

# Alex M. Ganose

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## Education and Training

### Lawrence Berkeley National Laboratory (2018 – present)

Postdoctoral scholar

Topic: Materials data mining

### University College London (2015 – 2018)

EngD in Molecular Modelling and Materials Science

Thesis title: “Atomic-scale insights into emerging photovoltaic absorbers.”

### University College London (2014 – 2015)

MRes. in Molecular Modelling and Materials Science, Distinction

Dissertation title: “Tailoring the band gap of SnO<sub>2</sub> for improved transparent electronic conducting properties in solar cells.”

### University College London (2010 – 2014)

MSci. in Natural Sciences (Organic Chemistry and Neuroscience), 1st Class Honours

Dissertation title: “Synthesis of novel covalent organic frameworks.”

## Awards

2018 Scopus Early Career Researcher Award

2018 Catlow Prize, UCL

2018 Materials Research Society Graduate Student Award (Gold)

2017 Materials Research Society Graduate Student Award (Silver)

2017 Best use of ARCHER (UK national supercomputer) Award

2015 Violet Horshall Prize, UCL

## Teaching

2015 – 2018: Supervised 11 final year research projects, UCL

2015 – 2018: Demonstrator for M<sup>3</sup>S Computational Labs, UCL

2015 – 2018: Demonstrator for 1<sup>st</sup> and 2<sup>nd</sup> year Inorganic Chemistry Workshops, UCL

## Publications

 23 published, 5 in submission, 560 citations, H-index of 12, [Google Citations](#)

1. N. H. Bashian, S. Zhou, M. Zuba, **A. M. Ganose**, J. W. Stiles, A. Ee, D. S. Ashby, D. O. Scanlon, L. F. J. Piper, B. S. Dunn, B. C. Melot, Correlated Polyhedral Rotations in the Absence of Polarons During Electrochemical Insertion of Lithium in ReO<sub>3</sub>, *ACS Energy Letters*, **3**, 2513–2519 (2018) doi: 10.1021/acsenergylett.8b01179
2. **A. M. Ganose**, A. J. Jackson, D. O. Scanlon, sumo: Command-line tools for plotting and analysis of periodic ab initio calculations, *Journal of Open Source Software*, **3**, 717 (2018) doi: 10.21105/joss.00717
3. A. J. Jackson, **A. M. Ganose**, A. Regoutz, R. G. Egdell, D. O. Scanlon, Galore: Broadening

and weighting for simulation of photoelectron spectroscopy, *Journal of Open Source Software*, **3**, 773 (2018) doi: 10.21105/joss.00773

