Seán R. Kavanagh

PhD Researcher

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Flash Summary

- Published 20 peer-reviewed papers over 3 years in high-quality publications (Nature Photonics, Nature Communications, npj Comp Mater, Chemical Science, ACS Energy Letters, Materials Horizons, Matter…), including 9 as first-author and 5 as corresponding author.
- Several papers are the result of MSc / PhD projects I designed and supervised.
- UCL Mathematical & Physical Sciences (MAPS) Faculty Education Award, for Individual Excellence in academic supervision and personal tutoring.
- MRS Graduate Student Awards (Gold 2023, Silver 2022), *Materials Today Chemistry* Rising Star Award, eMRS Young Researcher Award, 2 eMRS Graduate Student Awards, Ramsay Medal (and Catlow Prize) for Best (Computational) Chemistry PhD student in UCL Chemistry 2022 – all typically awarded to final year students, all received in the 2nd & 3rd years of my 4-year PhD.

Education & Research Experience

2023-10 - **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 energy materials, primarily solar photovoltaics (incl. non-radiative recombination) but also batteries, thermoelectrics, LEDs/emission (exciton self-trapping), COFs, ferroelectrics, using DFT, GW+BSE and some ML.

- Designed & supervised >20 MSc & PhD projects, yielding papers in *Matter, npj Comp Mater, ACS Energy Lett*… alongside multiple prizes for excellent supervision.
- Month-long research stays (Max Planck and JSPS Awards; €1k & £3k) with Profs. Freysoldt (Germany) & Kumagai (Japan); paper in *Faraday Discussion,* 2 in submission.
- 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).
- Archer2 Pioneer Project Lead; notional value £110k.
- Peer reviewer for *J. Am. Chem. Soc.* (*JACS*), *Appl. Phys. Lett. (APL)*, *Matter, Phys. Rev. Appl., J. Phys. Chem. Lett. (JPCL), Phys. Rev. X (PRX) Energy, Comp. Phys. Comm., IOP Model. Simul. Mat. Sci. Eng.* and *J. Electroceramics* (JECR).
- Average 3.5 talks at each MRS Spring/Fall conference since Fall 2020 (1st year PhD).
- Session chair for MRS Fall CH02 (2021) and EN02 (2022) Symposia.
- Featured in the Irish Times: Irish Scientists Shine in Solar Cell Development.
- UCL MAPS Early Career Researcher (ECR) advisory committee member.

- UCL Resources for New Chemistry Researchers (Computational Chemistry) Tutor and 'Python for Chemical Modelling' module Graduate Teaching Assistant (GTA) at UCL.
- Developer of computational chemistry tools: ShakeNBreak, vaspup2.0 and doped, co-developer of sumo, surfaxe, easyunfold, PyTASER, CarrierCapture.jl …

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.

2019-05 - B.A. (Mod): Nanoscience, Physics And Chemistry of Advanced Materials
2015-09 *Trinity College Dublin* – Ireland
Graduated top-of-the-class (margin >10%), Gold Medal, with First Class Honours (88%).

- Henderson-Lloyd prize for the highest overall grade in the Class of 2019, in the Schools of Chemistry and Physics at Trinity College Dublin (margin >10%).
- Trinity Employability Award in Partnership with Intel (2018).
- Elected to Foundation Scholarship, the "most prestigious undergraduate award in Ireland" (€100,000 Value)(2017).
- Represented Trinity College Dublin in the Eurachem Analytical Measurement Competition, achieving 2nd place out of 20 (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.

Awards

- UCL Mathematical & Physical Sciences (MAPS) Faculty Education Award, for Individual Excellence in academic supervision and personal tutoring.

Research Excellence Awards

- MRS Gold Graduate Student Award & Future Leader 2023.
- *Materials Today Chemistry* Rising Star Award 2022.
- Materials Research Society (MRS) Future Leader 2022.
- European Materials Research Society (eMRS) Young Researcher Award 2022.
- MRS Graduate Student Award (Silver) 2022.
- Ramsay Medal for Top Chemistry PhD student in UCL & Catlow Prize for Top Computational Chemistry PhD – typically awarded to final year PhDs, both received in my 2nd-last year.
- eMRS Graduate Student Award 2021 (Symposium A) for outstanding research performance in the field of materials for energy applications.
- eMRS Graduate Student Award 2021 (Symposium F) for outstanding research performance in the field of earth-abundant next-generation solar cell materials.

