

# Seán R. Kavanagh

PhD Researcher

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## Flash Summary

- Published 18 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.
- Materials Today Chemistry Rising Star Award, MRS Graduate Student Award (Silver), 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 2<sup>nd</sup> & 3<sup>rd</sup> 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).
- Peer reviewer for *J. Am. Chem. Soc. (JACS)*, *Appl. Phys. Lett. (APL)*, *Matter*, *Phys. Rev. Appl.*, *J. Phys. Chem. Lett. (JPCL)*, *Comp. Phys. Comm.* and *J. Electroceramics (JECR)*.
- 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](#), [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 2<sup>nd</sup> 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

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

## Research Excellence Awards

- *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 2<sup>nd</sup>-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.

## Presentation Prizes & Awards

- Roy Prize for Best Graduate Student Oral Presentation at the RSC 40<sup>th</sup> 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<sub>2</sub> Solar Absorbers’
- Best Presentation Award at EMRS Spring 2022 – ‘Cation disorder engineering in AgBiS<sub>2</sub>’
- Excellent Talk Prize at MRS Fall 2020 – ‘Enhanced Optical Absorption via Mixed-Valent Doping of Vacancy-Ordered A<sub>3</sub>B<sub>2</sub>X<sub>9</sub> 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<sub>2</sub>Ag(Sb<sub>x</sub>Bi<sub>1-x</sub>)Br<sub>6</sub> Double Perovskite Alloys’.
- Best Poster Prize at UCL Chemistry PhD Poster Session (2021) – ‘Hidden spontaneous polarisation in the chalcogenide photovoltaic absorber Sn<sub>2</sub>SbS<sub>2</sub>l<sub>3</sub>’.

## Publications

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(1) **Kavanagh, S. R.** & Wang, Y. (co-authors); Burgués-Ceballos I.; Walsh, A.; Scanlon D., Konstantatos G. Cation Disorder Engineering Yields AgBiS<sub>2</sub> 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](#)) – 48 citations – [doi.org/10.1038/s41566-021-00950-4](https://doi.org/10.1038/s41566-021-00950-4)

(2) Huang, Y.; **Kavanagh, S. R.**; Scanlon, D. O.; Walsh, A.; Hoyer, R. L. Z. Perovskite-Inspired Materials for Photovoltaics and beyond — from Design to Devices. *Nanotechnology* **2021**, 32 (13), 132004.

(Authored Sections 1, 2 & 6) 87 citations (**most read/cited 2021 article in IOP Nanotechnology**) – [doi.org/10.1088/1361-6528/abcf6d](https://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) – [doi.org/10.1038/s41524-023-00973-1](https://doi.org/10.1038/s41524-023-00973-1)

(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 – [doi.org/10.21105/joss.04817](https://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.; Hoyer. Strong Absorption and Ultrafast Localisation in NaBiS<sub>2</sub> Nanocrystals with Slow Charge-Carrier Recombination. *Nature Communications* **2022** 13 (1), 1-13 – [doi.org/10.1038/s41467-022-32669-3](https://doi.org/10.1038/s41467-022-32669-3)

(6) **Kavanagh, S. R.** & Li, Z. (co-authors)... Friend, R. H.; Scanlon, D. O.; Walsh, A.; Hoyer, R. L. Z. Bandgap Lowering in Mixed Alloys of Cs<sub>2</sub>Ag(Sb<sub>x</sub>Bi<sub>1-x</sub>)Br<sub>6</sub> Double Perovskite Thin Films. *Journal of Materials Chemistry A* **2020**, 8 (41), 21780–21788 – 44 citations – [doi.org/10.1039/D0TA07145E](https://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 – 21 citations – [doi.org/10.1021/acsenergylett.1c00380](https://doi.org/10.1021/acsenergylett.1c00380)

