



# Michael W. Gaultois

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Research Fellow in Functional Materials Design

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## Employment

**2018–present** Research Fellow, Theme Lead in Experimental Inorganic Materials, *Leverhulme Research Centre for Functional Materials Design*, The Materials Innovation Factory, University of Liverpool, Liverpool, United Kingdom.

**2015–2017** **Marie Skłodowska–Curie International Fellow**, *University of Cambridge*, United Kingdom.  
Postdoctoral Associate, *St Catharine's College*, Cambridge, United Kingdom.  
Advisor: Professor **Dame Clare Grey**

## Education

**2011–2015** PhD Chemistry, *University of California*, Santa Barbara, CA, USA.  
**International Fulbright Science & Technology Fellow**, **NSERC Postgraduate Scholarship**  
Advisor: Professor **Ram Seshadri**  
Thesis: Design principles for oxide thermoelectrics  
Created a database of thermoelectric materials and developed online visualization tools, extracted trends and insight, and developed material selection guidelines and design principles.

**2009–2011** MSc Chemistry, *University of Saskatchewan*, Saskatoon, SK, Canada.  
**Julie Payette–NSERC Research Scholarship**  
Advisor: Professor **Andrew P. Grosvenor**  
Thesis: Final-state Effects in X-ray Spectra from Transition Metal Oxides and Silicates  
Prepared and characterized amorphous and crystalline inorganic materials using X-ray absorption and photoelectron spectroscopy at synchrotron radiation facilities.

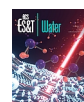
**2004–2009** BSc Chemistry (Honours), *University of Alberta*, Edmonton, AB, Canada.  
Advisor: Professor **Arthur Mar**  
Thesis: Anionic Ga–Ga bonding in RE–Co–Ga systems (RE = Gd, Tb, Dy, Ho, Er)  
Thesis: Anion-stabilized differential fractional site occupancy in ternary Zr–Si–As  
Created isothermal ternary phase diagrams, grew single crystals and determined the structures of novel intermetallic phases, and used ab initio calculations to determine the electronic structure.

## Publications

With [DOI](#) links where available.

78. Site-Net: Using global self-attention and real-space supercells to capture long-range interactions in crystal structures Michael Moran, Michael W. Gaultois, Vladimir Gusev, Matthew J. Rosseinsky. [[arXiv 2209.08190](#)]
77. A database of experimentally measured lithium solid electrolyte conductivities evaluated with machine learning. Cameron J. Hargreaves, Michael W. Gaultois, Luke M. Daniels, Emma J. Watts, Vitaliy A. Kurlin, Michael Moran, Yun Dang, Rhun Morris, Alexandra Morscher, Kate Thompson, Matthew A.

