Seán R. Kavanagh

PhD Researcher

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Education & Research Experience

2020-02 - 2023-09 **- Ph.D.: Computational Materials Science**

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 and PhD research projects, producing a publication in *Matter* and 3 others in preparation, alongside prizes in recognition of 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* (JECR).
- Session chair (in-person) for MRS Fall *Solid-State Chemistry of New Materials* (CH02) Symposium.
- 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 - 2018-09 **- Research Assistant**

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

Trinity College Dublin – Ireland

Graduated top-of-the-class (margin >10%), Gold Medal, with First Class Honours (88%).

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

- 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.
- UCL Mathematical & Physical Sciences (MAPS) Faculty Education Award, for Individual Excellence in academic supervision and personal tutoring.
- Shortlisted for the International Conference on Defects in Semiconductors (ICDS) 2021 Corbett Prize (typically awarded to Associate Professors).
- 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).
- 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.
- École Polytechnique Fédérale Lausanne (EPFL) SeeFuturePV 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).
- The nominee of the Royal Society and the UCL Provost to attend the tri-annual Chemistry Nobel Laureate Meeting in Lindau, Germany.
- 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).
- 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*'.
- 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 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** (March Issue 'Hero' Image, featured on many news sites)
doi.org/10.1038/s41566-021-00950-4

(2) Huang, Y.-T.; **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) – 32 citations (one of the* ***most read/cited articles in IOP Nanotechnology****)*
doi.org/10.1088/1361-6528/abcf6d
- Spotlighted in ***Nature Physics*** (link), before publication.

(3) **Kavanagh, S. R.** & Li, Z. (co-authors); Napari, M.; Palgrave, R. G.; Abdi-Jalebi, M.; Andaji-Garmaroudi, Z.; Davies, D. W.; Laitinen, M.; Julin, J.; Isaacs, M. A.; 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. *J. Mater. Chem. A* **2020**, *8* (41), 21780–21788 – *24 citations*
doi.org/10.1039/D0TA07145E

(4) **Kavanagh, S. R.;** Walsh, A.; Scanlon, D. O. Rapid Recombination by Cadmium Vacancies in CdTe. *ACS Energy Lett.* **2021**, 6 (4), 1392–1398 – *8 citations*
doi.org/10.1021/acsenergylett.1c00380.

(5) **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** – *4 citations*
doi.org/10.1039/D1MH00764E

(6) **Kavanagh, S. R.**; Scanlon, D. O.; Walsh, A.; Freysoldt, C. Impact of Metastable Defect Structures on Carrier Recombination in Solar Cells. *Faraday Discuss.* **2022**, Accepted Manuscript
https://doi.org/10.1039/D2FD00043A

(7) 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**
doi.org/10.1039/d1sc03775g

(8) 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

(9) Jaśkaniec, S.; **Kavanagh, S. R.**; Coelho, J.; Ryan, S.; Hobbs, C.; Walsh, A.; Scanlon, D. O.; Nicolosi, V. Solvent Engineered Synthesis of Layered SnO for High-Performance Anodes. *npj 2D Materials and Applications* **2021**, *5* (1), 1–9 – *5 citations*
doi.org/10.1038/s41699-021-00208-1

(10) 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
doi.org/10.1021/acsaem.1c03534

(11) 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

(12) Antonelli, T.; … **Kavanagh, S. R.**; …; Scanlon, D. O.; King, P. D. C. Orbital-Selective Band Hybridisation at the Charge Density Wave Transition in Monolayer $TiTe_2$. *arXiv:2203.15560 [cond-mat]* **2022** (Submitted to npj Quantum Materials)
https://doi.org/10.48550/arXiv.2203.15560

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

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' (Talk) Chosen to represent 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)

See YouTube channel for recorded talks.

3rd Year PhD:
'Efficient Ultrathin AgBiS2 Solar Cells via Cation Disorder Engineering' (Talk) @ IOP & SuperSolar Advances in Photovoltaics 2022 (Only student speaker), MRS Spring 2022 (Graduate Student Award Final)

'Impact of Metastable Defect Structures on Carrier Recombination in Solar Cells' (Invited Talk) @ Colorado School of Mines, MRS Spring 2022

Referees

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