Alex M. Ganose

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Summary

I am an early career researcher working on designing and understanding **solid-state materials** from **computational techniques**. I primarily use **quantum mechanical** simulations applied in a **high-throughput** approach to screen thousands of materials for **renewable energy** applications. Some areas I have worked on include **photovoltaics**, **thermoelectrics**, **photocatalysts**, and **batteries**. I am currently a researcher for the **Materials Project** working on a computationally efficient framework for calculating **electron transport** properties. I am also interested in applying **machine learning** and **data mining** to challenges in materials science.

Education and Training

Lawrence Berkeley National Laboratory (2018 – present)
Postdoctoral scholar, The Materials Project
Topic: Materials data mining, electron transport properties,

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_2 for improved transparent electronic conducting properties in solar cells."

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

Awards

2019 Springer Thesis Prize
2018 Scopus Early Career Researcher Award
2018 Maths and Physical Sciences Postgraduate Research Prize, UCL
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

2019 – 2020: Materials Project workshop instructor
2018 – 2020: Mentored 3 SULI research projects, LBNL
2015 – 2018: Supervised 11 final year research projects, UCL
2015 – 2018: Demonstrator for M^3S Computational Labs, UCL

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

Publications *30 published, 7 in submission, > 900 citations, H-index of 17, Google scholar*

1. **Ganose, A. M.**; Jain, A. Robocrystallographer: Automated Crystal Structure Text Descriptions and Analysis. *MRC* **2019**, 1–8 doi:10.1557/mrc.2019.94
2. Karim, M. M. S.; **Ganose, A. M.**; Pieters, L.; Leung, W. 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_2SnX_6 Vacancy Ordered Double Perovskites. *Chem. Mater.* **2019**, 31 (22), 9430–9444 doi: 10.1021/acs.chemmater.9b03267
3. 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** doi:10.1021/jacs.9b06346
4. 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_2 Using Soft and Hard X-Ray Photoelectron Spectroscopy in Combination with Density Functional Theory. *Phys. Rev. Materials* **2019**, *3* (2), 025001 doi: 10.1103/PhysRevMaterials.3.025001
5. 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: 10.1021/acs.chemmater.8b05036
6. 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: 10.1021/acsaem.8b01809
7. 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: 10.1039/C9TC01325C
8. 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: 10.1039/C8TA00751A
9. 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. *Chemistry of Materials* **2018**, *30* (2), 472–483 doi: 10.1021/acs.chemmater.7b04516
10. 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: 10.1021/acs.chemmater.8b01549
11. **Ganose, A. M.**; J Jackson, A.; O Scanlon, D. Sumo: Command-Line Tools for Plotting and Analysis of Periodic Ab Initio Calculations. *JOSS* **2018**, *3* (28), 717 doi: 10.21105/joss.00717.
12. J Jackson, A.; **Ganose, A. M.**; Regoutz, A.; G. Egdell, R.; O Scanlon, D. Galore: Broadening and Weighting for Simulation of Photoelectron Spectroscopy. *JOSS* **2018**, *3* (26), 773 doi: 10.21105/joss.00773
13. **Ganose, A. M.**; Matsumoto, S.; Buckeridge, J.; Scanlon, D. O. Defect Engineering of Earth-Abundant Solar Absorbers BiSI and BiSeI. *Chemistry of Materials* **2018**, *30* (11), 3827–3835 doi: 10.1021/acs.chemmater.8b01135
14. **Ganose, A. M.**; Gannon, L.; Fabrizi, 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 $ZrTe_3$ with Ni Intercalation. *Phys. Rev. B* **2018**, *97* (15), 155103 doi: 10.1103/PhysRevB.97.155103
15. 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_3. *ACS Energy Lett.* **2018**, *3* (10), 2513–2519 doi: 10.1021/acsenergylett.8b01179
16. Savory, C. N.; **Ganose, A. M.**; Scanlon, D. O. Exploring the PbS–Bi_2S_3 Series for Next

Generation Energy Conversion Materials. *Chemistry of Materials* **2017**, *29* (12), 5156–5167. doi: 10.1021/acs.chemmater.7b00628

17. 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. *Chemistry of Materials* **2017**, *29* (8), 3663–3670 doi: 10.1021/acs.chemmater.7b00464
18. **Ganose, A. M.**; Savory, C. N.; Scanlon, D. O. Electronic and Defect Properties of $(CH_3NH_3)_2Pb(SCN)_2I_2$ Analogues for Photovoltaic Applications. *J. Mater. Chem. A* **2017**, *5* (17), 7845–7853 doi: 10.1039/C7TA01688C
19. 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_2. *Physical Review B* **2017**, *96* (8), 085205 doi: 10.1103/PhysRevB.96.085205
20. 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. *Inorganic Chemistry* **2016**, *55* (7), 3393–3400 doi: 10.1021/acs.inorgchem.5b02749
21. 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: 10.1039/C6TA03376H
22. Quackenbush, N. F.; Paik, H.; Wahila, M. J.; Sallis, S.; Holtz, M. E.; Huang, X.; **Ganose, A.**; Morgan, B. J.; Scanlon, D. O.; Gu, Y.; et al. Stability of the M2 Phase of Vanadium Dioxide Induced by Coherent Epitaxial Strain. *Physical Review B* **2016**, *94* (8), 085105 doi: 10.1103/PhysRevB.94.085105
23. 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_2SnI_6 and Cs_2TeI_6. *Journal of the American Chemical Society* **2016**, *138* (27), 8453–8464 doi: 10.1021/jacs.6b03207
24. 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: 10.1039/C6CC03895F
25. **Ganose, A. M.**; Scanlon, D. O. Band Gap and Work Function Tailoring of SnO_2 for Improved Transparent Conducting Ability in Photovoltaics. *J. Mater. Chem. C* **2016**, *4*, 1467–1475 doi: 10.1039/C5TC04089B
26. **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. *Chemistry of Materials* **2016**, *28* (7), 1980–1984 doi: 10.1021/acs.chemmater.6b00349
27. **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: 10.1039/C5TA09612J
28. **Ganose, A. M.**; Savory, C. N.; Scanlon, D. O. Beyond Methylammonium Lead Iodide: Prospects for the Emergent Field of ns^2 Containing Solar Absorbers. *Chem. Commun.* **2016** doi: 10.1039/C6CC06475B
29. 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 $SrRu_2O_6$. *Physical Review B* **2015**, *92* (10), 104413 doi: 10.1103/PhysRevB.92.104413
30. **Ganose, A. M.**; Savory, C. N.; Scanlon, D. O. $(CH3NH_3)_2Pb(SCN)_2I_2$: A More Stable Structural Motif for Hybrid Halide Photovoltaics? *J. Phys. Chem. Lett.* **2015**, *6* (22), 4594–4598 doi: 10.1021/acs.jpclett.5b02177

Conference Presentations (Oral) *23 total at national and international level*

Five select presentations:

1. **Invited** "Defect and carrier transport properties of emerging bismuth-based photovoltaics", *American Chemical Society*, San Diego, USA (2019)
2. **Invited** "Computational approaches for smart high-throughput calculations and machine learning", *CECAM*, Liverpool, UK (2019)
3. **Invited "**Electronic transport properties from first-principles calculations", *Seminar*, University of Warwick, UK (2019)
4. **Invited** "Defect chemistry of emerging photovoltaic absorbers", *Seminar*, University of California Santa Barbara, USA (2019)
5. **Invited** "Defect chemistry of emerging materials for photovoltaics", *Seminar*, Colorado State University, USA (2018)

Other Skills

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

References

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