Hayley Weir

380 Roth Way, Stanford, CA 94305
hweir@stanford.edu

Education

2017-Present | PhD Chemical Physics, **Stanford University**
- Advisor: Todd J. Martinez
- Graduate Classes: Programming Abstractions in C++ (CS 106b), Parallel Computing (CME 213), Scientific Python (CS 193), Advanced Quantum Mechanics (CHEM 275).

2013-17 | MSci Chemistry with Molecular Physics, **Imperial College London**
- First-Class Honours (overall average grade: 79%; master's thesis grade: 85%)
- Relevant Classes: Maths and Physics I & II, Python Programming I & II, Robot Chemistry, Complexity, Quantum Mechanics I & II, Statistical Thermodynamics I, II & III, Molecular Reaction Dynamics.

Research Experience

2017-Present | PhD Research Projects, **Stanford University** | Advisor: Prof. Todd J. Martinez
- Hand-drawn chemical structures recognition with neural image captioning approach for educational and research app.
  - > Implemented natural language processing and computer vision algorithms to recognise hand-drawn molecular structures.
  - > Designed and promoted a data collection app to generate a hand-drawn dataset for training. Collected over 6,000 labelled images of hand-drawn structures. Developed image augmentation and degradation pipelines for data regularisation.
  - > Fine tuning and ensemble learning to achieve an accuracy of ∼80% on hand-drawn hydrocarbon molecule recognition with only 400 hand-drawn images.
- Simulated excited state quantum dynamics of *cis*-stilbene with *ab initio* electronic structure algorithms.
  - > Analysed trajectories and linked results to existing literature and ongoing experimental collaborations. Proposed future experiments for selective chemical design for targeted applications such as chemical synthesis and molecular motors.
- Applied quantum chemistry algorithms and quantum computing approach to compress machine learning datasets.
  - > Represented MNIST and other image datasets as a wavefunction to reduce information of dataset by exploiting structure in the data. Attended 4 day Rigetti quantum computing workshop at Lawrence Livermore National Lab.
- Developed single and multi GPU-accelerated code of coupled cluster quantum chemistry algorithm in team of six.

2016-17 | Master's Research Project, **Imperial College London** | Advisor: Prof. Alexei Kornyshev
- Carried out full theoretical analysis of two novel electrotuneable nanoplasmonic device.
  - > Developed theory of assembly of nanoparticles at an interface to dramatically improve match with higher level of theory.
  - > Defended research findings to professors in presentation, oral exam and thesis. Achieved highest thesis grade in cohort.

Summer 2016 | Undergraduate Research Project, **Massachusetts Institute of Technology** | Advisor: Prof. Troy Van Voorhis
- Developed a mean field theoretical method to investigate OLED kinetics as an alternative to Kinetic Monte Carlo.
  - > Determined the effect of disorder on unimolecular and bimolecular reaction rate constants.
  - > One of two Imperial chemistry students awarded an eight week scholarship to undertake a research project at MIT.

Summer 2015 | Undergraduate Research Project, **Imperial College London** | Advisor: Prof. Michael Bearpark
- Studied retinal-like molecule with quantum chemistry algorithms to explore vision mechanism in the eye.

Skills

IT Skills | Python, C++, CUDA, LaTeX; Bash; Keras, TensorFlow, RDKit, OpenCV; Quantum chemistry packages.

Awards and Honours

2020 | Outstanding Graduate Student Poster, **Virtual Conference on Theoretical Chemistry**

2017 | Award for Excellence in Physical Chemistry, **Imperial College London**

2017 | Dean's List, **Imperial College London**

2016 | International Research Opportunity Project Scholarship, **Massachusetts Institute of Technology**

Journal Publications

Raucci, U., **Weir, H.**, Bannwarth, C., Sanchez, D., and Martínez, T.J., The Chiral Photochemistry of Achiral Molecules: The Emblematic Case of Stilbene and Stiff-Stilbene, *In Prep.*

Williams, M., Forbes, R., **Weir, H.**, Veyrinas, K., MacDonell, R.J., Boguslavskiy, A.E., Schuurman, M.S., Stolow. A. and Martínez, T.J., Unmasking the *cis*-Stilbene Phantom State with ab-initio Multiple Spawning and Time-Resolved Photoelectron Spectroscopy, *In Prep.*

Weir, H., Thompson, K., Choi, B., Woodward, A., Braun, A. and Martínez, T.J., ChemPix: Automated Recognition of Hand-drawn Hydrocarbon Structures Using Deep Learning, *Submitted*

Raucci, U., Valentini, A., Pieri, E., **Weir, H.**, Seritan, S. and and Martínez, T.J., Voice-controlled quantum chemistry. *Nat. Comput. Sci.* 1, 42–45 (2021).

van den Berg, J.L., Neumann, K.I., Harrison, J.A., **Weir, H.**, Hohenstein, E.G., Martinez, T.J. and Zare, R.N., Strong, nonresonant AC Field enhances photoisomerisation of *cis*-stilbene in solution, *J. Phys. Chem. A* 124, 5999–6008 (2020).

