

# List of Publications for Brent C. Melot

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## In press, or submitted:

- i S. Zhou, E. Howard, K. Nolan, M. T. Sougrati, and B. C. Melot Hydrothermal Preparation, Crystal Chemistry, and Redox Properties of Iron Muscovite Clay (under review)

## Independent Publications:

59. A. J. Clough, J. Skelton, C. A. Downes, A. de la Rosa, J. W. Yoo, A. Walsh, B. C. Melot, and S. C. Marinescu Metallic Conductivity in a Two Dimensional Cobalt Dithiolene Framework *J. Am. Chem. Soc.* (2017) [doi]
58. A. J. Neer, J. Milam-Guerrero, J. E. So, B. C. Melot, K. A. Ross, Z. Hulvey, C. M. Brown, A. A. Sokol, D. O. Scanlon, Ising Magnetism on the Octahedral Sublattice of a Cobalt-containing Garnet and the Potential for Quantum Criticality *Phys. Rev. B.* **95** (2017) 144419 [doi]
57. Y. Tulchinsky, C. Hendon, K. Lomachenko, E. Borfecchia, B. C. Melot, M. Hudson, J. Tarver, M. Korzynski, A. Stubbs, J. Kagan, C. Lamberti, C. Brown, M. Dinca, Reversible Capture and Release of Elemental Halogens with a Redox-Active Metal-Organic Framework *J. Am. Chem. Soc.* **139** (2017) 5992–5997 [doi]
56. Investigating the Mechanism of Reversible Lithium insertion into Anti-NASICON  $\text{Fe}_2(\text{WO}_4)_3$  G. Barim, B. C. Melot, R. L. Brutchey *ACS Appl. Mater. Interfaces* **9** (2017) 10813–10819 [doi]
55. R. Hoye, P. Schultz, L. Schelhaus, A. Holder, K. Stone, J. Perkins, D. Vigil-Fowler, S. Siol, D. O. Scanlon, A. Walsh, B. C. Melot, R. Kurchin, Y. Wang, J. Shi, F. Marques, J. Berry, W. Tumas, S. Lany, V. Stevanovic, M. Toney, T. Buonassi Perovskite-inspired photovoltaic materials: Toward best practices in materials characterization and calculations *Chem. Mater.* **29** (2017) 1964–1988 [doi]
54. K. K. Bass, L. Evergreen, S. Zhou, S. E. Bradforth, M. E. Thompson, and B. C. Melot Room Temperature Free Exciton Emission in Films of  $\text{Cs}_3\text{Bi}_2\text{Br}_9$  *Inorg. Chem.* **56** (2017) 4245 [doi]
53. C. H. Hendon, F. Pradaux-Caggiano, L. E. Hatcher, W. J. Gee, D. L. Cruickshank, C. C. Wilson, D. R. Carbery, A. Walsh, and B. C. Melot, Magnetic coupling in a hybrid Mn (II) acetylene dicarboxylate *Phys. Chem. Chem. Phys.* **18** (2016) 33329–33334 [doi]
52. M. Marisa, S. Zhou, B. C. Melot, G. Peaslee, J. R. Neilson Paracrystalline Disorder from Phosphate Ion Orientation and Substitution in Synthetic Bone Mineral *Inorganic Chemistry* **55** (2016) 12290–12298
51. S. Zhou, G. Barim, B. J. Morgan B. C. Melot, and R. L. Brutchey Influence of Rotational Distortions on Li- and Na-ion Intercalation in  $\text{Fe}_2(\text{MoO}_4)_3$  *Chem. Mater.*, **28** (2016) 4492–4500 [doi]
50. B. Lopez-Bermudez, W. G. Zeier, S. Zhou, D. O. Scanlon, B. J. Morgan, and B. C. Melot Lithium-ion conductivity in  $\text{Li}_6\text{Y}(\text{BO}_3)_3$ : a thermally and electrochemically robust solid electrolyte *J. Mater. Chem. A* **4** (2016) 6972–6979 [doi]
49. E. Uman, M. Colonna-Dashwood, L. Colonna-Dashwood, M. Perger, C. Klatt, S. Leighton, B. Miller, K. T. Butler, B. C. Melot, R. W. Speirs, and C. H. Hendon The effect of bean origin and temperature on grinding roasted coffee *Sci. Rep.* **6** (2016) 24483 [doi]
48. M. M. Butala, K. R. Danks, M. A. Lumley, S. Zhou, B. C. Melot, and R. Seshadri MnO Conversion in Li-ion Batteries: In Situ Studies and the Role of Messtructuring *ACS Appl. Mater. Interfaces* **8** (2016) 6496–6503 [doi]
47. D. Russel, A. J. Neer, B. C. Melot, and S. Derakhshan Long Range Antiferromagnetic ordering in B-site Ordered Double Perovskite;  $\text{Ca}_2\text{ScOs}_6$  *Inorg. Chem.* **155** (2016) 2240–245 [doi]
46. E. E. Rodriguez, H. Cao, R. Haiges, B. C. Melot Single crystal magnetic structure and susceptibility of  $\text{CoSe}_2\text{O}_5$  *J. Solid State Chem.* **236** (2016) 39–44 [doi]
45. K. M. Ø. Jensen, X. Yang, J. Vidal Laveda, W. G. Zeier, K. A. See, M. Di Michiel, B. C. Melot, S. A. Corr and S. J. L. Billinge X-Ray Diffraction Computed Tomography for Structural Analysis of Electrode Materials in Batteries *J. Electrochem. Soc.* **162** (2015) A1310–A1314 [doi]
44. S. Zhou, W. G. Zeier, M. Kemei, M. T. Sougrati, M. Mechlenberg, K. Page, and B. C. Melot Hydrothermal preparation and Magnetic Properties of  $\text{NaFeSi}_2\text{O}_6$  Nanowires *Inorg. Chem.* **53** (2014) 12396–12401 [doi]

