

# Seán R. Kavanagh

PhD Researcher

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## Education & Research Experience

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### 2020-02 - Ph.D.: Computational Materials Science

2023-09 Supervisors: Profs David Scanlon (University College London) & Aron Walsh (Imperial College London), UK

Focused on defect processes in solar photovoltaic materials (thermodynamics & non-radiative recombination).

- Supervised several MSc & PhD research projects, producing a publication in *Matter*, 2 papers submitted and 3 in preparation, alongside prizes for research excellence.
- Month-long research stay (via a Max Planck Travel Award; €1k) with Prof. Christoph Freysoldt at MPIE, Germany, for a collaboration on dynamic behaviour of defects.
- Lead tester of VASP (most widely-used computational materials science code in the UK & worldwide) for Archer2 (new UK National Supercomputer), and lead research consultant for procurement of UCL HPC & GPU upgrades 2021/2022 (>£1 million).
- Peer reviewer for the *Journal of the American Chemical Society* (JACS), *Applied Physics Letters* (APL), *Matter* and the *Journal of Electroceramics* (JECE).
- Session chair (in-person) for MRS Fall Chemistry of New Materials (CH02) Symposium.
- 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: [vaspup2.0](#) and [doped](#), co-developer of [sumo](#), [surfaxe](#) and contributions to many others.

### 2018-05 - Research Assistant

2018-09 NOKIA Bell Labs, Dublin, Ireland

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

### 2015-09 - B.A. (Mod): Nanoscience, Physics And Chemistry of Advanced Materials

2019-05 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).

## 2009-09 - High School

**2015-05** 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.
- eMRS Young Researcher Award 2022.
- MRS Graduate Student Award (Silver) 2022.
- 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).

## Travel Awards & Grants

- Max Planck Travel Award (€1k) for a research stay with Prof. Christoph Freysoldt at Max-Planck-Institut für Eisenforschung (MPIE), Germany.
- 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

- Best Presentation Award at EMRS Spring 2022 – ‘*Cation disorder engineering in AgBiS<sub>2</sub>*’
- 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 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 chalcogenide photovoltaic absorber  $Sn_2SbS_2I_3$ ’.

## 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  $AgBiS_2$  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](#)) – 11 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) 53 citations (one of the **most read/cited articles 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.** & 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  $NaBiS_2$  Nanocrystals with Slow Charge-Carrier Recombination. *Nature Communications* (Accepted)

(4) **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  $Cs_2Ag(Sb_xBi_{1-x})Br_6$  Double Perovskite Thin Films. *J. Mater. Chem. A* **2020**, 8 (41), 21780–21788 – 31 citations

[doi.org/10.1039/D0TA07145E](https://doi.org/10.1039/D0TA07145E)

(5) **Kavanagh, S. R.**; Walsh, A.; Scanlon, D. O. Rapid Recombination by Cadmium Vacancies in CdTe. *ACS Energy Lett.* **2021**, 6 (4), 1392–1398 – 10 citations

[doi.org/10.1021/acsenergylett.1c00380](https://doi.org/10.1021/acsenergylett.1c00380).

(6) **Kavanagh, S. R.**; Savory, C. N.; Scanlon, D. O.; Walsh, A. Hidden Spontaneous Polarisation in the Chalcogenide Photovoltaic Absorber  $Sn_2SbS_2I_3$ . *Materials Horizons* **2021**, 8 (10), 2709-2716 – **Outside Front Cover, October Issue** – 6 citations

[doi.org/10.1039/D1MH00764E](https://doi.org/10.1039/D1MH00764E)

(7) **Kavanagh, S. R.**; Scanlon, D. O.; Walsh, A.; Freysoldt, C. Impact of Metastable Defect Structures on Carrier Recombination in Solar Cells. *Faraday Discuss.* **2022**

<https://doi.org/10.1039/D2FD00043A>

(8) Krajewska, C.J.; **Kavanagh, S. R.**; Stranks, S. D.; Walsh, A.; Scanlon, D. O.; Palgrave, R.G. Enhanced Visible Light Absorption in Layered  $\text{Cs}_3\text{Bi}_2\text{Br}_9$  through Mixed-Valent Sn(II) / Sn(IV) Doping. *Chemical Science* **2021**, 12 (44), 14686–14699 – **Outside Front Cover, November Issue**, 4 citations

[doi.org/10.1039/d1sc03775g](https://doi.org/10.1039/d1sc03775g)

(9) Mosquera-Lois, I.; **Kavanagh, S. R.** In Search of Hidden Defects. *Matter* 4 (8), 2602–2605 **2021** – *From an MSc Project I designed & supervised.*

[doi.org/10.1016/j.matt.2021.06.003](https://doi.org/10.1016/j.matt.2021.06.003)

(10) 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 – 5 citations

[doi.org/10.1038/s41699-021-00208-1](https://doi.org/10.1038/s41699-021-00208-1)

(11) 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

[doi.org/10.1021/acsaem.1c03534](https://doi.org/10.1021/acsaem.1c03534)

(12) 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

<https://doi.org/10.1039/D1CP05373F>

(13) Antonelli, T.; ... **Kavanagh, S. R.**; ...; Scanlon, D. O.; King, P. D. C. Orbital-Selective Band Hybridisation at the Charge Density Wave Transition in Monolayer  $\text{TiTe}_2$ . *arXiv:2203.15560 [cond-mat]* **2022** (Under review at *npj Quantum Materials*)

<https://doi.org/10.48550/arXiv.2203.15560>

(14) 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. *J Mater. Chem. A* **2022** 10 (25), 13500–13507

<https://doi.org/10.1039/D2TA02993F>

(15) **Kavanagh, S. R.** & Mosquera-Lois, I. (co-authors); Walsh, A.; Scanlon, D. O. Identifying the Ground State Structures of Defects in Solids. *arXiv: 2207.09862 [cond-mat]* **2022** (Under review at *npj Computational Materials*)

<https://doi.org/10.48550/arXiv.2207.09862>

(16) Wang, X.; Ganose, A. M.; **Kavanagh, S. R.**; Walsh, A. Band Versus Polaron: Charge Transport in Antimony Chalcogenides. *arXiv:2206.15389 [cond-mat]* **2022** (Under review at *ACS Energy Letters*) <https://doi.org/10.48550/arXiv.2206.15389>

Extra: **Kavanagh, S. R.** [High-Throughput Material Modelling - The Key to Accelerated Discovery of Advanced Energy Technologies?](#) *Energy Journal*, 2020. (Student Publication)

## Conference Talks & Posters

### 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' (Talk) Chosen to represent 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)

See YouTube channel for recorded talks.

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

'Efficient Ultrathin  $\text{AgBiS}_2$  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**)

'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 ( $\text{Cs}_2\text{TiX}_6$ )' (Talk) @ eMRS Spring 2022 (**Young Researcher Award**), (Poster) @ EPFL SeeFuturePV (**Young Scientist Travel Award**)

## 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. ([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))