Hayley Weir

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Education

PhD Chemical Physics, **Stanford University** 2017-Present

Automating and Democratizing Photochemical Design using Machine Learning and Quantum Chemistry

- Classes: Machine Learning for Chemical and Dynamical Data, Programming Abstractions in C++, Parallel Computing, Scientific Python, Advanced Quantum Mechanics.
- Peaker Award for diversity, equity and inclusion efforts in the Department of Chemistry.

BSc/MSci Chemistry with Molecular Physics, **Imperial College London** 2013-17

Theoretical Investigations in Nanoplasmonics of Micro- and Nanostructured Electrode Systems

- First-Class Honours, highest Master's thesis grade in cohort (85%), Award for Excellence in Physical Chemistry, Dean's List.

Research Experience

Graduate Researcher, **Stanford University** | Advisor: Prof. Todd Martínez 2017-Present

- Hand-drawn Chemical Structure Recognition with Machine Learning (featured on *C&EN*, *Chemistry World* and *AIP Scilight*)
  - Crowd-sourced 7.5 K photographs of real-world hand-drawn chemical structures and generated 1M image synthetic dataset.
  - Built an image-to-SMILES neural network consisting of a CNN encoder and LSTM decoder network with beam search and attention.
  - Applied fine-tuning and ensemble learning to reach ∼80% accuracy using only 400 real-world hand-drawn hydrocarbon images.
  - Combined molecule recognition software with augmented reality molecular visualisation to create MolAR iPhone application.
- Photodynamics simulations of *cis*-Stilbene with GPU-Accelerated Quantum Chemistry
  - Modelled and analysed 1000s of trajectories to probe the fundamental photoisomerization mechanism of a prototypical molecule, applied new understanding to design highly symmetric molecular motor.
  - Collaborated with three independent experimental groups to understand and explain their data and propose future experiments.
  - Assembled team of students and postdocs to update, test and package *aimsprop*, a Python program for automating simulation analysis.

AI Resident, **X, the moonshot factory** (formerly Google[x]) January - June 2022

- Designing binders for protein targets with generative language models
  - Built a transformer-based supervised variational autoencoder (SVAE) and compared it to existing ML models for binder prediction.
  - Implemented latent space interpolation and hill climb for the SVAE to generate strong binders; submitted for experimental validation.
  - Discovered unwanted bias signal dominated experimental training data, brainstormed methods to reduce bias with experimentalists.
  - Active contributor and reviewer for Google's codebase, observing software development best practices including writing unit tests, linting and continuous integration.

Master's Researcher, **Imperial College London** | Advisor: Prof. Alexei Kornyshev 2016-17

- Coded a Fresnel-based model from scratch to analyse two novel electrotuneable nanoplasmonic smart window devices.

Summer Researcher, **Massachusetts Institute of Technology** | Advisor: Prof. Troy Van Voorhis Summer 2016

- Developed a theoretical framework to understand efficiency roll-off in OLEDs, which was later experimentally validated.

Summer Researcher, **Imperial College London** | Advisor: Prof. Michael Bearpark Summer 2015

- Studied the vision mechanism in the eye with quantum chemistry simulations.

Technical Skills

Programming/HPC	(*proficient*) Python; (*familiar*) C/C++, CUDA, Bash/Shell, Git, LaTex, SLURM
Python Libraries	(*proficient*) RDKit, OpenCV, Matplotlib, NumPy; (*familiar*) Keras, Tensorflow, PyTorch, Pandas, Plotly
Chemistry Software	(*proficient*) TeraChem, VDM; (*familiar*) Gaussian, BAGEL

Other Experience

Diversity Equity and Inclusion Initiatives 2019-Present

- Co-founded Women of STEM, a social media page featuring weekly interviews of women in STEM careers. Co-organised the first *Stanford Theoretical Chemistry PhD Preview Day* and *Stanford Chemistry Preview Day* aimed at groups who are historically under-represented in STEM. Hosted students for Science Accelerating Girls' Engagement in STEM (SAGE) 2020.

President of Imperial College London Chemistry Society 2015-16

- Led a team of nine committee members, managed a £16,000 budget and negotiated £4000 in corporate sponsorship. Executed events for over 500 students and staff including seminar series with 300 regular attendees.