Fales, B.S., Curtis, E.R, Johnson, K.G, Lahana, D., Seritan, S., Wang, Y., **Weir, H.**, Martínez, T.J. and Hohenstein, E.G., Performance of Coupled-Cluster Singles and Doubles on Modern Stream Processing Architectures. *J. Chem. Theory Comput.* 16, 4021–4028 (2020).

Weir, H., Williams, M., Parrish, R.M., Hohenstein, E.G. and Martínez, T.J. Nonadiabatic Dynamics of Photoexcited cis-Stilbene Using Ab Initio Multiple Spawning. *J. Phys. Chem. B* 124, 5476–5487 (2020).

McIsaac, A.R., Vaissier Welborn, V., Einzinger, M. Geva, N., **Weir, H.**, Baldo, M.A., and Van Voorhis, T., Investigation of External Quantum Efficiency Roll-off in OLEDs Using the Mean Field Steady State Kinetic Model, *J. Phys. Chem. C* 124, 14424–14431 (2020).

Sikdar, D., **Weir, H.**, and Kornyshev, A. A., Optical response of electro-tuneable 3D superstructures of plasmonic nanoparticles self-assembling on transparent columnar electrodes, *Opt. Express*, 27, 26483-26498, (2019).

Weir, H., Edel, J. B., Kornyshev, A. A. and Sikdar, D. Towards Electrotuneable Nanoplasmonic Fabry-Perot Interferometer. *Scientific Reports.* 8, 565, (2018).

Conference Contributions

Weir, H., Williams, M., Parrish, R. and Martínez, T.J. Nonadiabatic Dynamics of Photoexcited *cis*-Stilbene Using Ab Initio Multiple Spawning. Virtual Conference of Theoretical Chemistry, July 2020 (Poster and Lightening Talk).

Weir, H. and Wang, Y. Developing Tools for Chemical Research and Education using Machine Learning and Virtual Reality. Center for Molecular Analysis and Design Symposium 2020 (Poster).

Weir, H., Williams, M., Parrish, R. and Martínez, T.J. Elucidating the Photochemistry of *cis*-Stilbene with *ab initio* Multiple Spawning. Northern California Theoretical Chemistry Meeting, Berkeley CA, March 2019 (Poster).

Weir, H., Williams, M., Parrish, R. and Martínez, T.J. Nonadiabatic Simulation of *cis*-Stilbene with FOMO-CASCI in the 400 Femtosecond Regime. West Coast Theoretical Chemistry Symposium, Stanford CA, March 2018 (Poster).

Teaching Experience

2017-18	Teaching Assistant, **Stanford University** • Accelerated Chemical Principles • Spectroscopy Laboratory • Analytical Chemistry
2011-13	Maths Tutoring, Football Coaching and Sailing Instructing, **Steyning Grammar School & Sussex Yacht Club**

Other Experience

2019-Present — Women of STEM co-founder

- Run social media page featuring weekly interviews with women in STEM careers. Aim to inspire young girls to pursue science and engineering subjects by providing female role models in the field. instagram.com/women.of.stem

2015-16 — President of Imperial College London Chemistry Society

- Led a team of nine committee members, managed a £16,000 budget, executed events for over 500 chemistry students and staff, negotiated £4000 in corporate sponsorship.
- Organised seminar series regularly attracting 300 attendees - confirmed speakers included: Nobel Laureate, Sir Harry Kroto, FRS; first British astronaut, Dr Helen Sharman OBE; and former government drugs advisor, Prof. David Nutt.

2013-17 — Imperial College London Women's Football 1st Team

- Finished 2nd in division of British University Club Sports league. Former captain of school football team, achieving second place in the Sussex school's league.

2012-13 — Deputy Head Girl of Steyning Grammar School

- Organised social, academic and charity events for school and sixth form of 2000 students. Raised £8000 for charity.

2011-13 — Sailing Racing

- Competed in team of five in the Sonar World Championships in Rochester, NY and achieved 2nd place in the Under 25 category at Cowes Week. Presented a talk with team on the main stage at Alexandra Palace to over 200 people. Attained RYA dinghy sailing instructor qualification.