- Wright, Beluvalli-Eshwarappa Prasad, Frédéric Blanc, Chris M. Collins, Catriona A. Crawford, Benjamin B. Duff, Jae Evans, Jacinthe Gamon, Guopeng Han, Bernhard T. Leube, Hongjun Niu, Arnaud J. Perez, Aris Robinson, Oliver Rogan, Paul M. Sharp, Elvis Shoko, Manel Sonni, William J. Thomas, Andriy Vasylenko, Lu Wang, Matthew J. Rosseinsky, and Matthew S. Dyer. (Under review)
76. Andriy Vasylenko, Dmytro Antypov, Vladimir Gusev, Michael W. Gaultois, Matthew S. Dyer, and Matthew J. Rosseinsky. Element selection for functional materials discovery by integrated machine learning of atomic contributions to properties. (Under review) [[arXiv 2202.01051](#)]
75. Elena Derunova, Jacob Gayles, Yan Sun, Michael W. Gaultois, and Mazhar N. Ali. Fermi surface geometry. (Under review) [[arXiv 2007.05525](#)]
74. Michael W. Gaultois and T. Wesley Surta. “Spark plasma sintering routes to consolidated inorganic functional materials,” in *Comprehensive Inorganic Chemistry III*; Jan Reedijk and Kenneth Poeppelemeier, Eds. (In press) [[doi](#)]
73. Random projections and kernelised leave one cluster out cross-validation: Universal baselines and evaluation tools for supervised machine learning for material properties. *Digital Discovery* (In press) [[doi](#)]
72. Bernhard T. Leube, Christopher Collins, Luke M. Daniels, Benjamin B. Duff, Yun Dang, Ruiyong Chen, Michael W. Gaultois, Troy Manning, Frédéric Blanc, Matthew S. Dyer, John B. Claridge, and Matthew J. Rosseinsky. Cation disorder and large tetragonal supercell ordering in the Li-rich argyrodite  $\text{Li}_7\text{Zn}_{0.5}\text{SiS}_6$ . *Chem. Mater.* 34:4073–4087, 2022. [[doi](#)]
71. Rémi Pétuya, Samantha Durdy, Dmytro Antypov, Michael W. Gaultois, Neil G. Berry, George R. Darling, Alexandros P. Katsoulidis, Matthew S. Dyer, and Matthew J. Rosseinsky. Machine learning prediction of metal-organic framework guest accessibility from linker and metal chemistry *Angew. Chem. Int. Ed.* 61:e202114573 (6pp), 2022. [[doi](#)]  
**“Hot paper” in metal-organic frameworks**
70. Jacinthe Gamon, Matthew S. Dyer, Benjamin B. Duff, Andriy Vasylenko, Luke M. Daniels, Michael W. Gaultois, Frédéric Blanc, John B. Claridge, and Matthew J. Rosseinsky.  $\text{Li}_{4.3}\text{AlS}_{3.3}\text{Cl}_{0.7}$ : A sulfide-chloride lithium ion conductor with highly disordered structure and increased conductivity. *Chem. Mater.* 33:8733–8744, 2021. [[doi](#)]
69. Francesca C.N. Firth, Michael W. Gaultois, Yue Wu, Joshua Stratford, Dean S. Keeble, Clare P. Grey, and Matthew J. Cliffe. Exploring the role of cluster formation in UiO family Hf metal-organic frameworks with *in situ* X-ray pair distribution function analysis *J. Am. Chem. Soc.* 143:19668–19683, 2021. [[doi](#)]
68. Adam M. Tollitt, Rebecca Vismara, Luke M. Daniels, Dmytro Antypov, Michael W. Gaultois, Alexandros P. Katsoulidis, and Matthew J. Rosseinsky. High-throughput discovery of a rhombohedral twelve-connected zirconium-based metal-organic framework with ordered terephthalate and fumarate linkers. *Angew. Chem. Int. Ed.* 60:26939–26946, 2021. [[doi](#)]
67. Ahmed Moustafa, Alex Evans, Simmon Hofstetter, Jenny Boutros, Parastoo Pourrezaei, Cheng Zhang, Laura Patterson-Fortin, Charles Laing, Carter Goertzen, Richard Smith, Kenneth R. Code, Ning Cheng, Peter E. R. Blanchard, Nathan Bettman, Raquibul Alam, Kerry McPhedran, Zohreh Fallah, Edward Roberts, and Michael W. Gaultois. Operando studies of iodine species in an advanced oxidative water treatment reactor. *ACS ES&T Water* 1:2293–2458, 2021. [[doi](#)]  
**Cover Article**
66. Andriy Vasylenko, Jacinthe Gamon, Benjamin B. Duff, Vladimir V. Gusev, Luke M. Daniels, John B. Claridge, Frédéric Blanc, Michael W. Gaultois, Matthew S. Dyer, and Matthew J. Rosseinsky. Element selection for crystalline inorganic solid discovery guided by unsupervised machine learning of experimentally explored chemistry. *Nat. Commun.* 12:5561 (12pp), 2021. [[doi](#)]