43. K. K. Bass, R. E. McAnally, S. Zhou, P. I. Djurovich, M. E. Thompson, and B. C. Melot Influence of Moisture on the Preparation, Crystal Structure, and Photophysical Properties of Organohalide Perovskites *Chem. Comm.* **50** (2014) 15819–15822 [[doi](#)]
42. T. W. Day, W. G. Zeier, D. R. Brown, B. C. Melot, and G. J. Snyder Determining Conductivity and Mobility Values of Individual Components in Multiphase Composite  $\text{Cu}_{1.97}\text{Ag}_{0.03}\text{Se}$  *Appl. Phys. Lett.* **105** (2014) 172103 [[doi](#)]
41. S. Zhou, G. King, D. O. Scanlon, M. T. Sougrati, and B. C. Melot Low Temperature Preparation and Electrochemical Properties of  $\text{LiFeSi}_2\text{O}_6$  *J. Electrochem. Soc.* **161** (2014) A1642–A1647 [[doi](#)]
40. W. G. Zeier, S. Zhou, B. Lopez-Bermudez, K. Page, and B. C. Melot Dependence of Li-ion conductivity and activation energies on the crystal structure and ionic radii in  $\text{Li}_6\text{M}\text{La}_2\text{Ta}_2\text{O}_{12}$  *ACS Appl. Mater. Interfaces* **6** (2014) 10900–10907 [[doi](#)]
39. S. P. Culver, F. A. Rabuffetti, S. Zhou, M. Mecklenburg, Y. Song, B. C. Melot, and R. L. Brutchey Low-Temperature Synthesis of  $\text{AMoO}_4$  ( $A = \text{Ca}, \text{Sr}, \text{Ba}$ ) Scheelite Nanocrystals *Chem. Mater.* **25** (2013) 4129–4134 [[doi](#)]
38. L. Tao, G. Rouse, J. R. Neilson, B. C. Melot T. M. McQueen, C. Masquelier Magnetic Structures of  $\text{LiMBO}_3$  ( $M = \text{Mn}, \text{Fe}, \text{Co}$ ) lithiated transition metal borates *Inorg. Chem.* **52** (2013) 11966–11974 [[doi](#)]

