

# Alex M. Ganose

Department of Materials  
Faculty of Engineering  
Imperial College London  
South Kensington Campus, London SW7 2AZ

email: [a.ganose@imperial.ac.uk](mailto:a.ganose@imperial.ac.uk)  
web: [utf.github.com](https://utf.github.com)

phone: +44 7868 274 499

## EMPLOYMENT

2021– *Imperial College London*  
EPSRC Research Fellow  
Role: Independent research fellow studying renewable energy materials.

## EDUCATION AND TRAINING

2018–2021 *Lawrence Berkeley National Laboratory*  
Postdoctoral scholar, The Materials Project  
Topic: Data-driven methods, electron transport, many-body lattice dynamics

2015–2018 *University College London*  
EngD in Molecular Modelling and Materials Science  
Thesis title: “Atomic-scale insights into emerging photovoltaic absorbers.”

2014–2015 *University College London*  
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.”

2010–2014 *University College London*  
MSci. in Natural Sciences (Organic Chemistry and Neuroscience), First class  
Dissertation title: “Synthesis of novel covalent organic frameworks.”

## FUNDING

2021– EPSRC Postdoctoral Fellowship (PI, £378,578)  
Imperial College London

2021– Marie Skłodowska-Curie Individual Fellowship (PI, €212,933)  
Imperial College London  
*Declined for EPSRC Fellowship*

## AWARDS

2019 Springer Thesis Prize (£1,500)  
2019 Chemistry of Materials Lectureship and Best Paper Award (£600)  
2019 UCL Maths and Physical Sciences Postgraduate Research Prize  
2018 Scopus Early Career Researcher Award (£1,500)

2018	UCL Catlow Prize
2018	Gold MRS Graduate Student Award, MRS 2018 Spring Meeting (\$400)
2017	Silver MRS Graduate Student Award, MRS 2017 Fall Meeting (\$200)
2017	Best use of ARCHER (UK national supercomputer) Award (£3,000)
2017	Best Poster Prize, UCL Department of Chemistry
2017	Best Poster Prize, UCL Department of Chemistry
2015	UCL Violet Horshall Prize (£200)

#### SUPERVISING & MENTORING

2021–	Co-mentor for a PhD student, University of Illinois at Urbana-Champaign
2020–	Co-supervisor for Berkeley Undergraduate Summer Intern, LBNL
2018–	Mentored 5 undergraduate research projects, LBNL
2015–2018	Supervised 11 final year research projects, UCL

#### TEACHING, DEMONSTRATING & OUTREACH

2020–	Delivered 2-day data science seminar for the LBNL Director's Apprenticeship Program for underrepresented high school students in STEM
2019–	Materials Project workshop instructor in data science and machine learning, LBNL
2015–2018	Demonstrator for M <sup>3</sup> S Computational Chemistry Labs, UCL
2015–2018	Supervisor for 1 <sup>st</sup> and 2 <sup>nd</sup> year Inorganic Chemistry Workshops, UCL

#### CONFERENCE ORGANISATION

2018	Assistant organiser for TYC 5 <sup>th</sup> Energy Workshop: From Atoms to Applications, with 99 attendees ranging from established academics, to PDRAs, PhD and undergraduate students, and representation by Senior Editors from Nature and Nature Materials. The programme featured invited talks from established leaders in the field from the US, Europe, and Asia.
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#### PROFESSIONAL MEMBERSHIPS

Member of the RSC, Member of the ACS, Member of the MRS

#### INVITED SEMINARS & COLLOQUIA

A\*STAR (Singapore, 2020), University of Bath (UK, 2020); Imperial College London (UK, 2020), University of Warwick (UK, 2019); University of California, Santa Barbara (USA, 2019); Colorado State University, (USA, 2018); Thomas Young Centre (UK, 2017); Diamond Light Source (UK, 2017)

#### SELECTED CONFERENCE PRESENTATIONS (*international only*)

2020	<i>Invited</i>	An efficient approach for calculating thermoelectric transport properties, <i>Virtual Conference on Thermoelectrics</i>
2019	<i>Invited</i>	Defect and carrier transport properties of emerging bismuth-based

