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Department of Chemistry
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APPOINTMENTS

Assistant Professor Sep 2019 – Present
University of Massachusetts Amherst, United States

Postdoctoral Fellow with Prof Danna Freedman May 2015 – Aug 2019
Northwestern University, United States

Postdoctoral Fellow with Dr Jacob Overgaard Mar 2015 – May 2015
Aarhus University, Denmark

Research Associate with Dr Alistair Fielding Nov 2014 – Feb 2015
University of Manchester, United Kingdom

EDUCATION

PhD in Inorganic Chemistry (Thesis: Anisotropy in Molecular Magnetism) Sep 2010 – Oct 2014
Nanoscience Doctoral Training Centre, University of Manchester, United Kingdom
Advisors: Prof David Collison, Prof Eric McInnes, and Prof Richard Winpenny

MChem in Chemistry with Forensic Science Sep 2006 – Aug 2010
University of Manchester, United Kingdom

AWARDS AND HONORS

Lilly Teaching Fellowship Apr 2024
National Science Foundation CAREER Award Dec 2022

PUBLICATIONS

Independent Research:

10. High-pressure synthesis and recovery of single crystals of the metastable manganese carbide, MnC_x
Marshall, P. V.; Thiel, S. D.; Cote, E. E.; Arigbede, J.; Whitaker, M. L.; Walsh, J. P. S. *Chem. - Eur. J.*, **2024**.
 9. High-pressure polymorphism in silver ferrite delafossite, AgFeO_2
Manganaro, N. S.; Ambos, S. D.; DeCapua, M.; Thiel S. D.; Mitchell, W. E.; Liu, Z.; Zhang, D.; Nguyen, P. Q. H.; Lavina, B.; Alp, E. E.; Yan, J.; Walsh, J. P. S. *Inorg. Chem.*, **2024**, 63, 9763–9770.
 8. Shock compression experiments using the DiPOLE 100-X laser on the high energy density instrument at the European X-ray free electron laser: Quantitative structural analysis of liquid Sn
Gorman, M. G.; [...] Pereira, K. A.; [...] Walsh, J. P. S. [...] McMahon, M. I. *J. Appl. Phys.*, **2024**, 135, 165902.
 7. Combined first-principles and experimental investigation into the reactivity of co-deposited chromium-carbon samples under pressure
Marshall, P. V.; Thiel, S. D.; Cote, E. E.; Hrubiak, R.; Whitaker, M. L.; Meng, Y.; Walsh, J. P. S. *ACS Mater. Au*, **2024**, 4, 393–402.
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6. **Designing magnetic properties in CrSBr through hydrostatic pressure and ligand substitution**
Telford, E. J.; Chica, D. G.; Ziebel, M. E.; Xie, K; Manganaro, N. S.; Huang, C.-Y.; Cox, J.; Dismukes, A. H.; Zhu, X.; Walsh, J. P. S.; Cao, T.; Dean, C. R.; Roy X. *Adv. Physics Res.*, **2023**, 5, 2300036.
5. **First-principles investigation of phase stability in substoichiometric zirconium carbide under high pressure**
Thiel, S. D.; Walsh, J. P. S. *Adv. Theory Simul.*, **2022**, 33, 9601–9607.
4. **X-ray diffraction methods for high-pressure solid-state synthesis**
Thiel, S. D.; Tamarius, A. D.; Walsh, J. P. S. *Compr. Inorg. Chem. III*, **2022**, 220–221.
3. **High-pressure synthesis of cobalt cementite, Co₃C**
Marshall, P. V.; Alptekin, Z.; Thiel, S. D.; Smith, J.; Meng, Y.; Walsh, J. P. S. *Chem. Mater.*, **2021**, 33, 9601–9607.
2. **"Pink"-beam X-ray powder diffraction profile and its use in Rietveld refinement**
Von Dreele, R. B.; Clarke, S. M.; Walsh, J. P. S. *J. Appl. Crystallogr.*, **2021**, 54, 3–6.
1. **Anisotropic structural collapse of Mg₃Sb₂ and Mg₃Bi₂ at high pressure**
Calderón-Cueva, M.; Peng, W.; Clarke, S. M.; Ding, J.; Brugman, B. L.; Levental, G.; Balodhi, A.; Rylko, M.; Delaire, O.; Walsh, J. P. S.; Dorfman, S. M.; Zevalkink, A. *Chem. Mater.*, **2021**, 33, 567–573.

