

Seán R. Kavanagh

PhD Researcher

E-mail: sean.kavanagh.19@ucl.ac.uk

Website: seankavanagh.com

Google Scholar: bit.ly/3pBMxOG

Twitter: [@Kavanagh_Sean](https://twitter.com/Kavanagh_Sean)

Talks: youtube.com/c/SeánRKavanagh (>20k views) **Slides:** speakerdeck.com/kavanase

Flash Summary

- Published over 26 peer-reviewed papers in 3 years in top-tier journals (*Nature Photonics*, *Nature Communications*, *npj Comp Mater*, *Chemical Science*, *ACS Energy Letters*, *Materials Horizons*, *Matter*, *Phys Rev B*, *PRX Energy*...), including 10 as first-author and 5 as corresponding author.
- Several papers are the result of MSc / PhD projects I designed and supervised.
- MRS Graduate Student Awards (Gold 2023, Silver 2022), *Materials Today Chemistry* Rising Star Award, E-MRS Young Researcher Award, 2 E-MRS Graduate Student Awards, Ramsay Medal (and Catlow Prize) for Best (Computational) Chemistry PhD student in UCL Chemistry 2022.
- UCL Mathematical & Physical Sciences Education Award (& Associate Fellowship of the Higher Education Authority), for 'excellence in academic supervision and personal tutoring'.

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, excitons, COFs, ferroelectrics... using DFT, GW+BSE, RPA...

- Designed & supervised >20 MSc/PhD projects, yielding papers in *JACS*, *Phys Rev Lett*, *npj Comp Mater*, *ACS Energy Lett*, *Matter*... Multiple prizes for supervision excellence.
- Month-long visits (Max Planck & JSPS Awards; €1k & £3k) w/Profs Kumagai (Japan) & Freysoldt (Germany); papers in *Faraday Discussions*, *PRX Energy*. 2 more 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).
- Successful Archer2 Pioneer Project Grant lead author; value £110k.
- Peer reviewer for *J. Am. Chem. Soc. (JACS)*, *Appl. Phys. Lett. (APL)*, *Matter*, *Phys. Rev. Appl. (PRA)*, *J. Phys. Chem. Lett. (JPCL)*, *Phys. Rev. X (PRX) Energy*, *Phys. Rev. Mater. (PRM)*, *ACS Nano Lett.*, *Comp. Phys. Comm.*, *IOP Model. Simul. Mat. Sci. Eng.*, *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.
- Warden/Proctor in Imperial College undergraduate halls (2021-2023); responsibilities of supporting student mental health & wellbeing, discipline and event organisation.
- Mentored several visiting researchers (from Newcastle University, UPC Barcelona, FHI Berlin, Universidad de Santiago...) in defect computation & characterization.

- Featured in the Irish Times: [Irish Scientists Shine in Solar Cell Development](#). iNews...
- UCL Mathematical and Physical Sciences (MAPS) Faculty Early Career Researcher (ECR) advisory committee member, and ECR Forum Awards judge.
- UCL Resources for Computational Chemistry Researchers Tutor and 'Python for Chemical Modelling' module Post-Graduate Teaching Assistant (PGTA) at UCL.
- Developer of computational chemistry tools: [ShakeNBreak](#), [doped](#), [easyunfold](#), [PyTASER](#) and [vaspup2.0](#), contributor to [sumo](#), [surfaxe](#), [CarrierCapture.jl](#)...
- Outreach: [Pint of Science Invited Speaker](#) 2023, "[I'm an Engineer, Get me Out of Here!](#)" (UKRI, bp & Cavendish Nuclear), [YouTube](#) tutorials...

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*

Summa Cum Laude; top-of-the-class (margin >10%), Gold Medal, First Class Honours (88%)

- Henderson-Lloyd prize for the highest overall grade in the Schools of Chemistry and Physics at Trinity College Dublin (by a margin of over 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.
- Associate Fellowship of the Higher Education Authority (AFHEA), awarded for meeting UK Professional Standards in higher education teaching and learning support.
- EPSRC Pioneer Award (lead author) for Archer2 supercomputing resources (2023); value £110k.
- 2023 UCL [Open Science & Scholarship Award](#)

Research Excellence Awards

- Materials Research Society (MRS) Graduate Student Award (Gold) 2023.
- *Materials Today Chemistry* Rising Star Award 2022.