65. Quinn D. Gibson, Tianqi Zhao, Luke M. Daniels, Helen C. Walker, Ramzy Daou, Sylvie Hébert, Marco Zanella, Matthew S. Dyer, John B. Claridge, Ben Slater, Michael W. Gaultois, Furio Corà, Jonathan Alaria, Matthew J. Rosseinsky. Low thermal conductivity in a modular inorganic material with bonding anisotropy and mismatch. *Science* 373:1017–1022, 2021. [[doi](#)]
64. Chris M. Collins, Luke M. Daniels, Quinn Gibson, Michael W. Gaultois, Michael Moran, Richard Feetham, Michael J. Pitcher, Matthew S. Dyer, Charlene Delacotte, Marco Zanella, Claire. A. Murray, Gyorgyi Glodan, Olivier Pérez, Denis Pelloquin, Troy D. Manning, Jonathan Alaria, George R. Darling, John B. Claridge, and Matthew J. Rosseinsky. Discovery of a low thermal conductivity oxide guided by probe structure prediction and machine learning. *Angew. Chem. Int. Ed.* 60:16457–16465, 2021. [[doi](#)]
63. Stefan Maier, Michael W. Gaultois, Nami Matsubara, Wesley Surta, Françoise Damay, Sylvie Hébert, Vincent Hardy, David Berthebaud, and Franck Gascoin. Sb-5s lone pair dynamics and collinear magnetic ordering in  $\text{Ba}_2\text{FeSbSe}_5$ . *Phys. Rev. B* 103:054115 (7pp), 2021. [[doi](#)]
62. Philip A. E. Murgatroyd, Kieran Routledge, Samantha Durdy, Michael W. Gaultois, T. Wesley Surta, Matthew S. Dyer, John B. Claridge, Stanislav N. Savvin, Denis Pelloquin, Sylvie Hébert, and Jonathan Alaria. Chemically controllable magnetic transition temperature and magneto-elastic coupling in MnZnSb compounds. *Adv. Funct. Mater.* 31(17):202100108 (9pp), 2021. [[doi](#)]
61. Aikaterini Vriza, Angelos B. Canaj, Rebecca Vismara, Laurence J. Kershaw Cook, Troy D. Manning, Michael W. Gaultois, Peter A. Wood, Vitaliy Kurlin, Neil Berry, Matthew S. Dyer, and Matthew J. Rosseinsky. One class classification as a practical approach for accelerating  $\pi - \pi$  co-crystal discovery. *Chem. Sci.* 12:1702–1719, 2021. [[doi](#)]
60. Cameron J. Hargreaves, Matthew S. Dyer, Michael W. Gaultois, Vitaliy A. Kurlin, and Matthew J. Rosseinsky. The Earth Mover’s Distance as a metric for the space of inorganic compositions. *Chem. Mater.* 32:10610–10620, 2020. [[doi](#)]
- Cover Article**
59. Dragos Neagu, Evangelos I. Papaioannou, Bernhard Tjaden, Xuekun Lu, Cheuk-Man Mak, Michael W. Gaultois, Brian Ray, Paul Shearing, and Ian S. Metcalfe. Tracking the evolution of a single composite particle during redox cycling for application in  $\text{H}_2$  production. *Sci. Rep.* 10:5266 (9pp), 2020. [[doi](#)]
58. Andrew M. T. Moore, James P. Kennett, William M. Napier, Ted E. Bunch, James C. Weaver, Malcolm LeCompte, A. Victor Adedeji, Paul Hackley, Gunther Kletetschka, Robert E. Hermes, James H. Wittke, Joshua J. Razink, Michael W. Gaultois, and Allen West. Evidence of cosmic impact at Abu Hureyra, Syria at the Younger Dryas onset (~12.8 ka): High-temperature melting at  $>2200^\circ\text{C}$ . *Sci. Rep.* 10:4185 (22pp), 2020. [[doi](#)]
- Top 15 “Most Read Articles” of 2020**
57. Computationally guided discovery of the sulfide  $\text{Li}_3\text{AlS}_3$  in the Li–Al–S phase field: Structure and lithium conductivity. Jacinthe Gamon, Benjamin B. Duff, Matthew S. Dyer, Christopher Collins, Luke M. Daniels, T. Wesley Surta, Paul M. Sharp, Michael W. Gaultois, Frédéric Blanc, John Bleddyn Claridge, and Matthew J. Rosseinsky. *Chem. Mater.* 31:9699–9714, 2019. [[doi](#)]
56. Geneva Laurita, Danilo Puggioni, Daniel Hickox-Young, James M. Rondinelli, Michael W. Gaultois, Katherine Page, Leo K. Lamontagne, and Ram Seshadri. Uncorrelated Bi off-centering and the insulator-to-metal transition in ruthenium  $\text{A}_2\text{Ru}_2\text{O}_7$  pyrochlores *Phys. Rev. Mater.* 3:095003 (9pp), 2019. [[doi](#)]
55. Erin Finley, Michael W. Gaultois, and Jakoah Brgoch. Unlocking the key to persistent luminescence with X-ray absorption spectroscopy: A local structure investigation of Cr-substituted spinel-type phosphors *Phys. Chem. Chem. Phys.* 21:19349–19358, 2019. [[doi](#)]