Competitive Sport and Coaching 2011-17

- Sonar Sailing World Championships; dinghy sailing instructor; Imperial College Women's Soccer Team; high school soccer team captain.

Conference Contributions and Talks

Poster	American Conference on Theoretical Chemistry, Lake Tahoe	July 2022
Talk	Tech Forum, X the moonshot factory	March 2022
Invited talk	Pitzer Center Theoretical Chemistry Seminar, UC Berkeley	Oct 2021
Poster	57th Symposium on Theoretical Chemistry, University of Würzburg / Virtual	Sept 2021
Poster & Lightening Talk	BATChem, Virtual - *Honorable Mention Lightning Talk*	July 2021
Poster	Center for Molecular Analysis and Design Symposium, Stanford University	Sept 2020
Poster & Lightening Talk	Virtual Conference of Theoretical Chemistry - *Outstanding Graduate Student Poster*	July 2020
Poster	Northern California Theoretical Chemistry Meeting, UC Berkeley	March 2019
Poster	West Coast Theoretical Chemistry Symposium, Stanford University	March 2018

Journal Publications

[-] Raucci, U., **Weir, H.**, Seritan, S., Sakshuwong, S., Martínez, T.J., Natural user interfaces for quantum chemistry, *In Prep. for Annual Review of Physical Chemistry*

[-] Jones, C.M., Kirsh, J., Thompson, K., List, N.H., Walker, A.R., **Weir, H.**, Boxer, S.G., and Martínez, T.J., Dimming the lights in GFP: High-throughput, in silico mutagenesis and machine learning predict the fluorescence of green fluorescent protein variants, *In Prep.*

[-] Saha, S., **Weir, H.**, Nunes, J.P.F., Martínez, T.J., Centurion, M., Ultrafast Electron Diffraction of cis-Stilbene, *In Prep.*

[11] Sakshuwong, S., **Weir, H.**, Raucci, U., Martínez, T.J., Bringing Chemistry to Life with Augmented Reality and Machine Learning, *The Journal of Chemical Physics*, 156, 204801 (2022).
- Published as part of the special issue on Chemical Design by Artificial Intelligence, and selected as Featured.

[10] Raucci, U., **Weir, H.**, Bannwarth, C., Sanchez, D., Martínez, T.J., Chiral photochemistry of achiral molecules, *Nautre Communications*, 13, 1–7 (2022).

[9] Williams, M., Forbes, R., **Weir, H.**, Veyrinas, K., MacDonell, R.J., Boguslavskiy, A.E., Schuurman, M.S., Stolow. A., Martínez, T.J., Unmasking the *cis*-Stilbene Phantom State via Vacuum Ultraviolet Time-Resolved Photoelectron Spectroscopy and Ab Initio Multiple Spawning, *The Journal of Physical Chemistry Letters*, 12, 6363-6369 (2021).

[8] **Weir, H.**, Thompson, K., Choi, B., Woodward, A., Braun, A., Martínez, T.J., ChemPix: Automated Recognition of Hand-drawn Hydrocarbon Structures Using Deep Learning, *Chemical Science*, 12, 10622–10633 (2021).
- Featured in Chemical Science's Most popular 2021 physical and theoretical chemistry articles.

[7] Raucci, U., Valentini, A., Pieri, E., **Weir, H.**, Seritan, S., Martínez, T.J., Voice-controlled quantum chemistry. *Nature Computational Science*, 1, 42–45 (2021).
- Published in the first issue of Nature Computational Science.

[6] van den Berg, J.L., Neumann, K.I., Harrison, J.A., **Weir, H.**, Hohenstein, E.G., Martínez, T.J., Zare, R.N., Strong, nonresonant AC Field enhances photoisomerisation of *cis*-stilbene in solution, *The Journal of Physical Chemistry A*, 124, 5999–6008 (2020).

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

[4] **Weir, H.**, Williams, M., Parrish, R.M., Hohenstein, E.G., Martínez, T.J. Nonadiabatic Dynamics of Photoexcited cis-Stilbene Using Ab Initio Multiple Spawning. *The Journal of Physical Chemistry B*, 124, 5476–5487 (2020).
- Published as part of The Journal of Physical Chemistry virtual special issue "Peter J. Rossky Festschrift".

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

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

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