

Dr Seán R. Kavanagh, MRSC, Sch.

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Talks: youtube.com/c/SeánRKavanagh (>20k views)

Slides: speakerdeck.com/kavanase

Flash Summary

- Published 50 peer-reviewed papers in 5 years in top-tier journals (*Nature Photonics*, *Nature Communications* (x2), *Joule*, *Energy & Environ Sci*, *ACS Energy Letters* (x5), *npj Comput Mater* (x2), *Materials Horizons*, *Matter...*), including 13 as first-author and 9 as corresponding author.
- Several papers are the result of MSc / PhD projects I designed and supervised.
- APS & IOP Computational Physics Thesis Prizes, MRS Graduate Student Awards (Gold 2023, Silver 2022), *Materials Today Chemistry* Rising Star Award, E-MRS Young Researcher Award, 2 E-MRS Graduate Student Awards, Ramsay Medal (and Catlow Prize) for Best (Computational) Chemistry PhD student in UCL Chemistry 2022.
- UCL Mathematical & Physical Sciences Education Award (& Associate Fellowship of the Higher Education Authority), for 'excellence in academic supervision and personal tutoring'.

Research Experience

- Present** **Harvard Environmental Fellowship (HUCE)(Cambridge, MA, USA)**
2024-02 Hosted by Prof Boris Kozinsky (*Materials Intelligence Research Group, Harvard University*)
Modelling defects in solid-state materials using machine-learned force-fields (MLFFs).
- UCL nominee and further shortlisted for the [Schmidt Science Fellowship](#), [Lindemann Fellowship](#), and [Fulbright Scholarship](#) 2024, accepting the Harvard [HUCE Fellowship](#).
 - Developer and tester of the widely-used [NequIP](#) & [Allegro](#) MLFF architectures.
- 2024-02** - **Ph.D.: Computational Materials Science (London, UK)**
2020-02 Profs David Scanlon (*University College London*) & Aron Walsh (*Imperial College London*)
Modelling defects, disorder and bulk properties of solid-state materials, primarily solar photovoltaics (incl. non-radiative recombination) but also batteries, thermoelectrics, LEDs/emission, excitons, COFs, ferroelectrics... using DFT, GW+BSE, RPA...
- Designed & supervised >20 MSc/PhD projects, with papers in *JACS*, *Phys Rev Lett*, *npj Comp Mater*, *ACS Energy Lett*, *Matter...* and prizes for supervision excellence.
 - Month-long visits (Max Planck & JSPS Awards; €1k & £3k) w/Profs Kumagai (Japan) & Freysoldt (Germany); papers in *Faraday Discussions*, *PRX Energy*.
 - Lead tester of VASP (most widely-used computational materials science code worldwide) for Archer2 (UK National Supercomputer), and lead research consultant for procurement of UCL HPC & GPU upgrades 2021/2022 (>£1 million).
 - Successful Archer2 Pioneer Project Grant lead author; value £110k.
 - Featured in the Irish Times: [Irish Scientists Shine in Solar Cell Development](#)

- UCL Resources for Computational Chemistry Researchers Tutor and 'Python for Chemical Modelling' module Post-Graduate Teaching Assistant (PGTA) at UCL.

2018-09 - Research Assistant

2018-05 NOKIA Bell Labs, Dublin, Ireland

Research project employing chemical and electrochemical techniques to fabricate microporous, structured surfaces for efficient heat dissipation from 5G devices.

Education

2019-05 - B.A. (Mod): Nanoscience, Physics And Chemistry of Advanced Materials

2015-09 Trinity College Dublin – Ireland

Summa Cum Laude; top-of-the-class (margin >10%), Gold Medal, First Class Honours (88%)

- Henderson-Lloyd prize for the highest overall grade in the Schools of Chemistry and Physics at Trinity College Dublin.
- Elected to Foundation Scholarship, the “most prestigious undergraduate award in Ireland” (€100,000 Value)(2017).

2015-05 - High School

2009-09 Castleknock College - Dublin, Ireland

10th highest performer in the nationwide High School Leaving exams out of 58,000 students; amongst only 7 students to achieve 100% in Chemistry, and 3 for 100% in Maths.