4. A. E. Maughan, **A. M. Ganose**, M. Almaker, D. O. Scanlon, and J. R. Neilson, Anharmonicity and Octahedral Tilting in Hybrid Vacancy-Ordered Double Perovskites, *Chemistry of Materials*, **30**, 472–483 (2018) doi: 10.1021/acs.chemmater.7b04516
5. **A. M. Ganose**, S. Matsumoto, J. Buckeridge, and D. O. Scanlon, Defect engineering of earth-abundant solar absorbers BiSI and BiSeI, *Chemistry of Materials*, **30**, 3827–3835 (2018) doi: 10.1021/acs.chemmater.8b01135
6. **A. M. Ganose**, L. Gannon, F. Fabrizi, H. Nowell, S. A. Barnett, H. Lei, X. Zhu, C. Petrovic, D. O. Scanlon, and M. Hoesch, Local corrugation and persistent charge density wave in ZrTe<sub>3</sub> with Ni intercalation, *Physical Review B*, **97**, 155103 (2018) doi: 10.1103/PhysRevB.97.155103
7. Z. Wang, **A. M. Ganose**, C Niu, and D. O. Scanlon, First-principles insights into tin-based two-dimensional hybrid halide perovskites for photovoltaics, *Journal of Materials Chemistry A*, **6**, 5652–5660 (2018) doi: 10.1039/C8TA00751A
8. A. E. Maughan, **A. M. Ganose**, A. M. Candia, J. T. Granger, D. O. Scanlon, and J. R. Neilson, Anharmonicity and Octahedral Tilting in Hybrid Vacancy-Ordered Double Perovskites, *Chemistry of Materials*, **30**, 472–483 (2018) doi: 10.1021/acs.chemmater.7b04516
9. D. Biswas, **A. M. Ganose**, R. Yano, J. M. Riley, L. Bawden, O.J. Clark, J. Feng, L. Collins-Mcintyre, M.T. Sajjad, W. Meevasana, T.K. Kim, M. Hoesch, J.E. Rault, T. Sasagawa, D. O Scanlon, P. D. C. King, Narrow-band anisotropic electronic structure of ReS<sub>2</sub>, *Physical Review B*, **96**, 085205 (2017) doi: 10.1103/PhysRevB.96.085205
10. C. N. Savory, **A. M. Ganose**, and D. O. Scanlon, Exploring the PbS-Bi<sub>2</sub>S<sub>3</sub> series for next generation energy conversion materials, *Chemistry of Materials*, **29**, 5156–5167 (2017) doi: 10.1021/acs.chemmater.7b00628
11. **A. M. Ganose**, C. N. Savory, and D. O. Scanlon, Electronic and defect properties of (CH<sub>3</sub>NH<sub>3</sub>)<sub>2</sub>Pb(SCN)<sub>2</sub>I<sub>2</sub> analogues for photovoltaic applications, *Journal of Materials Chemistry A*, **5**, 7845–7853 (2017) doi: 10.1021/acs.chemmater.7b00464
12. C. H. Hendon, K. T. Butler, **A. M. Ganose**, Y. Roman-Leshkov, D. O Scanlon, G. A. Ozin, A. Walsh, Electroactive Nanoporous Metal Oxides and Chalcogenides by Chemical Design, *Chemistry of Materials*, **29**, 3663–3670 (2017) doi: 10.1039/C7TA01688C
13. **A. M. Ganose**, C. N. Savory, and D. O. Scanlon, Beyond Methylammonium Lead Iodide: Prospects for the Emergent Field of *ns*<sup>2</sup> Containing Solar Absorbers, *Chemical Communications*, Accepted (2016) doi: 10.1039/C6CC06475B
14. C. N. Savory, **A. M. Ganose**, W. Travis, R. S. Atri, R. G. Palgrave and D. O. Scanlon, An Assessment of Silver Copper Sulphides for Photovoltaic Applications: Theoretical and Experimental Insights, *Journal of Materials Chemistry A*, **4**, 12648 (2016) doi: 10.1039/C6TA03376H
15. A. E. Maughan, **A. M. Ganose**, M. M. Bordelon, E. M. Miller, D. O. Scanlon, and J. R. Neilson, Defect Tolerance to Intolerance in the Vacancy Ordered Double Perovskite Semiconductors Cs<sub>2</sub>SnI<sub>6</sub> and Cs<sub>2</sub>TeI<sub>2</sub>, *Journal of the American Chemical Society*, **138**, 8453 (2016) doi: 10.1021/jacs.6b03207
16. N. F. Quackenbush, H. Paik, M. J. Wahila, S. Sallis, M. E. Holtz, X. Huang, **A. M. Ganose**, B. J. Morgan, D. O. Scanlon, Y. Gu, F. Xue, L.-Q. Chen, G. E. Sterbinsky, C. Schlueter, T.-L. Lee, J. C. Woicik, J.-H. Guo, J. D. Brock, D. A. Muller, D. A. Arena, D. G. Schlom, and L. F. J. Piper, The stability of the M2 phase of vanadium dioxide induced by coherent epitaxial strain, *Physical Review B*, **94**, 085105 (2016) doi: 10.1103/PhysRevB.94.085105
17. **A. M. Ganose**, M. Cuff, K. T. Butler, A. Walsh and D. O. Scanlon, Interplay of Orbital and Relativistic Effects in Bismuth Oxyhalides: BiOF, BiOCl, BiOBr and BiOI, *Chemistry of Materials*, **28**, 1980 (2016) doi: 10.1021/acs.chemmater.6b00349