- Ramsay Medal for Best Chemistry PhD student in UCL & Catlow Prize for Best Computational Chemistry PhD – typically awarded to final year PhDs, both received in my 2nd-last year.
- MRS [Future Leader](#) 2023.
- European Materials Research Society (E-MRS) Young Researcher Award 2022.
- Shortlisted for the International Conference on Defects in Semiconductors (ICDS) 2021 [Corbett Prize](#) (typically awarded to Associate Professors).
- MRS Graduate Student Award (Silver) 2022.
- MRS [Future Leader](#) 2022.
- Lindau Spirit Fellowship for highly-promising young researchers; awarded to 4 junior lecturers, 1 postdoctoral and 1 PhD researcher (me), at the Lindau Nobel Chemistry Laureate Meeting.
- E-MRS Graduate Student Award 2021 (Symposium A) for outstanding research performance in the field of materials for energy applications.
- E-MRS Graduate Student Award 2021 (Symposium F) for outstanding research performance in the field of earth-abundant next-generation solar cell materials.
 - In addition, MSc and PhD students I've supervised have won the Nyholm (Best Inorganic MSc Project in UCL Chemistry) & Sharp (Best Theoretical MSc Project in UCL Chemistry) prizes, and the Catlow Prize (Best Computational Chemistry PhD Student in UCL Chemistry); see <https://seankavanagh.com/teaching/>.

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.
- Best Poster Prize at the RSC International Conference on Materials Chemistry (MC16) – '*Tin & Titanium Vacancy-Ordered Halide Perovskites: Cs₂(Sn/Ti)X₆*'
- Excellent Talk Prize at MRS Fall 2022 – '*Impact of Cation Disorder in ABZ₂ Solar Absorbers*'
- Best Presentation Award at E-MRS Spring 2022 – '*Cation disorder engineering in AgBiS₂*'
- Excellent Talk Prize at MRS Fall 2020 – '*Enhanced Optical Absorption via Mixed-Valent Doping of Vacancy-Ordered A₃B₂X₉ 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 Cs₂Ag(Sb_xBi_{1-x})Br₆ Double Perovskite Alloys*'.
- Best Poster Prize at UCL Chemistry PhD Poster Session (2021) – '*Hidden spontaneous polarisation in the chalcogenide photovoltaic absorber Sn₂SbS₂I₃*'.

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.
- RenewPV travel grant for the International Workshop on Emerging Inorganic Chalcogenides Photovoltaics in Tallinn, Estonia 2023.

Publications (*h*-index = 13; October 2023)

I am a firm believer in open science, all publications are openly-available online; see [Google Scholar](#)

* = Corresponding Author

(1) **Kavanagh, S. R.** & Wang, Y. (joint 1st-authors); Burgués-Ceballos I.; Walsh, A.; Scanlon D., Konstantatos G. Cation Disorder Engineering Yields AgBiS₂ 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](#)) – 66 citations – 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) 104 citations (**most read/cited 2021 article in IOP Nanotechnology**) –

doi.org/10.1088/1361-6528/abcf6d

- Spotlights in *Nature Physics* ([link](#)), before publication.

(3) **Kavanagh, S. R.*** & Mosquera-Lois, I. (joint 1st-authors); Walsh, A.; Scanlon, D. O. Identifying the Ground State Structures of Defects in Solids. *npj Computational Materials* **2023** 9(25) – 12 citations –

doi.org/10.1038/s41524-023-00973-1

- Spotlights in *Nature Physics* News & Views (<https://www.nature.com/articles/s41567-023-02049-9>)

(4) **Kavanagh, S. R.*** & Mosquera-Lois, I. (joint 1st-authors); Walsh, A.; Scanlon, D. O. ShakeNBreak: Navigating the defect configurational landscape. *Journal of Open Source Software* **2022**, 7(80), 4817 – 7 citations – doi.org/10.21105/joss.04817

(5) **Kavanagh, S. R.** & Huang, Y. (joint 1st-authors); ... Unold, T.; Stranks S. D.; Rao, A.; Herz L. M.; Scanlon, D. O.; Walsh, A.; Hoyer. Strong Absorption and Ultrafast Localisation in NaBiS₂ Nanocrystals with Slow Charge-Carrier Recombination. *Nature Communications* **2022** 13 (1), 1-13 – 13 citations – doi.org/10.1038/s41467-022-32669-3