Selected Awards

- American Physical Society (APS) [Metropolis Award](#) for Outstanding Doctoral Thesis Work in Computational Physics 2024.
- UCL Mathematical & Physical Sciences (MAPS) Faculty Education Award, for Individual Excellence in academic supervision and personal tutoring.
- Institute of Physics (IOP) [Computational Physics PhD Thesis Prize](#) 2024.
- Materials Research Society (MRS) Graduate Student Award (Gold) 2023; (Silver) 2022.
- Associate Fellowship of the Higher Education Authority (AFHEA), awarded for meeting UK Professional Standards in higher education teaching and learning support.
- EPSRC Pioneer Award (lead author) for Archer2 supercomputing resources (2023); value £110k.
- UCL nominee and further shortlisted for the [Schmidt Science Fellowship](#), [Lindemann Fellowship](#), and [Fulbright Scholarship](#) 2024, before accepting Harvard [HUCE Fellowship](#).
- *Materials Today Chemistry* Rising Star Award 2022.
- Ramsay Medal & Catlow Prize for Best Chemistry PhD student in UCL.
- Lindau Spirit Fellowship for highly-promising young researchers, at the Lindau Nobel Chemistry Laureate Meeting 2022.
- European Materials Research Society (E-MRS) Young Researcher Award 2022 & Graduate Student Award (x2) 2021.

- MSc and PhD students I've supervised have won the Catlow Prize (Best Computational Chemistry PhD Student in UCL Chemistry) – Adair Nicolson – and the Nyholm (Best Inorganic MSc Project in UCL Chemistry) & Sharp (Best Theoretical MSc Project in UCL Chemistry) prizes.

Selected Publications

I am a firm believer in open science, all publications are openly-available online; see [Google Scholar](#)

* = Corresponding Author

Kavanagh, S. R.* et al.; doped: Python Toolkit for Robust and Repeatable Charged Defect Supercell Calculations. *Journal of Open Source Software (JOSS)* **2024**, 9 (96), 6433 – 42 citations – doi.org/10.21105/joss.06433

Mosquera-Lois, I. & **Kavanagh, S. R.*** (joint 1st-authors); Walsh, A.; Scanlon, D. O. Identifying the Ground State Structures of Defects in Solids. *npj Computational Materials* **2023** 9 (25) – 89 citations – doi.org/10.1038/s41524-023-00973-1

- Spotlighted in *Nature Physics* News & Views (<https://www.nature.com/articles/s41567-023-02049-9>)

Wang, Y. & **Kavanagh, S. R.** (joint 1st-authors) et al. Cation Disorder Engineering Yields AgBiS₂ Nanocrystals with Enhanced Optical Absorption for Efficient Ultrathin Solar Cells. *Nature Photonics* **2022**, 16 (3), 235-241 – several [news features](#) – 198 citations – doi.org/10.1038/s41566-021-00950-4

Kavanagh, S. R.*; Identifying Split Vacancy Defects with Machine-Learned Foundation Models and Electrostatics. *JPhys Energy (Emerging Leaders 2025, Invited Submission)* – doi.org/10.1088/2515-7655/ade916

Huang, Y. & **Kavanagh, S. R.** (joint 1st-authors) et al. Strong Absorption and Ultrafast Localisation in NaBiS₂ Nanocrystals with Slow Charge-Carrier Recombination. *Nature Communications* **2022** 13 (1), 1-13 – 65 citations – doi.org/10.1038/s41467-022-32669-3

Kavanagh, S. R.; Walsh, A.; Scanlon, D. O. Rapid Recombination by Cadmium Vacancies in CdTe. *ACS Energy Letters* **2021**, 6 (4), 1392–1398 – 75 citations – doi.org/10.1021/acseenergylett.1c00380

Kavanagh, S. R.*; Scanlon, D. O.; Walsh, A.; Freysoldt, C. Impact of Metastable Defect Structures on Carrier Recombination in Solar Cells. *Faraday Discussions* **2022**, 239, 339-356 – 36 citations – doi.org/10.1039/D2FD00043A

Kavanagh, S. R.* et al. Intrinsic Point Defect Tolerance in Selenium for Indoor and Tandem Photovoltaics. *Energy & Environmental Science* **2025**, 18, 4431-4446 – 7 citations – doi.org/10.1039/D4EE04647A

Selected Talks

I am a firm believer in open science, all recorded talks are openly-available online; see [YouTube](#)