- Shortlisted for the International Conference on Defects in Semiconductors (ICDS) 2021 Corbett Prize (typically awarded to Associate Professors).
    - In addition, MSc students I've supervised have won the Nyholm (Best Inorganic MSc Project in UCL Chemistry) & Sharp (Best Theoretical) prizes.

Travel Awards & Grants

- UCL-McGill-JSPS Core-to-core research collaboration grant (£3k) to visit Prof. Yu Kumagai in Tohoku University (October – November 2022), to extend our defect structure-searching work.
- Max Planck Travel Award (€1k) for a research stay with Prof. Christoph Freysoldt at Max-Planck-Institut für Eisenforschung (MPIE), Germany (October – November 2022).
- Thomas Young Centre (TYC) Junior Research Fellowship (JRF), 2021 (£1k).
- École Polytechnique Fédérale Lausanne (EPFL) Young Scientist Travel Award 2021.
- Royal Society of Chemistry (RSC) Researcher Development Grant, 2021.
- UCL Mathematical & Physical Sciences Faculty Early Career Researcher Travel Grant (£800).
- Royal Society and UCL Nominee to attend the tri-annual Nobel Chemistry Laureate Meeting in Lindau, Germany, at which I was awarded the Lindau Spirit Fellowship for highly-promising young researchers; given to 4 junior lecturers, 1 postdoc and 1 PhD (me).
- RSC Solid State Chemistry Group Travel Award 2022.

Presentation Prizes & Awards

- Roy Prize for Best Graduate Student Oral Presentation at the RSC 40th Anniversary Solid State Chemistry Group (SSCG) Meeting, 2021 (£250), judged by the invited speakers.
- Excellent Talk Prize at MRS Fall 2022 – '*Impact of Cation Disorder in ABZ_2 Solar Absorbers*'
- Best Presentation Award at EMRS Spring 2022 – '*Cation disorder engineering in $AgBiS_2$*'
- Excellent Talk Prize at MRS Fall 2020 – '*Enhanced Optical Absorption via Mixed-Valent Doping of Vacancy-Ordered $A_3B_2X_9$ Triple Perovskites*'.
- Excellent Talk Prize at SCI Materials for Energy Technology 2021 – '*Rapid Recombination by Cadmium Vacancies in CdTe*'.
- Best Poster at TYC Conference 2020, King's College London – '*Band Alignment of Antimony and Bismuth Silver-Bromide Double Perovskites*'.
- Excellent Poster Prize at RSC Materials Chemistry Poster Symposium 2021 – '*Bandgap Lowering in Lead-Free $Cs_2Ag(Sb_xBi_{1-x})Br_6$ Double Perovskite Alloys*'.
- Best Poster Prize at UCL Chemistry PhD Poster Session (2021) – '*Hidden spontaneous polarisation in the chalcohalide photovoltaic absorber $Sn_2SbS_2I_3$*'.

Publications

(1) **Kavanagh, S. R.** & Wang, Y. (co-authors)**;** Burgués-Ceballos I.; Walsh, A.; Scanlon D., Konstantatos G. Cation Disorder Engineering Yields $AgBiS_2$ Nanocrystals with Enhanced Optical Absorption for Efficient Ultrathin Solar Cells. *Nature Photonics* **2022**, 16 (3), 235-241
(March Issue 'Hero' Image, featured on many news sites) – *50 citations* – doi.org/10.1038/s41566-021-00950-4

(2) Huang, Y.; **Kavanagh, S. R.;** Scanlon, D. O.; Walsh, A.; Hoye, R. L. Z. Perovskite-Inspired Materials for Photovoltaics and beyond — from Design to Devices. *Nanotechnology* **2021**, *32* (13), 132004. *(Authored Sections 1, 2 & 6) 91 citations (**most read/cited 2021 article in IOP Nanotechnology**)* – doi.org/10.1088/1361-6528/abcf6d
- Spotlighted in ***Nature Physics*** (link), before publication.