- photovoltaics, ACS, San Diego, USA
- 2019 *Invited* Computational approaches for smart high-throughput calculations and machine learning, CECAM, Liverpool, UK
- 2018 Earth-Abundant Bismuth-Based Semiconductors as Novel Photovoltaics, MRS Spring Meeting, Arizona, USA
- 2018 High ZT Thermoelectrics Identified from Defect Screening of Complex Oxides, MRS Spring Meeting, Arizona, USA
- 2018 Beyond  $\text{CH}_3\text{NH}_3\text{PbI}_3$ : Prospects for Emergent Solar Absorbers, MRS Spring Meeting, Arizona, USA
- 2018 Improving the Stability of the Hybrid Perovskites – A New Structural Motif, MRS Spring Meeting, Arizona, USA
- 2018 Identification of high ZT thermoelectrics from complex oxide screening, ACS, New Orleans, USA
- 2018 Bismuth chalcogenides as earth-abundant and non-toxic photovoltaics, ACS, New Orleans, USA
- 2017 Screening of complex oxides for high ZT thermoelectrics, MRS Fall Meeting, Boston, USA
- 2017 *Invited* Non-toxic and earth-abundant bismuth chalcogenide photovoltaics, CAM-IES, London, UK
- 2016 Non-toxic and earth-abundant V–VI–VII semiconductors for solar cells, E-MRS Spring Meeting, Strasbourg, France
- 2016 Beyond  $\text{MAPbI}_3$ : the search for stable hybrid halide perovskites, E-MRS Spring Meeting, Strasbourg, France

PUBLICATIONS [GOOGLE SCHOLAR] 41 published, 4 in review, > 1800 citations, H-index of 21

1. **Ganose, A. M.**; Park, J.; Faghaninia, A.; Woods-Robinson, R.; Kristin A.P.; Jain, A.; Efficient calculation of carrier scattering rates from first principles. *Nat. Commun.* 2021, 12 2222 [DOI]
2. Shi, X.; Zhang, X.; **Ganose, A. M.**; Park, J.; Sun, C.; Chen, Z.; Lin, S.; Li, W.; Jain, A.; Pei, Y.; Compromise between band structure and phonon scattering in efficient n- $\text{Mg}_3\text{Sb}_{2-x}\text{Bi}_x$  thermoelectrics. *Mater. Today Phys.* 2021, 18 100362 [DOI]
3. **Ganose, A. M.**; Searle, A.; Jain, A.; Griffin, S.M.; IFermi: A python library for Fermi surface generation and analysis. *J. Open Source Softw.* 2021, 6 (59), 3089 [DOI]
4. **Ganose, A. M.**; Pan, H.; Horton, M.; Aykol, M.; Persson, K.; Zimmermann, N. E. R.; Jain, A., Benchmarking Coordination Number Prediction Algorithms on Inorganic Crystal Structures. *Inorg. Chem.* 2021, 60 (3), 1590–1603 [DOI]
5. Pöhls, J.H.; Chanakian, S.; Park, J.; **Ganose, A.M.**; Dunn, A.; Friesen, N.; Bhattacharya, A.; Hogan, B.; Bux, S.; Jain, A.; Mar, A.; Experimental validation of high thermoelectric performance in  $\text{RECuZnP}_2$  predicted by high-throughput DFT calculations. *Mater. Horiz.* 2021, 8, 209–215 [DOI]
6. Mattei, G.S.; Dagdelen, J.M.; Bianchini, M.; **Ganose, A.M.**; Jain, A.; Suard, E.; Fauth, F.; Masquelier, C.; Croguennec, L.; Ceder, G.; Persson, K.A.; Enumeration as a Tool for Structure Solution: A Materials Genomic Approach to Solving the Cation-Ordered Structure of  $\text{Na}_3\text{V}_2(\text{PO}_4)_2\text{F}_3$ . *Chem. Mater.* 2020, 32 (20), 8981–8992 [DOI]

