

JAMES P. S. WALSH

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University of Massachusetts Amherst
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

National Science Foundation CAREER Award **Dec 2022**

PUBLICATIONS

Independent Research:

4. **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.
3. **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**. (In press)
2. **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.
1. **"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.

Doctoral and Postdoctoral Research:

33. **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.
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**
Adelnia, 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.; Murn, 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.; Wolverson, 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 Co₂Ln₄ 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.; Kuppuswamy, 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

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| 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, California, USA) | Jul 2023 |
| 17. GSCCM Biennial Meeting 2023 (Chicago, Illinois, USA) | Jul 2023 |
| 16. Boston Regional Inorganic Colloquium (Harvard Medical School, Massachusetts, USA) | Dec 2022 |
| 15. Workshop of the IUCr Commission on High Pressure (Advanced Photon Source, Illinois, USA) | Dec 2022 |
| 14. Chemistry Department Seminar (Clemson University, North Carolina, USA) | Oct 2022 |
| 13. AEROMAT 2022 (Pasadena, California, USA) | Mar 2022 |
| 12. Rigaku High Pressure Workshop (Virtual) | July 2021 |
| 11. CDAC Webinar (Virtual) | Mar 2021 |
| 10. Special Seminar (Georgia Institute of Technology, Georgia, USA) | Feb 2019 |
| 9. Special Seminar (University of Massachusetts Amherst, Massachusetts, USA) | Jan 2019 |
| 8. Special Seminar (University of Michigan, Michigan, USA) | Dec 2018 |
| 7. Materials in Extreme Environments at ACS Fall 2018 (Boston, Massachusetts, USA) | Aug 2018 |

6. **Workshop of the IUCr Commission on High Pressure** (*Honolulu, Hawai'i, USA*) **Jul 2018**
5. **Special Seminar** (*Michigan State University, Michigan, USA*) **Jan 2018**
4. **HPCAT Beamline Review** (*Advanced Photon Source, Illinois, USA*) **Nov 2017**
3. **Workshop on Probing Materials Under Extreme Conditions** (*Advanced Photon Source, Illinois, USA*) **Oct 2017**
2. **Nuclear Resonant Scattering Workshop** (*Argonne National Laboratory, Illinois, USA*) **Nov 2016**
1. **Gordon Research Seminar: Research at High Pressure** (*Holderness School, Plymouth, New Hampshire, USA*) **Jul 2016**

TEACHING

CHEM 341:	Inorganic Chemistry (<i>Professor</i>)	F2020, F2021, F2022
CHEM 743:	Crystallography and Solid-State Chemistry (<i>Professor</i>)	S2021
CHEM 590M:	Materials Chemistry (<i>Professor</i>)	F2019, S2022

LEADERSHIP AND SERVICE

External Service:

Member of the Advanced Photon Source High Pressure Proposal Review Panel	2019 – Present
Member of the Advanced Photon Source Users Organization Steering Committee	2019 – 2022
Mentor for GSMI Cientifico Latino	2020 – Present
Reviewer for the NSF Graduate Research Fellowship Program	2020
Reviewer for the NDSEG Fellowship	2020
Ad Hoc Reviewer for NSF Division of Materials Research	2020 – Present

Campus Service:

Chemistry Graduate Admissions Committee	2019 – Present
Chemistry Graduate Recruitment Committee	2019 – Present
Chemistry Ad Hoc Bylaws Committee	2022 – Present