- (6) **Kavanagh, S. R.** & Li, Z. (joint 1st-authors)... Friend, R. H.; Scanlon, D. O.; Walsh, A.; Hoyer, R. L. Z. Bandgap Lowering in Mixed Alloys of $\text{Cs}_2\text{Ag}(\text{Sb}_x\text{Bi}_{1-x})\text{Br}_6$ Double Perovskite Thin Films. *Journal of Materials Chemistry A* **2020**, 8 (41), 21780–21788 – 59 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 – 34 citations – doi.org/10.1021/acseenergylett.1c00380
- (8) **Kavanagh, S. R.**; Savory, C. N.; Scanlon, D. O.; Walsh, A. Hidden Spontaneous Polarisation in the Chalcogenide Photovoltaic Absorber $\text{Sn}_2\text{SbS}_2\text{I}_3$. *Materials Horizons* **2021**, 8 (10), 2709–2716 – **Outside Front Cover, October Issue** – 18 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 – 13 citations – doi.org/10.1021/acs.jpcclett.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 – 13 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 $\text{Cs}_3\text{Bi}_2\text{Br}_9$ through Mixed-Valent Sn(II) / Sn(IV) Doping. *Chemical Science* **2021**, 12 (44), 14686–14699 – **Outside Front Cover, November Issue**, 18 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.* – 12 citations – doi.org/10.1016/j.matt.2021.06.003
- (13) 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 – 5 citations – doi.org/10.1021/acseenergylett.2c01464
- (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 – 11 citations – doi.org/10.1038/s41699-021-00208-1
- (15) 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 $\text{Sn}_2\text{SbS}_2\text{I}_3$. *Journal of the American Chemical Society* **2023** 145 (23) 12509–12517 – doi.org/10.1021/jacs.2c13336

- (16) 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 – 8 citations – doi.org/10.1021/acsaem.1c03534
- (17) Antonelli, T.; ... **Kavanagh, S. R.** et al. 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
- (18) 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. *Journal of Materials Chemistry A* **2023**, 11 (27), 14833–14839 – doi.org/10.1039/D3TA02429F
- (19) 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 – 7 citations – doi.org/10.1039/D2TA02993F
- (20) 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 – 21 citations – doi.org/10.1039/D1CP05373F
- (21) 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. *Journal of Materials Chemistry A* **2023**, 11 (25), 13353–13370 – doi.org/10.1039/D3TA00532A
- (22) Andreasen, J. W. ... **Kavanagh, S. R.** et al.
- Indium-free CIGS analogues. *Faraday Discussions* **2022**, 239, 85–111 – doi.org/10.1039/D2FD90055F
 - Bulk and surface characterisation techniques of solar absorbers. *Faraday Discussions* **2022**, 239, 180–201 – doi.org/10.1039/D2FD90056D
 - Novel chalcogenides, pnictides and defect-tolerant semiconductors. *Faraday Discussions* **2022**, 239, 287–316 – doi.org/10.1039/D2FD90057B
 - Materials design and bonding. *Faraday Discussions* **2022**, 239, 375–404 – doi.org/10.1039/D2FD90058K
- (23) Kumagai, Y.; **Kavanagh, S. R.**; Tsunoda, N.; Walsh, A.; Scanlon, D. O.; Oba, F. Alkali Mono-Pnictides: Potential High-efficiency Photovoltaic Materials. *PRX Energy* **2023**, 2, 043002 – doi.org/10.1103/PRXEnergy.2.043002
- (24) Mosquera-Lois, I.; **Kavanagh, S. R.**; Klarbring, J.; Tolborg, K.; Walsh, A. Imperfections are not OK: Free Energy of Point Defects in Crystals. *Chemical Society Reviews* (Invited Review) **2023**, 52, 5812–5826 – doi.org/10.1039/D3CS00432E

(25) **Kavanagh, S. R.** & Liga, S. M. (joint 1st-authors); Walsh, A.; Scanlon, D. O.; Konstantatos G. Environmentally-friendly mixed titanium/tin (IV) based vacancy-ordered double perovskites. *J. Phys. Chem. C*. (Special Issue on physicochemical properties of perovskites; in press) (Preprint: doi.org/10.26434/chemrxiv-2023-tqvh2-v2)

(26) Wang, X.; **Kavanagh, S. R.**; Walsh, A.; Scanlon, D. O. Four-electron Negative-U Vacancy Defects in Antimony Selenide. *Physical Review B* **2023**, 108, 134102 – doi.org/10.1103/PhysRevB.108.134102

(27) Zhu, B.; **Kavanagh, S. R.**; Scanlon, D. O.; easyunfold: A Python package for unfolding electronic band structures. *In submission to Journal of Open Source Software (JOSS)* – joss.theoj.org/papers/e874a8adc53c61f40573b2d707ebf1e4

(28) Don, C. H; Smiles, M. J.; **Kavanagh, S. R.**; Shalvey, T.; Scanlon, D. O.; Veal, T. Band gap and band alignment trends of antimony sulfur/selenide (Sb₂(S/Se)₃) solar cells. *In Submission*.