54. Roberta Pigliapochi, Liam O'Brien, Andrew J. Pell, Michael W. Gaultois, Yuri Janssen, Peter Khalifah, and Clare P. Grey. When do anisotropic magnetic susceptibilities lead to large NMR shifts? Exploring particle shape effects in the battery electrode material  $\text{LiFePO}_4$ . *J. Am. Chem. Soc.* 33:13089–13100, 2019. [[doi](#)]
53. Michael G. Ehrenreich, Zhixin Zeng, Stefan Burger, Mark R. Warren, Michael W. Gaultois, Jin-Chong Tan, and Gregor Kieslich. Mechanical properties of the ferroelectric metal-free perovskite  $[\text{MDABCO}](\text{NH}_4)\text{I}_3$ . *Chem. Commun.* 55:3911–3914, 2019. [[doi](#)]
52. Taylor D. Sparks, Aleksander Gurlo, Maged F. Bekheet, Michael W. Gaultois, Gennady Cherkashinin, Laetitia Laversenne, and David R. Clarke. High-temperature structure of  $\text{Co}_3\text{O}_4$ : Understanding spinel inversion using in situ and ex situ measurements. *Phys. Rev. B*, 99(10):104104 (10pp), 2019. [[doi](#)]
51. Hamish H. M. Yeung, Adam F. Sapnik, Felicity Massingberd-Mundy, Michael W. Gaultois, Yue Wu, Duncan A. X. Fraser, Sebastian Henke, Roman Pallach, Niclas Heidenreich, Oxana V. Magdysyuk, Nghia T. Vo, and Andrew L. Goodwin. Control of metal-organic framework crystallization by metastable intermediate pre-equilibrium species. *Angew. Chem. Int. Ed.*, 58(2):566–571, 2019. [[doi](#)]
50. Daniel Olds, Rebecca A. Mills, Marshall T. McDonnell, Jue Liu, Joshua R. Kim, Matthew T. Dunstan, Michael W. Gaultois, S. Michelle Everett, Matthew G. Tucker, and Katharine Page. A high temperature gas flow environment for neutron total scattering studies of complex materials. *Rev. Sci. Instrum.*, 89(9):092906 (7pp), 2018. [[doi](#)]
49. Taylor D. Sparks, Aleksander Gurlo, Michael W. Gaultois, and David R. Clarke. Revised model for thermopower and site inversion in  $\text{Co}_3\text{O}_4$  spinel. *Phys. Rev. B*, 98(2):024108 (7pp), 2018. [[doi](#)]
48. Anton O. Oliynyk, Michael W. Gaultois, Martin Hermus, Andrew J. Morris, Arthur Mar, and Jakoah Brogch. Searching for missing binary equiatomic phases: Complex crystal chemistry in the Hf–In system. *Inorg. Chem.*, 57(13):7966–7974, 2018. [[doi](#)]
47. Michael F. Groh, Matthew J. Sullivan, Michael W. Gaultois, Oliver Pecher, Kent J. Griffith, and Clare P. Grey. Interface Instability in  $\text{LiFePO}_4\text{--Li}_{3+x}\text{P}_{1-x}\text{Si}_x\text{O}_4$  all-solid-state batteries. *Chem. Mater.*, 30(17):5886–5895, 2018. [[doi](#)]
46. Yue Wu, David M. Halat, Fengxia Wei, Trevor Binford, Ieuan D. Seymour, Michael W. Gaultois, Sammy Shaker, John Wang, Clare P. Grey, and Anthony K. Cheetham. Mixed X-site formate-hypophosphite hybrid Perovskites. *Chem.–Eur. J.*, 24(44):11309–11313, 2018. [[doi](#)]
45. Christian Dietrich, Raimund Koerver, Michael W. Gaultois, Gregor Kieslich, Giannantonio Cibin, Jürgen Janek, and Wolfgang G. Zeier. Spectroscopic characterization of lithium thiophosphates by XPS and XAS: A model to help monitor interfacial reactions in all-solid-state batteries. *Phys. Chem. Chem. Phys.*, 20(30):20088–20095, 2018. [[doi](#)]
44. Ewa Marek, Wenting Hu, Michael W. Gaultois, Clare P. Grey, and Stuart A. Scott. The use of strontium ferrite in chemical looping systems. *Appl. Energy*, 223:369–382, 2018. [[doi](#)]
43. David M. Halat, Matthew T. Dunstan, Michael W. Gaultois, Sylvia Britto, and Clare P. Grey. Study of defect chemistry in the system  $\text{La}_{2-x}\text{Sr}_x\text{NiO}_{4+\delta}$  by  $^{17}\text{O}$  solid-state NMR spectroscopy and Ni K-Edge XANES. *Chem. Mater.*, 30(14):4556–4570, 2018. [[doi](#)]
42. Matthew J. Cliffe, Jeongjae Lee, Joseph A. M. Paddison, Sam Schott, Paromita Mukherjee, Michael W. Gaultois, Pascal Manuel, Henning Sirringhaus, Sian E. Dutton, and Clare P. Grey. Low-dimensional quantum magnetism in  $\text{Cu}(\text{NCS})_2$ : A molecular framework material. *Phys. Rev. B*, 97(14):144421 (10pp), 2018. [[doi](#)]