7. Dunn, A.; Wang, Q.; **Ganose, A. M.**; Dopp, D.; Jain, A. Benchmarking materials property prediction methods: the matbench test set and automatminer reference algorithm. *npj Comput. Mater.* 2020, 6 (1), 1–10 [DOI]
8. Park, J.; Xia, Y.; **Ganose, A. M.**; Jain, A.; Ozoliņš, V., High Thermoelectric Performance and Defect Energetics of Multipocketed Full Heusler Compounds. *Phys. Rev. Appl.* 2020, 14, 024064 [DOI]
9. Bashian, N.; Abdel-Latif, S.; Zuba, M.; Griffith, K.; **Ganose, A. M.**; Stiles, J.; Zhou, S.; Scanlon, D. O.; Piper, L.; Melot, B.; Transition Metal Migration Can Facilitate Ionic Diffusion in Defect Garnet-Based Intercalation Electrodes. *ACS Energy Lett.* 2020, 5 (5) 1448–1455 [DOI]
10. W. Gorai, P.; **Ganose, A. M.**; Faghaninia, A.; Jain, A.; Stevanovic, V., Computational discovery of promising new n-type dopable ABX Zintl thermoelectric materials. *Mater. Horiz.* 2020, 7 (7), 1809–1818 [DOI]
11. Spooner, K. B.; **Ganose, A. M.**; Scanlon, D. O. Assessing the limitations of transparent conducting oxides as thermoelectrics. *J. Mater. Chem. A* 2020, 8 (24), 11948–11957 [DOI]
12. Karim, M. M. S.; **Ganose, A. M.**; Pieters, L.; Winnie Leung, W. W.; Wade, J.; Zhang, L.; Scanlon, D. O.; Palgrave, R. G.; Anion Distribution, Structural Distortion, and Symmetry-Driven Optical Band Gap Bowing in Mixed Halide Cs<sub>2</sub>SnX<sub>6</sub> Vacancy Ordered Double Perovskites. *Chem. Mater.* 2019, 31 (22) 9430–9444 [DOI]
13. **Ganose, A. M.**; Jain, A.; Robocrystallographer: Automated Crystal Structure Text Descriptions and Analysis. *MRS Commun.* 2019, 9 (3) 874–881 [DOI]
14. Fallon, K. J.; Budden, P.; Salvadori, E.; **Ganose, A. M.**; Savory, C. N.; Eyre, L.; Dowland, S.; Ai, Q.; Goodlett, S.; Risko, C.; et al. Exploiting excited-state aromaticity to design highly stable singlet fission materials. *J. Am. Chem. Soc.* 2019, 141 (35) 13867–13876 [DOI] (\*41 citations)
15. Fabian, D. M.; **Ganose, A. M.**; Ziller, J. W.; Scanlon, D. O.; Beard, M. C.; Ardo, S.; Influence of One Specific Carbon–Carbon Bond on the Quality, Stability, and Photovoltaic Performance of Hybrid Organic–Inorganic Bismuth Iodide Materials. *ACS Appl. Energy Mater.* 2019, 2 (3), 1579–1587 [DOI]
16. Regoutz, A.; **Ganose, A. M.**; Blumenthal, L.; Schlueter, C.; Lee, T.-L.; Kieslich, G.; Cheetham, A. K.; Kerherve, G.; Huang, Y.-S.; Chen, R.-S.; et al. Insights into the electronic structure of OsO<sub>2</sub> using soft and hard x-ray photoelectron spectroscopy in combination with density functional theory. *Phys. Rev. Mater.* 2019, 3 (2), 025001 [DOI]
17. Maughan, A. E.; **Ganose, A. M.**; Scanlon, D. O.; Neilson, J. R.; Perspectives and design principles of vacancy-ordered double perovskite halide semiconductors. *Chem. Mater.* 2019, 31 (4), 1184–1195 [DOI] (\*47 citations)
18. Wang, Z.; **Ganose, A. M.**; Niu, C.; Scanlon, D. O.; Two-dimensional eclipsed arrangement hybrid perovskites for tunable energy level alignments and photovoltaics. *J. Mater. Chem. C* 2019, 7 (17), 5139–5147 [DOI]
19. Bashian, N. H.; Zhou, S.; Zuba, M.; **Ganose, A. M.**; Stiles, J. W.; Ee, A.; Ashby, D. S.; Scanlon, D. O.; Piper, L. F. J.; Dunn, B.; et al.; Correlated Polyhedral Rotations in the Absence of Polarons during Electrochemical Insertion of Lithium in ReO<sub>3</sub>. *ACS Energy Lett.* 2018, 3 (10), 2513–2519 [DOI]
20. **Ganose, A. M.**; J Jackson, A.; Scanlon, D. O.; sumo: Command-line tools for plotting and analysis of periodic ab initio calculations. *J. Open Source Softw.* 2018, 3 (28), 717 [DOI] (\*91 citations)