Doctoral and Postdoctoral Research:

32. **Computationally directed discovery of MoBi₂**
Altman, A. B., Tamerius, A. D., Koocher, N. Z., Meng, Y., Pickard, C. J., Walsh, J. P. S., Rondinelli, J. M., Jacobsen, S. D., Freedman, D. E. *J. Am. Chem. Soc.*, **2021**, 143, 214–222.
31. **NMR study of spin dynamics in V₇Zn and V₇Ni molecular rings**
Adelina, F.; Arosio, P.; Mariani, M.; Orsini, F.; Radaelli, A.; Sangregorio, C.; Borsa, F.; Walsh, J. P. S.; Winpenny, R. E. P.; Timco, G. A.; Lascialfari, A. *Appl. Magn. Reson.*, **2020**, 51, 1277–1293.
30. **Pressure-induced collapse of magnetic order in jarosite**
Klein, R. A.; Walsh, J. P. S.; Clarke, S. M.; Liu, Z.; Alp E. E.; Bi, W.; Meng, Y.; Altman, A. B.; Chow, P.; Xiao, Y.; Norman M. R.; Rondinelli, J. M.; Jacobsen, S. D.; Puggioni, D.; Freedman, D. E. *Phys. Rev. Lett.*, **2020**, 125, 077202.
29. **Goldschmidtite, (K,REE,Sr)(Nb,Cr)O₃: A new perovskite supergroup mineral found in diamond from Koffiefontein, South Africa**
Meyer, N. A.; Wenz, M. D.; Walsh, J. P. S.; Jacobsen, S. D.; Locock, A. J.; Harris, J. W. *Am. Mineral.*, **2019**, 104, 1345–1350.
28. **High-pressure synthesis of the BiVO₃ perovskite**
Klein, R. A.; Altman, A. B.; Saballos, R. J.; Walsh, J. P. S.; Tamerius, A. D.; Meng, Y.; Puggioni, D.; Rondinelli, J. M.; Jacobsen, S. D.; Freedman, D. E. *Phys. Rev. Mater.*, **2019**, 3, 064411.
27. **MnBi₂: A metastable high-pressure phase in the Mn–Bi system**
Walsh, J. P. S.; Clarke, S. M.; Tamerius, A. D.; Meng, Y.; Jacobsen, S. D.; Freedman, D. E. *Chem. Mater.*, **2019**, 31, 3083–3088.
26. **Insights into single-molecule magnet behavior from the experimental electron density of linear two-coordinate iron complexes**
Thomsen, M. K.; Nyvang, A.; Walsh, J. P. S.; Bunting, P. C.; Long, J. R.; Neese, F.; Atanasov, M.; Genoni, A.; Overgaard, J. *Inorg. Chem.*, **2019**, 58, 3211–3218.

25. **Controlling dimensionality in the Ni–Bi system with pressure**
Clarke, S. M.; Powderly, K. M.; Walsh, J. P. S.; Yu, T.; Wang, Y.; Meng, Y.; Jacobsen, S. D.; Freedman, D. E. *Chem. Mater.*, **2019**, *31*, 955–959.
24. **Discovery of Cu₃Pb**
Tamerius, A. D.; Clarke, S. M.; Gu, M.; Walsh, J. P. S.; Esters, M.; Meng, Y.; Hendon, C. H.; Rondinelli, J. M.; Jacobsen, S. D.; Freedman, D. E. *Angew. Chem., Int. Ed.*, **2018**, *57*, 12809–12813.
23. **Impact of pressure on magnetic order in jarosite**
Klein, R. A.; Walsh, J. P. S.; Clarke, S. M.; Guo, Y.; Bi, W.; Fabbris, G.; Meng, Y.; Haskel, D.; Alp, E. E.; Van Duyne, R. P.; Jacobsen, S. D.; Freedman, D. E. *J. Am. Chem. Soc.*, **2018**, *140*, 12001–12009.
22. **High-pressure synthesis: A new frontier in the search for next-generation intermetallic compounds**
Walsh, J. P. S.; Freedman, D. E. *Acc. Chem. Res.*, **2018**, *51*, 1315–1323.
21. **Evidence of spin canting, metamagnetism, negative coercivity and slow relaxation in a two-dimensional network of {Mn₆} cages**
Dendrinou-Samara, C.; Walsh, J. P. S.; Muryn, C. A.; Collison, D.; Winpenny, R. E. P.; Tuna, F. *Eur. J. Inorg. Chem.*, **2018**, 485–492.
20. **Molecular single-ion magnets based on lanthanides and actinides: Design considerations and new advances in the context of quantum technologies**
McAdams, S. G.; Ariciu, A.-M.; Kostopoulos, A. K.; Walsh, J. P. S.; Tuna, F. *Coord. Chem. Rev.*, **2017**, *346*, 216–239.
19. **Creating binary Cu–Bi compounds via high-pressure synthesis: A combined experimental and theoretical study**
Clarke, S. M.; Amsler, M.; Walsh, J. P. S.; Yu, T.; Wang, Y.; Meng, Y.; Jacobsen, S. D.; Wolverton, C.; Freedman, D. E. *Chem. Mater.*, **2017**, *29*, 5276–5285.
18. **Discovery of FeBi₂**
Walsh, J. P. S.; Clarke, S. M.; Meng, Y.; Jacobsen, S. D.; Freedman, D. E. *ACS Cent. Sci.*, **2016**, *2*, 867–871.
17. **Using Supramolecular Chemistry to Build Quantum Logic Gates (Preview Article)**
Walsh, J. P. S.; Freedman, D. E. *Chem*, **2016**, *1*, 668–669.
16. **Oximate-bridged copper(II) compounds: Syntheses, molecular structures, magnetic, thermal and spectroscopic properties**
Naskar, J. P.; Biswas, C.; Bandyopadhyay, N.; Walsh, J. P. S.; Tuna, F.; Zhu, M.; Lu, L. *J. Coord. Chem.*, **2016**, *69*, 2329–2341.
15. **Evidence of slow magnetic relaxation in Co(AcO)₂(py)₂(H₂O)₂**
Walsh, J. P. S.; Bowling, G.; Ariciu, A.-M.; Jailani, N. F. M.; Chilton, N. F.; Waddell, P. G.; Collison, D.; Tuna F.; Higham, L. J. *Magnetochemistry*, **2016**, *2*, 23.
14. **Dioxygen binding at a four-coordinate cobaltous porphyrin site in a metal–organic framework: structural, EPR, and O₂ adsorption analysis**
Gallagher, A. T.; Kelty, M. L.; Park, J. G.; Anderson, J. S.; Mason, J. A.; Walsh, J. P. S.; Collins, S. L.; Harris, T. D. *Inorg. Chem. Front.*, **2016**, *3*, 536–540.
13. **Magnetism and variable temperature and pressure crystal structures of a linear oligonuclear cobalt bis-semiquinonate**
Overgaard, J.; Møller, L. H.; Borup, M. A.; Tricoire, M.; Walsh, J. P. S.; Diehl, M.; Rentschler, E. *Dalton. Trans.*, **2016**, *45*, 12924–12932.