(29) **Kavanagh, S. R.**; A. Walsh; Scanlon, D. O.; doped: A Python package for modelling defects in solids. *In submission to Journal of Open Source Software (JOSS)* – doped.readthedocs.io

(30) Jagadish, K... **Kavanagh, S. R.**... Gasparini, N; Dubal, D; Rondiya, S. Interface Characterization Tools for Copper-based Quaternary Chalcogenides: Review and Prospects. *In Submission*.

(31) Aggarwal, S.; **Kavanagh, S. R.**; Woo, Y. W.; Ganose, A. M.; A. Walsh; PyTASER: Simulating transient absorption spectroscopy (TAS) with DFT. *In submission to Journal of Open Source Software (JOSS)* – pytaser.readthedocs.io

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

(33) Murdock, B.; Cen, J.; Squires, A. G.; **Kavanagh, S. R.**; Zhu, B.; Scanlon, D. O.; Tapia-Ruiz, N. How cationic substitution alters the bulk structure of the high-voltage LiNi_{0.5}Mn_{1.5}O₄ cathode: Systematic combined XRD and neutron diffraction study of LiNi_{0.5-x}M_xMn_{1.5}O₄ (M = Fe, Mg, x = 0.05-0.2). *In submission*.

Software

I am a firm believer in open science, all software developed is openly-available online; see [GitHub](https://github.com)

- **ShakeNBreak**: Navigating the defect configurational landscape. **Kavanagh, S. R.**; Mosquera-Lois, I. – <https://shakenbreak.readthedocs.io> (500 downloads/month)
- **doped**: Calculating point defects in solids. **Kavanagh, S. R.** – doped.readthedocs.io (500 downloads/month)
- **easyunfold**: Unfolding electronic band structures. Zhu, B. Z; **Kavanagh, S. R.** – <https://smtg-ucl.github.io/easyunfold> (150 downloads/month)

- **vaspup2.0**: VASP convergence testing (energy, forces, dielectrics...). Kavanagh, S. R. – <https://github.com/kavanase/vaspup2.0> (50 downloads/month)
- **PyTASER**: Simulating Transient Absorption Spectroscopy (TAS). Aggarwal, S.; Kavanagh, S. R.; Woo, Y.; Ganose, A. M.; Walsh, A. – <https://pytaser.readthedocs.io> (70 downloads/month)

Contributor:

- **sumo**: Plotting & analysing solid-state electronic/phonon structure – <https://smtg-ucl.github.io/sumo>
- **surfaxe**: Surface slab generation & analysis – <https://surfaxe.readthedocs.io>
- **CarrierCapture.jl**: Calculating non-radiative electron-hole recombination at defects – <https://wmd-group.github.io/CarrierCapture.jl>
- **py-sc-fermi**: Calculating defect concentrations – <https://py-sc-fermi.readthedocs.io>
- **pymatgen**: Computational materials analysis – <https://pymatgen.org/index.html>

Conference Talks & Posters

I am a firm believer in open science, all recorded talks are openly-available online; see [YouTube](#)

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 $\text{Cs}_2\text{Ag}(\text{Sb}_x\text{Bi}_{1-x})\text{Br}_6$ 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 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; E-MRS 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; E-MRS 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**); E-MRS 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, E-MRS Spring 2022, ETH Zürich Defects in Solids Workshop 2022

'Revealing excitonic behaviour in vacancy-ordered titanium perovskites (Cs₂TiX₆)' Talk @ E-MRS Spring 2022 (**Young Researcher Award**), MRS Fall 2022, Poster @ EPFL SeeFuturePV (**Young Scientist Travel Award**), APS March 2023

'Impact of Cation Disorder in ABZ₂ 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, RenewPV Workshop (Tallinn, Estonia)

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

'Tin & Titanium Vacancy-Ordered Halide Perovskites: Cs₂(Sn/Ti)X₆' **Invited Talk** @ MRS Spring 2023, Poster @ RSC International Conference on Materials Chemistry (MC16) (**Best Poster Prize**)

'Symmetry-Breaking and Reconstruction at Point Defects in Solids' **Invited Talk** @ Summer of Chemical Theory @ WashU 2023, **Invited Talk** @ [TimeMan Seminars](#), University of Lille

'Performance Boosters to Efficiency Killers; From bulk disorder to isolated defects' Talk @ MRS Spring 2023 (**Gold Graduate Student Award**), RSC International Conference on Materials Chemistry (MC16)

'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.bl@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)

Dr. Sinéad Griffin, Staff Scientist, Materials Science Division and Molecular Foundry, Berkeley Lab (sgriffin@lbl.gov)

Prof. Sir. Richard Catlow, Foreign Secretary & Vice President of the Royal Society and Professor of Computational and Materials Chemistry, UCL. (c.r.a.catlow@ucl.ac.uk)