21. Maughan, A. E.; **Ganose, A. M.**; Almaker, M. A.; Scanlon, D. O.; Neilson, J. R.; Tolerance factor and cooperative tilting effects in vacancy-ordered double perovskite halides. *Chem. Mater.* 2018, 30 (11), 3909–3919 [DOI]  
(\*51 citations)
22. **Ganose, A. M.**; Matsumoto, S.; Buckeridge, J.; Scanlon, D. O.; Defect engineering of earth-abundant solar absorbers BiSI and BiSeI. *Chem. Mater.* 2018, 30 (11), 3827–3835 [DOI]
23. **Ganose, A. M.**; Gannon, L.; Fabrizio, F.; Nowell, H.; Barnett, S. A.; Lei, H.; Zhu, X.; Petrovic, C.; Scanlon, D. O.; Hoesch, M.; Local corrugation and persistent charge density wave in ZrTe<sub>3</sub> with Ni intercalation. *Phys. Rev. B* 2018, 97 (15), 155103 [DOI]
24. Maughan, A. E.; **Ganose, A. M.**; Candia, A. M.; Granger, J. T.; Scanlon, D. O.; Neilson, J. R.; Anharmonicity and octahedral tilting in hybrid vacancy-ordered double perovskites. *Chem. Mater.* 2018, 30 (2), 472–483 [DOI]  
(\*46 citations; Chemistry of Materials Lectureship and Best Paper Award)
25. Jackson, A. J.; **Ganose, A. M.**; Regoutz, A.; G. Egde, R.; Scanlon, D. O.; Galore: Broadening and weighting for simulation of photoelectron spectroscopy. *J. Open Source Softw.* 2018, 3 (26), 773 [DOI]
26. Wang, Z.; **Ganose, A. M.**; Niu, C.; Scanlon, D. O.; First-principles insights into tin-based two-dimensional hybrid halide perovskites for photovoltaics. *J. Mater. Chem. A* 2018, 6 (14), 5652–5660 [DOI]  
(\*36 citations)
27. Biswas, D.; **Ganose, A. M.**; Yano, R.; Riley, J. M.; Bawden, L.; Clark, O. J.; Feng, J.; Collins-Mcintyre, L.; Sajjad, M. T.; Meevasana, W.; et al.; Narrow-band anisotropic electronic structure of ReS<sub>2</sub>. *Phys. Rev. B* 2017, 96 (8), 085205 [DOI]
28. Savory, C. N.; **Ganose, A. M.**; Scanlon, D. O.; Exploring the PbS–Bi<sub>2</sub>S<sub>3</sub> Series for Next Generation Energy Conversion Materials. *Chem. Mater.* 2017, 29 (12), 5156–5167 [DOI]
29. Hendon, C. H.; Butler, K. T.; **Ganose, A. M.**; Román-Leshkov, Y.; Scanlon, D. O.; Ozin, G. A.; Walsh, A.; Electroactive nanoporous metal oxides and chalcogenides by chemical design. *Chem. Mater.* 2017, 29 (8), 3663–3670 [DOI]
30. **Ganose, A. M.**; Savory, C. N.; Scanlon, D. O.; 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. *J. Mater. Chem. A* 2017, 5 (17), 7845–7853 [DOI]  
(\*35 citations)
31. **Ganose, A. M.**; Savory, C. N.; Scanlon, D. O.; Beyond methylammonium lead iodide: prospects for the emergent field of ns<sup>2</sup> containing solar absorbers. *Chem. Commun.* 2017, 53 (1) 20–44 [DOI]  
(\*273 citations, top 5% of all publications in journal)
32. Quackenbush, N. F.; Paik, H.; Wahila, M. J.; Sallis, S.; Holtz, M. E.; Huang, X.; **Ganose, A. M.**; Morgan, B. J.; Scanlon, D. O.; Gu, Y.; et al.; Stability of the M2 phase of vanadium dioxide induced by coherent epitaxial strain. *Phys. Rev. B* 2016, 94 (8), 085105 [DOI]  
(\*56 citations)
33. Maughan, A. E.; **Ganose, A. M.**; Bordelon, M. M.; Miller, E. M.; Scanlon, D. O.; Neilson, J. R.; 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>6</sub>. *J. Amer. Chem. Soc.* 2016, 138 (27), 8453–8464 [DOI]  
(\*205 citations)
34. **Ganose, A. M.**; Cuff, M.; Butler, K. T.; Walsh, A.; Scanlon, D. O.; Interplay of orbital and relativistic effects in bismuth oxyhalides: BiOF, BiOCl, BiOBr, and BiOI. *Chem. Mater.* 2016,