18. W. Travis, C. Knapp, C. N. Savory, **A. M. Ganose**, P. Kafourou, X. Song, Z. Sharif, J. K. Cockcroft, D. O. Scanlon, H. Bronstein and R. G. Palgrave, Hybrid Organic–Inorganic Coordination Complexes as Tunable Optical Response Materials, *Inorganic Chemistry*, **55**, 3393 (2016) doi: 10.1021/acs.inorgchem.5b02749
19. **A. M. Ganose**, K. T. Butler, A. Walsh and D. O. Scanlon, Relativistic Electronic Structure and Band Alignment of BiSI and BiSeI: Candidate Photovoltaic Materials, *Journal of Materials Chemistry A*, **4**, 2060 (2016) doi: 10.1039/C5TA09612J
20. Y. Hu, N. Goodeal, Y. Chen, **A. M. Ganose**, R. G. Palgrave, H. Bronstein, M. O. Blunt, Probing the chemical structure of monolayer covalent-organic frameworks grown via Schiff-base condensation reactions, *Chemical Communications*, **52**, 9941–9944 (2016)
21. **A. M. Ganose** and D. O. Scanlon, Band gap and work function tailoring of SnO<sub>2</sub> for improved transparent conducting ability in photovoltaics, *Journal of Materials Chemistry C*, **4**, 1467 (2016) doi: 10.1039/C5TC04089B
22. **A. M. Ganose**, C. N. Savory and D. O. Scanlon, (CH<sub>3</sub>NH<sub>3</sub>)<sub>2</sub>Pb(SCN)<sub>2</sub>I<sub>2</sub>: a more stable structural motif for hybrid halide photovoltaics?, *Journal of Physical Chemistry Letters*, **6**, 4594 (2015) doi: 10.1021/acs.jpcllett.5b02177
23. C. I. Hiley, D. O. Scanlon, A. A. Sokol, S. M. Woodley, **A. M. Ganose**, S. Angio, J. M. De Teresa, P. Manuel, D. D. Khalyavin, M. Walker, M. R. Lees, and R. I. Walton, Antiferromagnetism at T > 500K in the layered hexagonal ruthenate SrRu<sub>2</sub>O<sub>6</sub>, *Physical Review B*, **92**, 104413 (2015) doi: 10.1103/PhysRevB.92.104413

### Conference Presentations (Oral) (2016 – present)

1. **Contributed** “Improving the Stability of the Hybrid Perovskites – A New Structural Motif”, *MRS Spring Meeting*, Arizona, USA (2018)
2. **Contributed** “Earth-Abundant Bismuth-Based Semiconductors as Novel Photovoltaics”, *MRS Spring Meeting*, Arizona, USA (2018)
3. **Contributed** “High ZT Thermoelectrics Identified from Defect Screening of Complex Oxides”, *MRS Spring Meeting*, Arizona, USA (2018)
4. **Contributed** “Beyond CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub>: Prospects for Emergent Solar Absorbers”, *MRS Spring Meeting*, Arizona, USA (2018)
5. **Contributed** “Identification of high ZT thermoelectrics from complex oxide screening”, *American Chemical Society*, New Orleans, USA (2018)
6. **Invited** “Defect Chemistry of Emerging Materials for Photovoltaics”, *Seminar*, Colorado State University, USA (2018)
7. **Contributed** “Identification of high ZT thermoelectrics from complex oxide screening”, *American Chemical Society*, New Orleans, USA (2018)
8. **Contributed** “Bismuth chalcogenides as earth-abundant and non-toxic photovoltaics”, *American Chemical Society*, New Orleans, USA (2018)
9. **Contributed** “Computational screening of complex oxides for high performance thermoelectrics”, *Thomas Young Centre Student Day*, University College London, UK, (2018)
10. **Invited** “The search for transparent oxide thermoelectrics”, *Thomas Young Centre Lunchtime Get-Together*, University College London, UK (2017)
11. **Invited** “Searching for high ZT oxide thermoelectrics”, *Spectroscopy Village*, Diamond Light Source, UK (2017)
12. **Contributed** “Screening of complex oxides for high ZT thermoelectrics”, *MRS Fall Meeting*, Boston, USA (2017)
13. **Contributed** “Non-toxic and earth-abundant V–VI–VII semiconductors for solar cells”, *Advances in Photovoltaics*, London, UK (2017)
14. **Invited** “Non-toxic and earth-abundant bismuth chalcogenide photovoltaics”, *CAM-IES*, London, UK (2017)
15. **Contributed** “Non-toxic and earth-abundant V–VI–VII semiconductors for solar cells”, *E-MRS Spring Meeting*, Strasbourg, France (2016)
16. **Contributed** “Beyond MAPbI<sub>3</sub>: the search for stable hybrid halide perovskites”, *E-MRS Spring Meeting*, Strasbourg, France (2016)

17. **Contributed** "Tuning the band gap of SnO<sub>2</sub> for improved transparent conducting oxide properties in photovoltaics", *Material Chemistry Consortium Conference*, Cardiff, UK (2016)
18. **Contributed** "(CH<sub>3</sub>NH<sub>3</sub>)<sub>2</sub>Pb(SCN)<sub>2</sub>I<sub>2</sub>: a new more stable structural motif for hybrid halide photovoltaics?", *RSC Next Generation Materials for Solar Photovoltaics*, London, UK (2016).
19. **Contributed** "The search for non-toxic and earth-abundant solar absorbers", *SuperSolar Hub – Winter Technical Meeting*, London, UK (2016)

## Other Skills

Proficient at programming in Python, C++/Java/bash and using the command line.  
Experience using the LaTeX typesetting system.

## Personal Interests

Contributing to open source programming projects.  
Keen interest in art, music, technology, literature, and cycling.

## References

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