### Publications During Ph. D. and Postdoctoral Training:

37. P. T. Barton, M. C. Kemei, M. W. Gaultois, S. L. Moffitt, L. E. Darago, R. Seshadri, M. R. Suchomel, B. C. Melot Structural Distortion Below the Néel Temperature in Spinel  $\text{GeCO}_2\text{O}_4$  *Phys. Rev. B* **90** (2014) 064105 [[doi](#)]
36. B. C. Melot, D. O. Scanlon, M. Reynaud, G. Rouse, J.-N. Chotard, M. Henry, and J.-M. Tarascon Chemical and Structural Indicators of Large Redox Potentials in Fe-Based Positive Electrode Materials *ACS Appl. Mater. Interfaces* [[doi](#)]
35. M. Reynaud, M. Ati, S. Boulineau, M. T. Sougrati, B. C. Melot, G. Rouse, J.-N. Chotard and J.-M. Tarascon Bimetallic Sulfates  $\text{A}_2\text{M}(\text{SO}_4)_2 \cdot n\text{H}_2\text{O}$  ( $A = \text{Li}, \text{Na}$  and  $M = \text{Transition Metal}$ ): as New Attractive Electrode Materials for Li- and Na-Ion Batteries *ECS Trans.* **50** (2013) 11–19 [[doi](#)]
34. B. C. Melot and J.-M. Tarascon Design and Preparation of Materials for Advanced Electrochemical Storage *Acc. Chem. Res.* **46** (2013) 1226–1238 [[doi](#)]
33. N. Recham, G. Rouse, M. T. Sougrati, J.-N. Chotard, C. Frayret, S. Mariyappan, B. C. Melot, J.-C. Jumas, and J.-M. Tarascon Preparation and Characterization of a Stable  $\text{FeSO}_4\text{F}$ -Based Framework for Alkali Ion Insertion Electrodes *Chem. Mater.* **24** (2012) 4363–4370 [[doi](#)]
32. M. Ati, M. Sathiya, S. Boulineau, M. Reynaud, A. Abakumov, G. Rouse, B. C. Melot, G. Van Tendeloo, and J.-M. Tarascon Understanding and Promoting the Rapid Preparation of *triplite*- $\text{LiFeSO}_4\text{F}$  for use as a Large-Potential Fe Cathode *J. Am. Chem. Soc.* **44** (2012) 18380–18387 [[doi](#)]
31. A. V. Radha, J. D. Furman, M. Ati, B. C. Melot, J.-M. Tarascon and A. Navrotsky Understanding the Stability of Fluorosulfate Li-ion Battery Cathode Materials: A Thermochemical Study of  $\text{LiFe}_{1-x}\text{Mn}_x\text{SO}_4\text{F}$  ( $0 \leq x \leq 1$ ) Polymorphs *J. Mater. Chem.* **22** (2012) 24446–24452 [[doi](#)]
30. M. Reynaud, M. Ati, B. C. Melot, M. T. Sougrati, G. Rouse, J.-N. Chotard, and J.-M. Tarascon  $\text{Li}_2\text{Fe}(\text{SO}_4)_2$  as a 3.83 V positive electrode material *Electrochem. Comm.* **21** (2012) 77–80 [[doi](#)]
29. B. C. Melot, G. Rouse, J.-N. Chotard, M. Ati, M. C. Kemei, and J.-M. Tarascon Magnetic structure and properties of  $\text{NaFeSO}_4\text{F}$  and  $\text{NaCoSO}_4\text{F}$  *Phys. Rev. B* **85** (2012) 094415 [[doi](#)]
28. M. Reynaud, P. Barpanda, G. Rouse, J.-N. Chotard, B. C. Melot, N. Recham, and J.-M. Tarascon Synthesis and crystal chemistry of the  $\text{NaMSO}_4\text{F}$  family ( $M = \text{Mg}, \text{Fe}, \text{Co}, \text{Cu}, \text{Zn}$ ) *Solid State Sci.* **14** (2012) 15–20 [[doi](#)]
27. M. Ati, B. C. Melot, G. Rouse, J.-N. Chotard, and J.-M. Tarascon Synthesis and Electrochemical Properties of pure  $\text{LiFeSO}_4\text{F}$  in the *triplite* structure *Electrochem. Comm.* **13** (2011) 1280–1283 [[doi](#)]