(8) **Kavanagh, S. R.**; Savory, C. N.; Scanlon, D. O.; Walsh, A. Hidden Spontaneous Polarisation in the Chalcogenide Photovoltaic Absorber Sn<sub>2</sub>SbS<sub>2</sub>I<sub>3</sub>. *Materials Horizons* **2021**, 8 (10), 2709-2716 – **Outside Front Cover, October Issue** – 16 citations – [doi.org/10.1039/D1MH00764E](https://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<sub>2</sub>TiX<sub>6</sub>). *J. Phys. Chem. Lett.* **2022**, 13, 10965–10975 – [doi.org/10.1021/acs.jpcllett.2c02436](https://doi.org/10.1021/acs.jpcllett.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 – [doi.org/10.1039/D2FD00043A](https://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<sub>3</sub>Bi<sub>2</sub>Br<sub>9</sub> through Mixed-Valent Sn(II) / Sn(IV) Doping. *Chemical Science* **2021**, 12 (44), 14686-14699 – **Outside Front Cover, November Issue**, 15 citations – [doi.org/10.1039/d1sc03775g](https://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.* – 9 citations – [doi.org/10.1016/j.matt.2021.06.003](https://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 – 16 citations – [doi.org/10.1039/D1CP05373F](https://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 – 8 citations – [doi.org/10.1038/s41699-021-00208-1](https://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  $\text{La}_5\text{Ti}_2\text{AgS}_5\text{O}_7$  and  $\text{La}_5\text{Ti}_2\text{CuS}_5\text{O}_7$  for Green Hydrogen Production: Computational Insights. *ACS Applied Energy Materials* **2022**, 5 (2), 1992–2001 – 5 citations – [doi.org/10.1021/acsaem.1c03534](https://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  $\text{TiTe}_2$ . *npj Quantum Materials* **2022**, 7 (98), 1-10 – [doi.org/10.1038/s41535-022-00508-9](https://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 – [doi.org/10.1039/D2TA02993F](https://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 – [doi.org/10.1021/acsenergylett.2c01464](https://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 chalcogenide  $\text{Sn}_2\text{SbS}_2\text{I}_3$ . Under review at the *Journal of the American Chemical Society* (Preprint: [doi.org/10.26434/chemrxiv-2022-rkm8l](https://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  $\text{LiMn}_{1.5}\text{Ni}_{0.5}\text{O}_4$  (LMNO) Spinel Cathode. Under review at *Journal of Materials Chemistry A* (Preprint: [doi.org/10.26434/chemrxiv-2023-nk8lr](https://doi.org/10.26434/chemrxiv-2023-nk8lr))
- (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](https://doi.org/10.48550/arXiv.2302.04901))

(22) Nicolson, A.; **Kavanagh, S. R.**; Savory, C. N.; Watson, G. W.; Scanlon, D. O. Interplay of static and dynamic disorder in the mixed-metal chalcogenide  $\text{Sn}_2\text{SbS}_2\text{I}_3$ . Under review at the *Journal of the American Chemical Society* (Preprint: [doi.org/10.26434/chemrxiv-2022-rkm8l](https://doi.org/10.26434/chemrxiv-2022-rkm8l))

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

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

\* = Corresponding Author

## Conference Talks & Posters

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See YouTube channel for recorded talks.

### 1<sup>st</sup> 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  $\text{Cs}_2\text{Ag}(\text{Sb}_x\text{Bi}_{1-x})\text{Br}_6$  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  $\text{A}_3\text{B}_2\text{X}_9$  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  $\text{SnO}$  Nanoparticles for High-Performance Anodes' (Flash Talk) @ MRS Fall 2020

### 2<sup>nd</sup> 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  $\text{CdTe}$ ' 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 chalcogenide photovoltaic absorber  $\text{Sn}_2\text{SbS}_2\text{I}_3$ ' 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  $\text{CdTe}$ ' (**Invited Talk**) @ Dept. of Computational Materials Design at Max-Planck-Institut für Eisenforschung (MPIE; 2021)



**3<sup>rd</sup> Year PhD:**

'Efficient Ultrathin AgBiS<sub>2</sub> 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<sub>2</sub>TiX<sub>6</sub>)' 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<sub>2</sub> Solar Absorbers' Talk @ MRS Fall 2022 (**Excellent Talk Prize**), (**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

## Referees

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**Prof David Scanlon**, Chair of Computational Materials Design, UCL. ([d.scanlon@ucl.ac.uk](mailto:d.scanlon@ucl.ac.uk))

**Prof Aron Walsh**, Chair of Materials Design, Imperial College London. ([a.walsh@imperial.ac.uk](mailto:a.walsh@imperial.ac.uk))

**Dr Christoph Freysoldt**, Defect Chemistry and Spectroscopy Group, Max-Planck-Institut für Eisenforschung GmbH. ([freysoldt@mpie.de](mailto:freysoldt@mpie.de))

**Prof Yu Kumagai**, Professor in Multi-Functional Materials Science, Institute for Materials Research, Tohoku University. ([yu.kumagai.b1@tohoku.ac.jp](mailto:yu.kumagai.b1@tohoku.ac.jp))

**Prof Robert Hoyer**, Associate Professor of Inorganic Chemistry & Royal Academy of Engineering Research Fellow, University of Oxford. ([robert.hoyer@chem.ox.ac.uk](mailto:robert.hoyer@chem.ox.ac.uk))