'Modeling the Impact of Defects in Solids' Invited Seminar @ MIT Department of Materials Science & Engineering (DMSE) 2024, IIT Dhanbad 2024; Department of Chemistry, University of Cambridge 2024, Northwestern University 2025, Harvard University 2025, Fudan University 2025, Psi-k 2025

'Modelling Energy Surfaces of Defects in Solids with DFT and Machine Learning' Invited Talk @ APS March 2025, RSC Next-Gen PV January 2025, International Conference on Defects in Semiconductors (Beijing) 2025, STAC-15 (Tokyo) 2025

'Accurately Modelling Point Defects in Semiconductors: The Case of CdTe' Invited Talk @ APS March 2025

'Defect Structure Searching – Irea Mosquera-Lois and Seán Kavanagh on ShakeNBreak' Podcast Interview @ [JOSSCast #10](#)

'Imperfections are key: How supercomputers and machine learning help us to understand material defects' Invited Outreach Talk @ [Pint of Science Festival 2024](#)

'Performance Boosters to Efficiency Killers; From bulk disorder to isolated defects' Talk @ [MRS Spring 2023](#) (Gold Graduate Student Award), RSC International Conference on Materials Chemistry (MC16)

Selected Community Service

- [Psi-k C2 Working Group](#) Committee; *Materials and Devices for Energy*; funding distribution, symposium organizer for the Psi-k 2025 conference.
- Peer reviewer for *npj Computational Materials*, *Advanced Intelligent Discovery*, *J. Am. Chem. Soc. (JACS)*, *Appl. Phys. Lett. (APL)*, *Matter*, *Phys. Rev. Appl. (PRA)*, *J. Phys. Chem. Lett. (JPCL)*, *Phys. Rev. X (PRX) Energy*, *Phys. Rev. Mater. (PRM)*, *ACS Nano Lett.*, *Comp. Phys. Comm.*, *IOP Model. Simul. Mat. Sci. Eng.*, *JECR*...
- Active developer & maintainer of widely-used community codes; [doped](#), [pymatgen](#), [NequIP](#), [ShakeNBreak](#), [easyunfold](#) (see Software)
- [Mittal Family Climate Fellowship](#) at Harvard; Inaugural Review committee
- Session chair for MRS Fall CH02 (2021) and EN02 (2022) Symposia.
- Warden/Proctor in Imperial College undergraduate halls (2021-2023); responsibilities of supporting student mental health & wellbeing, discipline and event organisation.
- UCL Mathematical and Physical Sciences (MAPS) Faculty Early Career Researcher (ECR) advisory committee member, and ECR Forum Awards judge.
- Outreach: [Pint of Science Invited Speaker](#) 2023 & 2024, "[I'm an Engineer, Get me Out of Here!](#)" (UKRI, bp & Cavendish Nuclear), [YouTube](#) tutorials...

Selected Software

I am a firm believer in open science, all software developed is openly-available online; see [GitHub](#)

Core Developer:

- **doped**: Calculating point defects in solids. **Kavanagh, S. R.** – doped.readthedocs.io (>1k downloads/month)
- **ShakeNBreak**: Navigating the defect configurational landscape. **Kavanagh, S. R.;** Mosquera-Lois, I. – shakenbreak.readthedocs.io (>1k downloads/month)
- **easyunfold**: Unfolding electronic band structures. Zhu, B. Z; **Kavanagh, S. R.** – smtg-bham.github.io/easyunfold (1k downloads/month)
- **vaspup2.0**: VASP convergence testing (energy, forces, dielectrics...). **Kavanagh, S. R.** – github.com/kavanase/vaspup2.0 (100 downloads/month)
- **PyTASER**: Simulating Transient Absorption Spectroscopy (TAS). Aggarwal, S.; **Kavanagh, S. R.;** Woo, Y.; Ganose, A. M.; Walsh, A. – pytaser.readthedocs.io (100 downloads/month)

Contributor:

- **pymatgen**: Computational materials analysis – pymatgen.org
- **NequIP & Allegro**: Equivariant graph neural network interatomic potentials – github.com/mir-group/nequip & github.com/mir-group/allegro
- **CarrierCapture.jl**: Calculating non-radiative electron-hole recombination at defects – wmd-group.github.io/CarrierCapture.jl
- **sumo**: Plotting & analysing solid-state electronic/phonon structure – smtg-bham.github.io/sumo