Shu Fay Ung

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

su2254@columbia.edu • shufay.github.io

Education

- **Columbia University** — **New York, NY**
  Ph.D. Chemical Physics — *Expected August 2026*
  - Advisor: David Reichman
- **Columbia University** — **New York, NY**
  MPhil. Chemical Physics — *February 2025*
  - Cumulative GPA: 4.1
- **California Institute of Technology** — **Pasadena, CA**
  B.Sc. Physics — *June 2021*
  - Advisor: Garnet Chan
  - Cumulative 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*
  - 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

- 2022-2023 Jack Miller Teaching Award
- 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

[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** — **Malaysia**
  USAPPS — *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.
- Served as copywriter, designer, photographer, and copy editor before being appointed co-editor-in-chief.

Skills

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

References

David Reichman **Advisor**
Centennial Professor of Chemistry, Columbia University
drr2103@columbia.edu

Joonho Lee **Collaborator**
Assistant Professor, Harvard University
joonholee@g.harvard.edu