41. Michael W. Gaultois, Matthew T. Dunstan, Adam W. Bateson, Martin S. C. Chan, and Clare P. Grey. Screening and characterization of ternary oxides for high-temperature carbon capture. *Chem. Mater.*, 30(8):2535–2543, 2018. [doi]
40. Arobendo Mondal, Michael W. Gaultois, Andrew J. Pell, Marcella Iannuzzi, Clare P. Grey, Jürg Hutter, and Martin Kaupp. Large-scale computation of nuclear magnetic resonance shifts for paramagnetic solids using CP2K. *J. Chem. Theory Comput.*, 14(1):377–394, 2018. [doi]  
**Cover Article**
39. Matthew T. Dunstan, Hannah L. Schlogelhofer, John M. Griffin, Matthew S. Dyer, Michael W. Gaultois, Cindy Y. Lau, Stuart A. Scott, and Clare P. Grey. Ion dynamics and CO<sub>2</sub> absorption properties of Nb-, Ta-, and Y-Doped Li<sub>2</sub>ZrO<sub>3</sub> studied by solid-state NMR, thermogravimetry, and first-principles calculations. *J. Phys. Chem. C*, 121(40):21877–21886, 2017. [doi]
38. Clayton Cozzan, Geneva Laurita, Michael W. Gaultois, Marcus Cohen, Alexander A. Mikhailovsky, Mahalingam Balasubramanian, and Ram Seshadri. Understanding the links between composition, polyhedral distortion, and luminescence properties in green-emitting  $\beta$ -Si<sub>6-z</sub>Al<sub>z</sub>O<sub>z</sub>N<sub>8-z</sub>:Eu<sup>2+</sup> phosphors. *J. Mater. Chem. C*, 5(38):10039–10046, 2017. [doi]
37. Shijing Sun, Zeyu Deng, Yue Wu, Fengxia Wei, Furkan H. Isikgor, Federico Brivio, Michael W. Gaultois, Jianyong Ouyang, Paul D. Bristowe, Anthony K. Cheetham, and Gregor Kieslich. Variable temperature and high-pressure crystal chemistry of perovskite formamidinium lead iodide: A single crystal x-ray diffraction and computational study. *Chem. Commun.*, 53(54):7537–7540, 2017. [doi]
36. Wei Meng, Roberta Pigliapochi, Paul M. Bayley, Oliver Pecher, Michael W. Gaultois, Ieuan D. Seymour, Han-Pu Liang, Wenqian Xu, Kamila M. Wiaderek, Karena W. Chapman, and Clare P. Grey. Unraveling the complex delithiation and lithiation mechanisms of the high capacity cathode material V<sub>6</sub>O<sub>13</sub>. *Chem. Mater.*, 29(13):5513–5524, 2017. [doi]
35. Matthew Cliffe, Elizabeth J. Castillo-Martinez, Yue Wu, Jeongjae Lee, Alexander C. Forse, Francesca C. N. Firth, Peyman Z. Moghadam, David Fairen-Jimenez, Michael W. Gaultois, Joshua A. Hill, Oxana V. Magdysyuk, Ben Slater, Andrew L. Goodwin, and Clare P. Grey. Metal-organic nanosheets formed via defect-mediated transformation of a hafnium metal-organic framework. *J. Am. Chem. Soc.*, 139(15):5397–5404, 2017. [doi]
34. Anton O. Oliynyk, Erin Antono, Taylor D. Sparks, Leila Ghadbeigi, Michael W. Gaultois, Bryce Meredig, and Arthur Mar. High-throughput machine-learning-driven synthesis of full-heusler compounds. *Chem. Mater.*, 28(20):7324–7331, 2016. [doi]
33. Anton O. Oliynyk, Taylor D. Sparks, Michael W. Gaultois, Leila Ghadbeigi, and Arthur Mar. Gd<sub>12</sub>Co<sub>5.3</sub>Bi and Gd<sub>12</sub>Co<sub>5</sub>Bi, Crystalline doppelgänger with low thermal conductivities. *Inorg. Chem.*, 55(13):6625–6633, 2016. [doi]
32. Matthew T. Dunstan, Serena A. Maugeri, Wen Liu, Matthew G. Tucker, Oluwadamilola O. Taiwo, Belen Gonzalez, Phoebe K. Allan, Michael W. Gaultois, Paul R. Shearing, David A. Keen, Anthony E. Phillips, Martin T. Dove, Stuart A. Scott, John S. Dennis, and Clare P. Grey. In situ studies of materials for high temperature CO<sub>2</sub> capture and storage. *Faraday Discuss.*, 192:217–240, 2016. [doi]
31. Michael W. Gaultois, Anton O. Oliynyk, Arthur Mar, Taylor D. Sparks, Gregory J. Mulholland, and Bryce Meredig. Web-based machine learning models for real-time screening of thermoelectric materials properties. *APL Mater.*, 4(5):053213 (11pp), 2016. [doi]  
**Top 15 “Most Read Articles” of 2016, Cover Article**
30. Leo K. Lamontagne, Geneva Laurita, Michael W. Gaultois, Michael Knight, Leila Ghadbeigi, Taylor D. Sparks, Markus E. Gruner, Rossitza Pentcheva, Craig M. Brown, and Ram Seshadri. High thermopower with metallic conductivity in *p*-type Li-substituted PbPdO<sub>2</sub>. *Chem. Mater.*, 28(10):3367–3373, 2016. [doi]