(3) **Kavanagh, S. R.*** & Mosquera-Lois, I. (co-authors); Walsh, A.; Scanlon, D. O. Identifying the Ground State Structures of Defects in Solids. *npj Computational Materials* **2023** 9(25) – *5 citations* – doi.org/10.1038/s41524-023-00973-1
- Spotlighted in ***Nature Physics*** News & Views (https://www.nature.com/articles/s41567-023-02049-9)

(4) **Kavanagh, S. R.*** & Mosquera-Lois, I. (co-authors); Walsh, A.; Scanlon, D. O. ShakeNBreak: Navigating the defect configurational landscape. *Journal of Open Source Software* **2022**, 7(80), 4817 – *5 citations* – doi.org/10.21105/joss.04817

(5) **Kavanagh, S. R.** & Huang, Y. (co-authors)**;** … Unold, T.; Stranks S. D.; Rao, A.; Herz L. M.; Scanlon, D. O.; Walsh, A.; Hoye. Strong Absorption and Ultrafast Localisation in $NaBiS_2$ Nanocrystals with Slow Charge-Carrier Recombination. *Nature Communications* **2022** 13 (1), 1-13 – *4 citations* – doi.org/10.1038/s41467-022-32669-3

(6) **Kavanagh, S. R.** & Li, Z. (co-authors)… Friend, R. H.; Scanlon, D. O.; Walsh, A.; Hoye, R. L. Z. Bandgap Lowering in Mixed Alloys of $Cs_2Ag(Sb_xBi_{1-x})Br_6$ Double Perovskite Thin Films. *Journal of Materials Chemistry A* **2020**, *8* (41), 21780–21788 – *48 citations* – doi.org/10.1039/D0TA07145E

(7) **Kavanagh, S. R.;** Walsh, A.; Scanlon, D. O. Rapid Recombination by Cadmium Vacancies in CdTe. *ACS Energy Letters* **2021**, 6 (4), 1392–1398 – *27 citations* – doi.org/10.1021/acsenergylett.1c00380

(8) **Kavanagh, S. R.;** Savory, C. N.; Scanlon, D. O.; Walsh, A. Hidden Spontaneous Polarisation in the Chalcohalide Photovoltaic Absorber $Sn_2SbS_2I_3$. *Materials Horizons* **2021,** 8 (10), 2709-2716 – **Outside Front Cover, October Issue** – *16 citations* – doi.org/10.1039/D1MH00764E

(9) **Kavanagh, S. R.*;** Savory, C. N.; Liga, S. M.; Konstantatos G.; Scanlon, D. O.; Walsh, A. Frenkel Excitons in Vacancy-ordered Titanium Halide Perovskites (Cs_2TiX_6). *J. Phys. Chem. Lett.* **2022**, 13, 10965–10975 – *7 citations* – doi.org/10.1021/acs.jpclett.2c02436

(10) **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 – *8 citations* – doi.org/10.1039/D2FD00043A

(11) Krajewska, C.J.; **Kavanagh, S. R.;** Stranks, S. D.; Walsh, A.; Scanlon, D. O.; Palgrave, R.G. Enhanced Visible Light Absorption in Layered $Cs_3Bi_2Br_9$ through Mixed-Valent Sn(II) / Sn(IV) Doping.

Chemical Science **2021**, 12 (44), 14686-14699 – **Outside Front Cover, November Issue,** *16 citations* – doi.org/10.1039/d1sc03775g

(12) Mosquera-Lois, I.; **Kavanagh, S. R.*** In Search of Hidden Defects. *Matter* **2021** *4 (8), 2602-2605* – *From an MSc Project I designed & supervised.* – *10 citations* – doi.org/10.1016/j.matt.2021.06.003

(13) Wang, X.; Li, Z.; **Kavanagh, S. R.;** Ganose, A. M.; Walsh, A. Lone Pair Driven Anisotropy in Antimony Chalcogenide Semiconductors. *Physical Chemistry Chemical Physics* **2022**, *24* (12), 7195–7202 – *18 citations* – doi.org/10.1039/D1CP05373F

(14) Jaśkaniec, S.; **Kavanagh, S. R.;** Walsh, A.; Scanlon, D. O.; Nicolosi, V. Solvent Engineered Synthesis of Layered SnO for High-Performance Anodes. *npj 2D Mater. Appl.* **2021**, *5* (1), 1–9 – *9 citations* – doi.org/10.1038/s41699-021-00208-1

(15) Brlec, K.; **Kavanagh, S. R.;** Savory, C. N.; Scanlon, D. O. Understanding the Photocatalytic Activity of $La_5Ti_2AgS_5O_7$ and $La_5Ti_2CuS_5O_7$ for Green Hydrogen Production: Computational Insights. *ACS Applied Energy Materials* **2022**, *5* (2), 1992–2001 – 5 citations – doi.org/10.1021/acsaem.1c03534