12. **Discovery of a superconducting Cu–Bi intermetallic compound via high-pressure synthesis**
Clarke, S. M.; Walsh, J. P. S.; Amsler, M.; Malliakas, C. D.; Yu, T.; Goedecker, S.; Wang, Y.; Wolverton, C.; Freedman, D. E. *Angew. Chem., Int. Ed.*, **2016**, *55*, 13446–13449.
11. **Electronic structure of a mixed-metal fluoride-centered triangle complex: A potential qubit component**
Walsh, J. P. S.; Meadows, S. B.; Ghirri, A.; Moro, F.; Jennings, M.; Smith, W. F.; Graham, D. M.; Kihara, T.; Nojiri, H.; Vitorica-Yrezabal, I. J.; Timco, G. A.; Collison, D.; McInnes, E. J. L.; Winpenny, R. E. P. *Inorg. Chem.*, **2015**, *54*(24), 12019–12026.
10. **Hexanuclear 3d–4f neutral Co^{II}Ln^{III} clusters: Synthesis, structure, and magnetism**
Goura, J.; Chakraborty, A.; Walsh, J. P. S.; Tuna, F.; Chandrasekhar, V. *Cryst. Growth Des.*, **2015**, *15*(7), 3157–3165.
9. **P–C bond cleavage-assisted lanthanide phosphate coordination polymers**
Goura, J.; Walsh, J. P. S.; Tuna, F.; Halder, R.; Maji, T. K.; Chandrasekhar, V. *Cryst. Growth Des.*, **2015**, *15*(6), 2555–2560.
8. **Discrete and polymeric cobalt organophosphates: isolation of a 3-D cobalt phosphate framework exhibiting selective CO₂ capture**
Gupta, S. K.; Kuppaswamy, S.; Walsh, J. P. S.; McInnes, E. J. L.; Murugavel, R. *Dalton Trans.*, **2015**, *44*, 5587–5601.
7. **A synthetic strategy for switching the single ion anisotropy in tetrahedral Co(II) complexes**
Vaidya, S.; Upadhyay, A.; Kumar Singh, S.; Gupta, T.; Tewary, S.; Langley, S. K.; Walsh, J. P. S.; Murray, K. S.; Rajaraman, G.; Shanmugam, M. *Chem. Comm.*, **2015**, *51*, 3739–3742.
6. **Structural, magnetic and catalytic properties of cobalt chromite obtained through precursor method**
Gingasu, D.; Mandru, I.; Culita, D. C.; Patron, L.; Calderon-Moreno, J.-M.; Osiceanu, P.; Preda, S.; Oprea, O.; Parvulescu, V.; Teodorescu, V.; Walsh, J. P. S. *Mater. Res. Bull.*, **2015**, *62*, 52–64.
5. **Self-assembly of a 3d–5f trinuclear single-molecule magnet from a pentavalent uranyl complex**
Chatelain, L.; Walsh, J. P. S.; Pécaut, J.; Tuna, F.; Mazzanti, M. *Angew. Chem.*, **2014**, *53*(49), 13434–13438.
4. **Synthesis, structure, and magnetism of non-planar heptanuclear lanthanide(III) complexes**
Goura, J.; Walsh, J. P. S.; Tuna, F.; Chandrasekhar, V. *Dalton Trans.*, **2014**, *44*, 1142–1149.
3. **Relationships between electron density and magnetic properties in water-bridged dimetal complexes**
Overgaard, J.; Walsh, J. P. S.; Hathwar, V. R.; Jørgensen, M. R. V.; Hoffman, C.; Platts, J. A.; Piltz, R.; Winpenny, R. E. P. *Inorg. Chem.*, **2014**, *53*(21), 11531–11539.
2. **On the possibility of magneto-structural correlations: Detailed studies of dinickel carboxylate complexes**
Walsh, J. P. S.; Sproules, S.; Chilton, N. F.; Barra, A.-L.; Timco, G. A.; Collison, D.; McInnes, E. J. L.; Winpenny, R. E. P. *Inorg. Chem.*, **2014**, *53*(16), 8464–8472.
1. **Tetranuclear lanthanide(III) complexes in a seesaw geometry: Synthesis, structure, and magnetism**
Goura, J.; Walsh, J. P. S.; Tuna, F.; Chandrasekhar, V. *Inorg. Chem.*, **2014**, *53*(7), 3385–3391.