29. Taylor D. Sparks, Michael W. Gaultois, Anton Oliynyk, Jakoah Brgoch, and Bryce Meredig. Data mining our way to the next generation of thermoelectrics. *Scr. Mater.*, 111:10–15, 2016. [[doi](#)]
28. Michael W. Gaultois, Jason E. Douglas, Taylor D. Sparks, and Ram Seshadri. Single-step preparation and consolidation of reduced early-transition-metal oxide/metal *n*-type thermoelectric composites. *AIP Adv.*, 5(9):097144 (11pp), 2015. [[doi](#)]
27. Kristin A. Denault, Jakoah Brgoch, Simon D. Kloss, Michael W. Gaultois, Joan Siewenie, Katharine Page, and Ram Seshadri. Average and local structure, Debye temperature, and structural rigidity in some oxide compounds related to phosphor hosts. *ACS Appl. Mater. Interfaces*, 7(13):7264–7272, 2015. [[doi](#)]
26. Michael W. Gaultois, Moureen C. Kemei, Jaye K. Harada, and Ram Seshadri. Rapid preparation and magnetodielectric properties of trirutile Cr<sub>2</sub>WO<sub>6</sub>. *J. Appl. Phys.*, 117(1):014105 (5pp), 2015. [[doi](#)]
25. Jakoah Brgoch, Michael W. Gaultois, MMahalingam Balasubramanian, Katharine Page, Byung-Chul Hong, and Ram Seshadri. Local structure and structural rigidity of the green phosphor beta-SiAlON:Eu<sup>2+</sup>. *Appl. Phys. Lett.*, 105(18):181904 (4pp), 2014. [[doi](#)]
24. Phillip T. Barton, Moureen C. Kemei, Michael W. Gaultois, Stephanie L. Moffitt, Lucy E. Darago, Ram Seshadri, Matthew R. Suchomel, and Brent C. Melot. Structural distortion below the Neel temperature in spinel GeCo<sub>2</sub>O<sub>4</sub>. *Phys. Rev. B*, 90(6):064105 (7pp), 2014. [[doi](#)]
23. Gregor Kieslich, Ulrich Burkhardt, Christina S. Birkel, Igor Veremchuk, Jason E. Douglas, Michael W. Gaultois, Ingo Lieberwirth, Ram Seshadri, Galen D. Stucky, Yuri Grin, and Wolfgang Tremel. Enhanced thermoelectric properties of the *n*-type Magneli phase WO<sub>2.90</sub>: reduced thermal conductivity through microstructure engineering. *J. Mater. Chem. A*, 2(33):13492–13497, 2014. [[doi](#)]
22. Adam J. Hauser, Jeremy M. Lucy, Michael W. Gaultois, Molly R. Ball, Jennifer R. Soliz, Yongseong Choi, Oscar D. Restrepo, Wolfgang Windl, John W. Freeland, Daniel Haskel, Patrick M. Woodward, and Fengyuan Yang. Magnetic structure in epitaxially strained Sr<sub>2</sub>CrReO<sub>6</sub> thin films by element-specific XAS and XMCD. *Phys. Rev. B*, 89(18):180402(R) (6pp), 2014. [[doi](#)]
21. Kristin A. Denault, Jakoah Brgoch, Michael W. Gaultois, Alexander Mikhailovsky, Ralf Petry, Holger Winkler, Steven P. DenBaars, and Ram Seshadri. Consequences of optimal bond valence on structural rigidity and improved luminescence properties in Sr<sub>x</sub>Ba<sub>2-x</sub>SiO<sub>4</sub>:Eu<sup>2+</sup> orthosilicate phosphors. *Chem. Mater.*, 26(7):2275–2282, 2014. [[doi](#)]
20. Michael W. Gaultois and Taylor D. Sparks. How much improvement in thermoelectric performance can come from reducing thermal conductivity? *Appl. Phys. Lett.*, 104(11):113906 (4pp), 2014. [[doi](#)]
19. Gregor Kieslich, Christina S. Birkel, Jason E. Douglas, Michael Gaultois, Igor Veremchuk, Ram Seshadri, Galen D. Stucky, Yuri Grin, and Wolfgang Tremel. SPS-assisted preparation of the Magneli phase WO<sub>2.90</sub> for thermoelectric applications. *J. Mater. Chem. A*, 1(42):13050–13054, 2013. [[doi](#)]
18. Moureen C. Kemei, Phillip T. Barton, Stephanie L. Moffitt, Michael W. Gaultois, Joshua A. Kurzman, Ram Seshadri, Matthew R. Suchomel, and Young-Il Kim. Crystal structures of spin-Jahn-Teller-ordered MgCr<sub>2</sub>O<sub>4</sub> and ZnCr<sub>2</sub>O<sub>4</sub>. *J. Phys.: Condens. Matter*, 25(32):326001 (7pp), 2013. [[doi](#)]
17. Michael W. Gaultois, Taylor D. Sparks, Christopher K. H. Borg, Ram Seshadri, William D. Bonificio, and David R. Clarke. Data-driven review of thermoelectric materials: Performance and resource considerations. *Chem. Mater.*, 25(15):2911–2920, 2013. [[doi](#)]  
**Top 20 “Most Read Articles” of May–June, Cover Article of August**
16. Michael W. Gaultois, Phillip T. Barton, Christina S. Birkel, Lauren M. Misch, Efrain E. Rodriguez, Galen D. Stucky, and Ram Seshadri. Structural disorder, magnetism, and electrical and thermoelectric properties of pyrochlore Nd<sub>2</sub>Ru<sub>2</sub>O<sub>7</sub>. *J. Phys.: Condens. Matter*, 25(18):186004 (10pp), 2013. [[doi](#)]