(16) Antonelli, T.; … **Kavanagh, S. R.**; …; Scanlon, D. O.; King, P. D. C. Orbital-Selective Band Hybridisation at the Charge Density Wave Transition in Monolayer $TiTe_2$. *npj Quantum Materials* **2022**, *7* (98), 1-10 – doi.org/10.1038/s41535-022-00508-9

(17) Huang J.; Golomb M. J.; **Kavanagh, S. R.;** Tolborg K.; Ganose A. M.; Walsh A. Band Gap Opening from Displacive instabilities in Layered Covalent-Organic Frameworks. *Journal of Materials Chemistry A* **2022** *10* (25), 13500–13507 – *5 citations* – doi.org/10.1039/D2TA02993F

(18) Wang, X.; Ganose, A. M.; **Kavanagh, S. R.;** Walsh, A. Band Versus Polaron: Charge Transport in Antimony Chalcogenides. *ACS Energy Letters* **2022** *7 (9), 2954–2960 – 3 citations* – doi.org/10.1021/acsenergylett.2c01464

(19) Nicolson, A.; Breternitz, J.; **Kavanagh, S. R.**; Tomm, Y.; Morita, K.; Squires, A.; Tovar, M.; Walsh, A.; Schorr, S.; Scanlon, D. O. Interplay of static and dynamic disorder in the mixed-metal chalcohalide $Sn_2SbS_2I_3$. *Journal of the American Chemical Society* **2023** (Accepted, preprint: doi.org/10.26434/chemrxiv-2022-rkm8l)

(20) Cen, J.; Zhu, B.; **Kavanagh, S. R.**; Squires, A.; Scanlon, D. O. Intrinsic Defect Chemistry of High-Voltage $LiMn_{1.5}Ni_{0.5}O_4$ (LMNO) Spinel Cathode. *Journal of Materials Chemistry A* **2023** Advance Article – https://doi.org/10.1039/D3TA00532A

(21) Wang, X.; **Kavanagh, S. R.;** Walsh, A.; Scanlon, D. O. Four-electron Negative-U Vacancy Defects in Antimony Selenide. Under review at *Physical Review Letters* (Preprint: doi.org/10.48550/arXiv.2302.04901)

(22) Nicolson, A.; **Kavanagh, S. R.**; Savory, C. N.; Watson, G. W.; Scanlon, D. O. Cu_2SiSe_3 as a promising solar absorber: harnessing cation dissimilarity to avoid killer antisites. Under review at *Journal of Materials Chemistry A* (ChemRxiv: https://doi.org/10.26434/chemrxiv-2023-7454p)

(23) Kumagai, O.; **Kavanagh, S. R.**; Tsunoda, N.; Walsh. A; Scanlon, D. O.; Oba. F Alkali Mono-Pnictides: Potential High-efficiency Photovoltaic Materials. Under review at *Advanced Energy Materials*

(23) **Kavanagh, S. R.***; Kumagai, O.; Scanlon, D. O.; Walsh. A High-Throughput Study of Symmetry-Breaking at Oxygen Vacancies in Oxides. In Submission.

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Conference Talks & Posters

See YouTube channel for recorded talks.

1st Year PhD:
'*Band Alignment of Antimony and Bismuth Silver-Bromide Double Perovskites*' Poster @ NanoGe Online Conference: Beyond Lead Halide Perovskites; TYC Conference 2020, King's College London (***Best Poster Prize***); Talk @ NanoGe ComPer 2020

'*Bandgap Lowering in Lead-Free $Cs_2Ag(Sb_xBi_{1-x})Br_6$ Double Perovskite Alloys*' Talk@ RSC Solid-State Chemistry ECR Conference; NanoGe Fall 2020 Poster @ NanoGe HOPV 2020; (Flash Talk) MRS Fall 2020; RSC Materials Chemistry Poster Symposium (***Excellent Poster Prize***)

'*Enhanced Optical Absorption via Mixed-Valent Doping of Vacancy-Ordered $A_3B_2X_9$ Triple Perovskites*' Talk @ MRS Fall 2020 (***Excellent Talk Prize***); NanoGe Fall 2020; MRS Spring 2021; (Invited Talk) @ Morgan Research Group, University of Bath; ***(Invited Talk)*** Centre for Plastic Electronics (CPE) Perovskite Symposium 2021; RSC SSCG 2021 ***(Roy Prize for Best Oral Presentation)***, ACS Fall 2021

'*Solvent Engineered Synthesis of Layered SnO Nanoparticles for High-Performance Anodes*' (Flash Talk) @ MRS Fall 2020

