Shu Fay Ung

MC 3141, Department of Chemistry, Columbia University 3000 Broadway, New York, NY 10027

Education

Columbia University

New York, NY

Ph.D. Chemical Physics

Expected May 2026

- Advisor: David Reichman

Columbia University

New York, NY

MPhil. Chemical Physics

Feb 2025

- Cumulative GPA: 4.1

California Institute of Technology

Pasadena, CA

B.Sc. Physics

June 2021

Advisor: Garnet ChanCumulative GPA: 4.0

Research Experience

Graduate Researcher, Columbia University

New York, NY

Advisor: David Reichman

August 2021 – Present

- Studying strongly-correlated electronic states in moiré materials, particularly in twisted bilayer transition metal dichalcogenides.

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

- Analyzed data from the CMS detector at the Large Hadron Collider (LHC) to obtain exclusion limits on the parameters of the hypothesized dark photon.
- Simulated the decay of dark photons to dimuons and the detector response using the CMS Software Framework (CMSSW).

Awards and Honors

- o 2022-2023 Jack Miller Teaching Award
- o 2022-2023 Blanche R. and David Kasindorf Fellowship Fund in Physical Chemistry, Columbia University
- o 2020 Donald and Trudy Bergen Math Scholarship, Caltech
- o 2020 John Stauffer SURF Fellowship, Caltech
- o 2017, 2018, 2019 Wylie Endowed Scholarship, Caltech
- o 2017 Pearson Outstanding Learner Awards Highest Mark in Malaysia for A Level Further Mathematics

Publications and Preprints

- [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), <u>arXiv:2308.03020</u>
- [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

- o 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. 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
- o 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. SURF Seminar Day, Caltech, 10/2020
- o Representation of molecular wavefunctions with plane wave bases. SURF Seminar Day, Caltech. 10/2019

Mentoring and Teaching Experience

Volunteer Mentor and Facilitator

Malaysia

USAPPS

September 2020 - Present

- Provide guidance for Malaysian students applying to U.S. colleges and volunteered for the annual USAPPs workshops.

Teaching Assistant

Columbia University & Caltech

- Columbia University, August 2021 December 2023
 - · CHEMGU 4230: Statistical Thermodynamics (Graduate)
 - · CHEMUN 1500: General Chemistry Lab (Undergraduate)
 - · CHEMUN 1507: Intensive General Chemistry Lab (Undergraduate)
- Caltech, January 2020 March 2020
 - · Ph 6: Physics Laboratory (Undergraduate)

Skills

- o Natural languages English (native), Mandarin (native), Malay (Limited working proficiency)
- Programming languages Python, C++, Julia, Q#, Bash, LATEX
- o Scientific software pySCF, Q-Chem, ipie, Qiskit
- o Miscellaneous Adobe Suite (Illustrator, InDesign, Photoshop, Lightroom)