Seán R. Kavanagh

PhD Researcher

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Twitter: @Kavanagh_Sean_

YouTube (Conference Talks): bit.ly/2U5YgLf

Slides: speakerdeck.com/kavanase

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 three others in preparation.
- UCL Resources for New Chemistry Researchers (Computational Chemistry) Tutor
- 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 at NOKIA Bell Labs, focused on the use of chemical and electrochemical techniques to fabricate a microporous, structured surface for the purpose of 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%), with First Class Honours (88%).

2009-09 - 2015-05 **High School**

Castleknock College - Dublin, Ireland

10th highest performer in the nationwide Leaving Certificate exams, out of 58,000 students; one of 7 students to achieve 100% in Chemistry, and one of 3 to achieve 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.
- Shortlisted for the International Conference on Defects in Semiconductors (ICDS) 2021 Corbett Prize (typically awarded to Associate Professors).
- Max Planck Travel Award for a research stay with Prof. Christoph Freysoldt at MPIE, Germany.
- École Polytechnique Fédérale Lausanne (EPFL) SeeFuturePV Young Scientist Travel Grant 2021.
- RSC Researcher Development Grant, to attend and present at ACS Fall 2021.
- 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) 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) – 19 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.

(2) **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 – *17 citations*
doi.org/10.1039/D0TA07145E

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

doi.org/10.1021/acsenergylett.1c00380.

(4) **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* Advance Article **2021** – **Outside Front Cover, October Issue**
doi.org/10.1039/D1MH00764E

(5) 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 (Accepted)* **2021** (Preprint: 10.33774/chemrxiv-2021-k2d20)

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

(7) 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.
doi.org/10.1038/s41699-021-00208-1

(8) **Kavanagh, S. R.** & Wang, Y. (co-authors)**;** Burgués-Ceballos I.; Walsh, A.; Scanlon D., Konstantatos G. Highly Efficient Extremely Thin Absorber Solar Cells enabled by Cation Disorder Engineering. *Nature Photonics* (Under Review)

(9) Wang, X.; Li, Z.; **Kavanagh, S. R.;** Ganose, A. M.; Walsh, A. Lone Pair Driven Anisotropy in Antimony Chalcogenide Semiconductors. *Journal of Chemical Physics* (Under Review)(Preprint: arXiv:2109.08117)

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

'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 Group, alongside 3 other speakers (all PIs).*

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

'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***)

See YouTube channel for recorded talks.

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 Ryan Enright, Senior Member of Technical Staff, Efficient energy transfer (ηet) Dept., Nokia – Bell Labs. (ryan.enright@nokia-bell-labs.com)