadena, CA**
Advisors: Peter Love (Tufts University), John Preskill *June 2019 – August 2019*
 - Worked on term reduction techniques (e.g. unitary partitioning) for solving electronic structure Hamiltonians via variational quantum algorithms.
 - Worked to extend the OpenFermion software library to include plane wave basis and plane wave dual basis electronic structure Hamiltonians for (i) non-periodic 3D systems, and (ii) periodic and non-periodic 2D systems.
- **Undergraduate Researcher, Caltech** **Pasadena, CA**
Advisor: Maria Spiropulu *June 2018 – March 2019*
 - Ran simulations and analyzed data from the CMS experiment at the Large Hadron Collider (LHC) to obtain exclusion limits in the dark photon parameter space.

Awards and Honors

- 2026 Pegram Award, Columbia University
- 2022-2023 Jack Miller Teaching Award, Columbia University
- 2022-2023 Blanche R. and David Kasindorf Fellowship Fund in Physical Chemistry, Columbia University

- 2020 Donald and Trudy Bergen Math Scholarship, Caltech
- 2020 John Stauffer SURF Fellowship, Caltech
- 2017, 2018, 2019 Wylie Endowed Scholarship, Caltech
- 2017 Pearson Outstanding Learner Awards - Highest Mark in Malaysia for A Level Further Mathematics

Publications and Preprints

(* indicates equal contributions and † indicates corresponding authors.)

- [6] **S.F. Ung**^{*†}, A. Mahajan^{*†}, D.R. Reichman[†]. *Study of the triangular-lattice Hubbard model with constrained-path quantum Monte Carlo*. *Phys. Rev. B* 114, 065112 (2026), [arXiv:2603.14808](#) (2026)
- [5] L. Peng, S. Liu, X. Zhang, X. Chen, C. Li, **S.F. Ung**, H.P. Cheng[†], G.K.L. Chan[†]. *Accurate crystal field Hamiltonians of single-ion magnets at mean-field cost*. *J. Phys. Chem. Lett.* 16, 12312-12320 (2025), [arXiv:2505.16905](#)
- [4] T. Jiang, M.K.A. Baumgarten, P.F. Loos, A. Mahajan, A. Scemama, **S.F. Ung**, J. Zhang, F.D. Malone, J. Lee[†]. *Improved modularity and new features in ipie: Toward even larger AFQMC calculations on CPUs and GPUs at zero and finite temperatures*. *J. Chem. Phys.* 161, 162502 (2024), [arXiv:2406.16238](#)
- [3] **S.F. Ung**[†], J. Lee[†], D.R. Reichman[†]. *Competing Generalized Wigner Crystal States in Moiré Heterostructures*. *Phys. Rev. B* 108, 245113 (2023), [arXiv:2308.03020](#)
- [2] R. Babbush[†], W.J. Huggins, D.W. Berry, **S.F. Ung**, A. Zhao, D.R. Reichman, H. Neven, A.D. Baczewski, and J. Lee[†]. *Quantum simulation of exact electron dynamics can be more efficient than classical mean-field methods*. *Nat. Commun.* 14, 4058 (2023), [arXiv:2301.01203](#)
- [1] A. Zhao, A. Tranter, W. Kirby, **S.F. Ung**, A. Miyake, and P.J. Love[†]. *Measurement reduction in variational quantum algorithms*. *Phys. Rev. A* 101, 062322 (2020), [arXiv:1908.08067](#)

Talks

- *Correlated electronic states in moiré heterostructures: insights from quantum chemistry*. Contributed talk at Materials Innovators Workshop, Columbia University, 01/2025
- *Correlated electronic states in moiré heterostructures*. Invited talk at Joonho Lee's group, Harvard University, 09/2024
- *Competing generalized Wigner crystal states in moiré heterostructures*. Contributed talk at American Physical Society March Meeting, Minneapolis, MN, 03/2024
- *Competing generalized Wigner crystal states in moiré heterostructures*. Invited talk at MRSEC IRG Symposium, Columbia University, 11/2023
- *Competing generalized Wigner crystal states in moiré heterostructures*. Invited talk at Physical Chemistry Seminar, Columbia University, 09/2023
- *Competing generalized Wigner crystal states in moiré heterostructures*. Invited talk at Joonho Lee's group, Harvard University, 08/2023
- *Spin-symmetry restored many-body perturbation theory*. Contributed talk at SURF Seminar Day, Caltech, 10/2020
- *Representation of molecular wavefunctions with plane wave bases*. Contributed talk at SURF Seminar Day, Caltech, 10/2019

Mentoring and Teaching Experience

- **Volunteer Mentor and Facilitator**
 ○ USAPPS

Malaysia
 September 2020 – Present

- Provide guidance for Malaysian students applying to U.S. colleges and volunteered at the annual USAPPs workshops.
- Paired with a mentee (now enrolled at the University of Pennsylvania) during the 2021 application cycle and met weekly to brainstorm, edit, and proofread application essays.

Teaching Assistant

New York, NY

Department of Chemistry, Columbia University

August 2021 – December 2023

- Wrote and graded problem sets; held weekly office hours; led exam review sessions; supervised experiments; graded lab reports; updated the lab manual.
 - CHEMGU 4230: Statistical Thermodynamics (Graduate)
 - CHEMUN 1500: General Chemistry Lab (Undergraduate)
 - CHEMUN 1507: Intensive General Chemistry Lab (Undergraduate)

Teaching Assistant

Pasadena, CA

Division of Physics, Mathematics, and Astronomy, Caltech

January 2020 – March 2020

- Supervised experiments; graded pre-lab assignments.
 - Ph 6: Physics Laboratory (Undergraduate)

Other Experience

President, 2020-21

Pasadena, CA

Caltech Undergraduate Physics Club

October 2019 – June 2021

- Organized talks by faculty and graduate students, graduate school application panels, and social events.

Co-Editor-in-Chief, 2020-21

Pasadena, CA

Caltech Big T Yearbook

October 2017 – June 2021

- Oversaw the publication of the annual yearbook.
- Contributed as a copywriter, designer, photographer, and copy editor before being appointed co-editor-in-chief.

Skills

- **Natural languages** English (native), Mandarin (native), Malay (proficient)
- **Programming languages** Python, C++, Julia, Q#, Bash, $\text{\LaTeX}$
- **Scientific software** pySCF, Q-Chem, ipie, trot, ITensor, Qiskit
- **Miscellaneous** Adobe Suite (Illustrator, InDesign, Photoshop, Lightroom)