15. James D. S. Walker, John R. Hayes, Michael W. Gaultois, Esther Rani Aluri, and Andrew P. Grosvenor. A case for oxygen deficiency in  $\text{Gd}_2\text{Ti}_{2-x}\text{Zr}_x\text{O}_7$  pyrochlore-type oxides. *J. Alloys Compd.*, 565:44–49, 2013. [[doi](#)]
14. Michael W. Gaultois and Andrew P. Grosvenor. XANES and XPS investigations of the local structure and final-state effects in amorphous metal silicates:  $(\text{ZrO}_2)_x(\text{TiO}_2)_y(\text{SiO}_2)_{1-x-y}$ . *Phys. Chem. Chem. Phys.*, 14(1):205–217, 2012. [[doi](#)]
13. Brianna R. Slater, Haiying Bie, Michael W. Gaultois, Stanislav S. Stoyko, and Arthur Mar. Rare-earth cobalt gallides  $\text{RE}_4\text{Co}_3\text{Ga}_{16}$  ( $\text{RE} = \text{Gd–Er, Y}$ ): Self-interstitial derivatives of  $\text{RE}_2\text{CoGa}_8$ . *Eur. J. Inorg. Chem.*, 2011(26):3896–3903, 2011. [[doi](#)]
12. Jessica A. Sigrist, James D. S. Walker, John R. Hayes, Michael W. Gaultois, and Andrew P. Grosvenor. Determining the effect of Ru substitution on the thermal stability of  $\text{CeFe}_{4-x}\text{Ru}_x\text{Sb}_{12}$ . *Solid State Sci.*, 13(11):2041–2048, 2011. [[doi](#)]
11. Jessica A. Sigrist, Michael W. Gaultois, and Andrew P. Grosvenor. Investigation of the Fe K-edge XANES spectra from  $\text{Fe}_{1-x}\text{Ga}_x\text{SbO}_4$ : Local versus nonlocal excitations. *J. Phys. Chem. A*, 115(10):1908–1912, 2011. [[doi](#)]
10. Jessica M. Peddle, Michael W. Gaultois, and Andrew P. Grosvenor. On the oxidation of  $\text{EuFe}_4\text{Sb}_{12}$  and  $\text{EuRu}_4\text{Sb}_{12}$ . *Inorg. Chem.*, 50(13):6263–6268, 2011. [[doi](#)]
9. Michael W. Gaultois and Andrew P. Grosvenor. XANES and XPS investigations of  $(\text{TiO}_2)_x(\text{SiO}_2)_{1-x}$ : the contribution of final-state relaxation to shifts in absorption and binding energies. *J. Mater. Chem.*, 21(6):1829–1836, 2011. [[doi](#)]
8. Michael W. Gaultois, John E. Greedan, and Andrew P. Grosvenor. Investigation of coordination changes in substituted transition-metal oxides by k-edge xanes: Beyond the pre-edge. *J. Electron Spectrosc. Relat. Phenom.*, 184(3-6):192–195, 2011. [[doi](#)]
7. Alina C. Sklad, M. W. Gaultois, and A. P. Grosvenor. Examination of  $\text{CeFe}_4\text{Sb}_{12}$  upon exposure to air: Is this material appropriate for use in terrestrial, high-temperature thermoelectric devices? *J. Alloys Compd.*, 505(1):L6–L9, 2010. [[doi](#)]
6. Michael W. Gaultois, Alina C. Sklad, and Andrew P. Grosvenor. Effects of metal substitution on the electronic structure of mixed ionic-electronic conduction materials. In Matthew Dalzell, editor, *Canadian Light Source Activity Report 2009*, pages 108–109. Houghton Boston, Saskatoon, SK, 2010. [[url](#)]
5. Michael W. Gaultois, Andrew P. Grosvenor, Peter E. R. Blanchard, and Arthur Mar. Ternary arsenides  $\text{Zr}(\text{Si}_x\text{As}_{1-x})\text{As}$  with  $\text{PbCl}_2$ -type ( $0 \leq x \leq 0.4$ ) and  $\text{PbFCl}$ -type ( $x = 0.6$ ) structures. *J. Alloys Compd.*, 492(1-2):19–25, 2010. [[doi](#)]
4. Michael W. Gaultois and Andrew P. Grosvenor. Coordination-induced shifts of absorption and binding energies in the  $\text{SrFe}_{1-x}\text{Zn}_x\text{O}_{3-\delta}$  system. *J. Phys. Chem. C*, 114(46):19822–19829, 2010. [[doi](#)]
3. Stephane Dufresne, Michael Gaultois, and William G. Skene. Environmentally friendly preparation of a conjugated polyazostilbene: A photophysical and electrochemical investigation. *Opt. Mater.*, 30(6):961–967, 2008. [[doi](#)]
2. Stephane Dufresne, Michael Gaultois, and William G. Skene. Disodium 5,5'-diamino-2,2'-ethylenedibenzenesulfonate tetrahydrate. *Acta Crystallogr., Sect. E*, 63:M2714–U772, 2007. [[doi](#)]
1. Stephane Dufresne, Michael Gaultois, and William G. Skene. Bis(triethylammonium) 4,4'-diaminotrans-stilbene-2,2'-disulfonate. *Acta Crystallogr., Sect. E*, 63:O3926–U1847, 2007. [[doi](#)]