INVITED LECTURES

30. Chemistry Department Seminar (<i>University of Rochester, NY, USA</i>)	May 2024
29. Advanced Photon Source Users Meeting (<i>Argonne National Laboratory, IL, USA</i>)	May 2024
28. Boston Regional Inorganic Colloquium (<i>University of New Hampshire, NH, USA</i>)	May 2024
27. Chemistry Department Seminar (<i>University at Buffalo, NY, USA</i>)	Apr 2024
26. Chemistry Department Seminar (<i>The Ohio State University, OH, USA</i>)	Feb 2024
25. Chemistry Department Seminar (<i>Michigan State University, MI, USA</i>)	Feb 2024

24. Chemistry Department Seminar (*University of Washington, WA, USA*) Jan 2024
23. Physics Department Seminar (*University of Nevada Las Vegas, NV, USA*) Jan 2024
22. NSF Professional Development Workshop in Ceramics (*Northeastern University, MA, USA*) Nov 2023
21. Chemistry Department Seminar (*University of Massachusetts Dartmouth, MA, USA*) Oct 2023
20. ARL-ARO Seminar Series (*Virtual*) Aug 2023
19. AIRAPT Biennial Meeting 2023 (*University of Edinburgh, UK*) Jul 2023
18. Materials Science Division Seminar (*Lawrence Livermore National Laboratory, CA, USA*) Jul 2023
17. GSCCM Biennial Meeting 2023 (*Chicago, IL, USA*) Jul 2023
16. Boston Regional Inorganic Colloquium (*Harvard Medical School, MA, USA*) Dec 2022
15. Workshop of the IUCr Commission on High Pressure (*Advanced Photon Source, IL, USA*) Dec 2022
14. Chemistry Department Seminar (*Clemson University, NC, USA*) Oct 2022
13. AEROMAT 2022 (*Pasadena, CA, USA*) Mar 2022
12. Rigaku High Pressure Workshop (*Virtual*) July 2021
11. CDAC Webinar (*Virtual*) Mar 2021
10. Special Seminar (*Georgia Institute of Technology, GA, USA*) Feb 2019
9. Special Seminar (*University of Massachusetts Amherst, MA, USA*) Jan 2019
8. Special Seminar (*University of Michigan, MI, USA*) Dec 2018
7. Materials in Extreme Environments at ACS Fall 2018 (*Boston, MA, USA*) Aug 2018
6. Workshop of the IUCr Commission on High Pressure (*Honolulu, HI, USA*) Jul 2018
5. Special Seminar (*Michigan State University, MI, USA*) Jan 2018
4. HPCAT Beamline Review (*Advanced Photon Source, IL, USA*) Nov 2017
3. Probing Materials Under Extreme Conditions Workshop (*Advanced Photon Source, IL, USA*) Oct 2017
2. Nuclear Resonant Scattering Workshop (*Argonne National Laboratory, IL, USA*) Nov 2016
1. Research at High Pressure GRC (*Holderness School, NH, USA*) Jul 2016