- 28 (7), 1980–1984 [DOI]  
(\*156 citations)
35. Travis, W.; Knapp, C. E.; Savory, C. N.; **Ganose, A. M.**; Kafourou, P.; Song, X.; Sharif, Z.; Cockcroft, J. K.; Scanlon, D. O.; Bronstein, H.; et al.; Hybrid organic–inorganic coordination complexes as tunable optical response materials. *Inorg. Chem.* 2016, 55 (7), 3393–3400 [DOI]
36. Savory, C. N.; **Ganose, A. M.**; Travis, W.; Atri, R. S.; Palgrave, R. G.; Scanlon, D. O.; An assessment of silver copper sulfides for photovoltaic applications: theoretical and experimental insights. *J. Mater. Chem. A* 2016, 4 (32), 12648–12657 [DOI]  
(\*35 citations)
37. Hu, Y.; Goodeal, N.; Chen, Y.; **Ganose, A. M.**; Palgrave, R. G.; Bronstein, H.; Blunt, M. O.; Probing the chemical structure of monolayer covalent-organic frameworks grown via Schiff-base condensation reactions. *Chem. Commun.* 2016, 52 (64), 9941–9944 [DOI]  
(\*45 citations)
38. **Ganose, A. M.**; Butler, K. T.; Walsh, A.; Scanlon, D. O.; Relativistic electronic structure and band alignment of BiSI and BiSeI: candidate photovoltaic materials. *J. Mater. Chem. A* 2016, 4 (6), 2060–2068 [DOI]  
(\*92 citations)
39. **Ganose, A. M.**; Scanlon, D. O.; Band gap and work function tailoring of SnO<sub>2</sub> for improved transparent conducting ability in photovoltaics. *J. Mater. Chem. C* 2016, 4, 1467–1475 [DOI]  
(\*136 citations)
40. **Ganose, A. M.**; Savory, C. N.; Scanlon, D. O.; (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? *J. Phys. Chem. Lett.* 2015, 6 (22), 4594–4598 [DOI]  
(\*107 citations)
41. Hiley, C. I.; Scanlon, D. O.; Sokol, A. A.; Woodley, S. M.; **Ganose, A. M.**; Sangiao, S.; De Teresa, J. M.; Manuel, P.; Khalyavin, D. D.; Walker, M.; et al.; Antiferromagnetism at T > 500 K in the layered hexagonal ruthenate SrRu<sub>2</sub>O<sub>6</sub>. *Phys. Rev. B* 2015, 92 (10), 104413 [DOI]  
(\*42 citations)

## COLLABORATORS

Prof. G. Jeffrey Snyder, Northwestern University; Prof. Sinéad Griffin, Berkeley Lab; Prof. Louis F. J. Piper, SUNY Binghamton; Prof. Brent C. Melot, University of South California; Prof. Aron Walsh, ICL; Prof. David J. Payne, ICL; Prof. Philip. D. C. King, St. Andrews; Prof. Timothy D. Veal, Stephenson Institute, University of Liverpool; Dr Robert G. Palgrave, UCL; Dr Hugo Bronstein, Cambridge; Dr Moritz Hoesch, DLS; Dr Tien-Lin Lee, DLS; Prof. Jamies R. Neilson, Colorado State University; Dr. Keith T. Bulter, Rutherford Appleton Laboratories; Dr. Ben Morgan, University of Bath; Prof. Christopher H. Hendon, University of Oregon; Dr. Prashun Gorai, Colorado School of Mines; Prof. Vladan Sevanovic, Colorado School of Mines; Prof. Kristin Persson, University of California, Berkeley; Prof. Yanzhong Pei, Tongji University; Dr. Arthur Mar, University of Alberta; Prof. Alexandra Zevalkink, Michigan State University; Prof. Peter G. Khalifah, Stony Brook University;

## REVIEWING DUTIES

Physical Review Letters, Physical Review B, Physical Review Applied, Physical Review Research, Physical Review Materials, Chemistry of Materials, Journal of the American Chemical Society,

Materials Horizons, Journal of Materials Chemistry, Nature Communications, npj Computational Materials

BOOKS

2020      Atomic-Scale Insights into Emergent Photovoltaic Absorbers (Springer Theses),  
*Springer*, 978-3030557072