2nd Year PhD:
'*UCL Chemistry & Light Highlight Seminar: Modelling Excited Molecules and Materials*' ***(Invited Talk)*** *Representing the 30-person Scanlon Research Group, alongside 3 other speakers (all Professors).*

'*Rapid Recombination by Cadmium Vacancies in CdTe*' Talk @ MRS Spring 2021; NanoGe HOPV 2021, RSC ECR 2021; ACS Fall 2021; eMRS Fall 2021 (***Graduate Student Award***); ICDS31; SCI Materials for Energy Tech (***Excellent Talk Prize***); MRS Fall 2021

'*Hidden spontaneous polarisation in the chalcohalide photovoltaic absorber $Sn_2SbS_2I_3$*' Talk @ MRS Spring 2021; ACS Fall 2021; eMRS Fall 2021 (***Graduate Student Award***); NanoGe HOPV 2021 Poster (***UCL Chemistry Best Poster Prize)***; MRS Fall 2021

*'Impact of Defect Dynamics on Device Performance: Case Study in CdTe' (**Invited Talk**)* @ Dept. of Computational Materials Design at Max-Planck-Institut für Eisenforschung (MPIE; 2021)

3rd Year PhD:
'Efficient Ultrathin AgBiS2 Solar Cells via Cation Disorder Engineering' Talk @ IOP & SuperSolar Advances in Photovoltaics 2022 (Sole student speaker), MRS Spring 2022 (***Graduate Student Award***); EPFL SeeFuturePV (***Young Scientist Travel Award***); eMRS Spring 2022 (***Best Presentation Award***), *(**Invited Talk**)* @ UCL Materials for the Future Mini-Symposium 2022

'Impact of Metastable Defect Structures on Carrier Recombination in Solar Cells' ***(Invited Talk)*** @ Colorado School of Mines, MRS Spring 2022, RSC Faraday Discussions, eMRS Spring 2022, ETH Zürich Defects in Solids Workshop 2022

'Revealing excitonic behaviour in vacancy-ordered titanium perovskites (Cs_2TiX_6)' Talk @ eMRS Spring 2022 (***Young Researcher Award***), MRS Fall 2022, Poster @ EPFL SeeFuturePV (***Young Scientist Travel Award***), APS March 2023

'Impact of Cation Disorder in ABZ_2 Solar Absorbers' Talk @ MRS Fall 2022 (***Excellent Talk Prize***), MRS Spring 2023, ***Invited Talk*** @ CDT-ACM Christmas Symposium 2022

'Identifying Ground State Structures of Defects in Solids' Talk @ MRS Fall 2022, Tohoku University 2022, Yokohama University 2022, UCL-JSPS Core-to-Core Biannual Conference 2022, GRC Defects in Semiconductors 2022, APS March 2023

4th Year PhD:
'Impact of Intrinsic & Extrinsic Defects on Optoelectronic Properties in Selenium' Talk @ MRS Spring 2023

'Symmetry-Breaking and Reconstruction at Point Defects in Perovskites' Talk @ MRS Spring 2023

'Tin & Titanium Vacancy-Ordered Halide Perovskites: $Cs_2(Sn/Ti)X_6$' ***Invited Talk*** @ MRS Spring 2023

'Symmetry-Breaking and Reconstruction at Point Defects in Solids' ***Invited Talk*** @ Summer of Chemical Theory @ WashU 2023

'Performance Boosters to Efficiency Killers; From bulk disorder to isolated defects' Talk @ MRS Spring 2023 (***Graduate Student Award (Gold)***)

'Shining a light on the future: supercomputers and AI in solar cell research' Invited Outreach Talk @ Pint of Science Festival 2023

Referees

Prof David Scanlon, Chair of Computational Materials Design, UCL. (d.scanlon@ucl.ac.uk)
Prof Aron Walsh, Chair of Materials Design, Imperial College London. (a.walsh@imperial.ac.uk)
Dr Christoph Freysoldt, Defect Chemistry and Spectroscopy Group, Max-Planck-Institut für Eisenforschung GmbH. (freysoldt@mpie.de)

Prof Yu Kumagai, Professor in Multi-Functional Materials Science, Institute for Materials Research, Tohoku University. (yu.kumagai.b1@tohoku.ac.jp)
Prof Robert Hoye, Associate Professor of Inorganic Chemistry & Royal Academy of Engineering Research Fellow, University of Oxford. (robert.hoye@chem.ox.ac.uk)