## Invited presentations

19. Lathom Lecture, *NSG Group*, Ormskirk, United Kingdom (25 September 2020).
18. Rational development and investigation of functional materials, *Max-Planck-Institut für Mikrostrukturphysik*, Halle, Germany (30 November 2018).
17. Parkin Prize Lecture, *British Crystallographic Association Spring Meeting*, Coventry, United Kingdom (27 March 2018).
16. Computer-assisted searches for new functional inorganic materials using high-throughput DFT and machine learning algorithms: thermoelectrics and CO<sub>2</sub> capture, *Institut de Ciència de Materials de Barcelona*, Barcelona, Spain (13 September 2017).
15. Possible structural origins of reversible CO<sub>2</sub> looping in complex metal oxides, *Department of Chemistry, Technische Universität München*, München, BY, Germany (5 December 2016).
14. Metrics for quantitative evaluation of material resource considerations, *99th Canadian Chemistry Conference, Workshop on Sustainable Approaches to Materials Research*, Halifax, NS, Canada (3–4 June 2016).
13. High throughput DFT screening and experimental characterization of CO<sub>2</sub> looping materials, *Khalifa University*, Abu Dhabi, United Arab Emirates (24 February 2016).
12. High throughput DFT screening and experimental characterization of CO<sub>2</sub> looping materials, *International Workshop on Advanced Materials*, Ras al-Khaimah, United Arab Emirates (21 February 2016).
11. Design principles for oxide thermoelectric materials, *Materials Research Outreach Program Symposium*, Santa Barbara, CA, USA (4 February 2015).
10. Site disorder in Ru pyrochlores and the search for oxide thermoelectric materials, *Lujan Neutron Scattering Center*, Los Alamos, NM, USA (22 January 2014).
9. Using low-temperature physical property measurements to predict high-temperature material performance, *Quantum Design Inc.*, San Diego, CA, USA (20 November 2013).
8. Big data for big problems: Visualizing large datasets for thermoelectric materials discovery, *Third Bilateral UCSB–Chalmers University Workshop on Materials Science and Engineering*, University of California, Santa Barbara, CA, USA (24 August 2013).
7. Data-driven thermoelectric materials discovery: Developing design principles for oxides, *Institute of Inorganic Chemistry and Analytical Chemistry, Johannes Gutenberg–Universität Mainz*, Mainz, RP, Germany (11 July 2013).
6. Data-driven thermoelectric materials discovery: Developing design principles for oxides, *Catalonia Institute for Energy Research, Universitat de Barcelona*, Barcelona, CT, Spain (9 July 2013).
5. Data-driven thermoelectric materials discovery: Developing design principles for oxides, *Unitat de Física dels Materials, Universitat Autònoma de Barcelona*, Barcelona, CT, Spain (8 July 2013).
4. Towards oxide-based thermoelectric materials, *Chemical Sciences Student Seminar, University of California*, Santa Barbara, CA, USA (23 October 2012).
3. Determination of local structure using total scattering and pair distribution function analysis, *Department of Chemistry, University of Saskatchewan*, Saskatoon, SK, Canada (5 June 2012).
2. Le rayonnement synchrotron et son application pour l'étude des oxydes et silicates métalliques, *L'Association francophone pour le savoir (ACFAS) 6e Forum du Savoir*, Saskatoon, SK, Canada (16 March 2011).



1. Presentation to the Governor General of Canada, Her Excellency the Right Honourable Michaëlle Jean, *Canadian Light Source Inc.*, Saskatoon, SK, Canada (24 August 2010).

## Selected awards and recognition

### 2022

- [Ramsay Trust Memorial Fellowship](#), *Society of Chemical Industry*.

### 2018

- Parkin Prize, for “outstanding contributions to promoting science,” *British Crystallographic Association*.

### 2016

- Runner up, Air Force Research Lab [Materials Science and Engineering Data Challenge](#) (\$5 000 prize).
- Chosen by the University of Cambridge to attend the Singapore National Research Foundation 2017 Global Young Scientists Summit. (5 nominees in Cambridge)

### 2015

- [Marie Skłodowska–Curie Individual Fellowship](#).

### 2014

- “Outstanding Oral Presentation” Award, *Functional Inorganic Solid State Materials Symposium, 97th Canadian Chemistry Conference and Exhibition*.
- Outstanding Service to the Department Award, *Department of Chemistry and Biochemistry, UCSB*
- Doctoral Student Travel Grant, *UCSB Academic Senate*

### 2013

- Sponsored by NSERC to attend the 2013 Lindau Nobel Laureate meeting. (5 nominees in Canada)

### 2012

- “Outstanding Poster” Award, *Materials Research Society (MRS) Fall Meeting*. (8 awarded)
- Graduate Thesis Award, for the most outstanding thesis in Physical and Engineering Sciences. *U. Saskatchewan*.
- Henry Taube Medal, for the “most significant overall contribution to research and scholarly activity,” *U. Saskatchewan*.
- Dow-MRL Outreach Outstanding Service Award, *UCSB*

### 2011

- [Vanier Canada Graduate Scholarship](#) (*declined*)
- [NSERC Alexander Graham Bell Canada Graduate Scholarship](#) (CGS-D) (*declined*)

## 2010

- **International Fulbright Science & Technology Award**, *U.S. Department of State*
- **Gerhard Herzberg Memorial Scholarship**, *U. Saskatchewan*
- **Julie Payette–NSERC Research Scholarship**, held at *U. Saskatchewan*

## Professional services

Reviewer for the following:

- ACS Petroleum Research Fund
- Alberta Agriculture and Forestry Strategic Research and Development Program
- Applied Physics Letters
- Chemistry of Materials
- Chemical Physics Reviews
- Computational Materials Science
- Dalton Transactions
- International Journal of Applied Ceramic Technology
- Inorganic Chemistry
- Journal of Alloys and Compounds
- Journal of Applied Physics
- Journal of Materials Chemistry
- Journal of Materials Chemistry A
- Journal of Materials Chemistry C
- Journal of Materials Science
- Journal of Physics and Chemistry of Solids
- Journal of the American Ceramic Society
- Materials Horizons
- Materials Letters
- Materials Research Express
- Nanoscale Research Letters
- Physica Status Solidi A
- Physical Chemistry Chemical Physics
- RSC Advances
- Science Advances
- Scientific Reports