26. M. Ati, B. C. Melot, G. Rousse, J-N. Chotard, P. Barpanda, and J-M. Tarascon Structural and Electrochemical Diversity in the  $\text{LiFe}_{1-\delta}\text{Zn}_\delta\text{SO}_4\text{F}$  solid solution: another 3.9V positive electrode based on Fe *Angew. Chem. Int. Ed.* **50** (2011) 10574–10577 [doi]
25. P. Barpanda, M. Ati, B. C. Melot, G. Rousse, J-N. Chotard, M-L. Doublet, M. T. Sougrati, S. A. Corr, J-C. Jumas, and J-M. Tarascon A 3.9V Fe-based fluorosulphate material for Li-ion batteries crystallizing in the *triplite* structure *Nat. Mater.* **10** (2011) 772–779 [doi]
24. B. C. Melot, J-N. Chotard, G. Rousse, M. Ati, M. Reynaud, and J-M. Tarascon, Synthesis, structure and magnetic properties of the  $\text{NaCoXO}_4\text{F}\cdot 2\text{H}_2\text{O}$  phases where  $X = \text{S}$  and  $\text{Se}$  *Inorg. Chem.* **50** (2011) 7662–7668 [doi]
23. B. C. Melot, G. Rousse, J.-N. Chotard, M. Ati, J. Rodríguez-Carvajal, M. C. Kemei, and J.-M. Tarascon Magnetic structure and properties of the Li-ion battery materials  $\text{FeSO}_4\text{F}$  and  $\text{LiFeSO}_4\text{F}$  *Chem. Mater.* **23** (2011) 2922–2930 [doi]
22. J. R. Neilson, D. E. Morse, B. C. Melot, D. P. Shoemaker, J. A. Kurzman, and R. Seshadri Understanding complex magnetic order through analyses of local atomic structure *Phys. Rev. B* **83** (2011) 094418 [doi]
21. B. C. Melot, L. E. Darago, R. Seshadri, A. Goldman, J. D. Furman, and E. E. Rodriguez Magnetic susceptibility and magnetodielectric phenomena in  $\text{CoSeO}_4$  *J. Phys.: Condens. Matter* **22** (2010) 506003 [doi]
20. S.-H. Kim, P. S. Halasymani, B. C. Melot, R. Seshadri, M. Green, A. Sefat, and D. Mandrus, An experimental and computational investigation of the polar ferrimagnet  $\text{VOSe}_2\text{O}_5$  *Chem. Mater.* **22** (2010) 50074–5083 [doi]
19. P. J. Saines, B. C. Melot, Ram Seshadri. and A. K. Cheetham, Synthesis, structure and magnetic phase transitions of the manganese succinate hybrid framework  $[\text{Mn}(\text{C}_4\text{H}_4\text{O}_4)]$  *Chem.-Eur. J.* **16** (2010) 7579–7585 [doi]
18. K. I. Lilova, A. Navrotsky, B. C. Melot, and R. Seshadri, Thermodynamics of  $\text{CoAl}_2\text{O}_4$ – $\text{CoGa}_2\text{O}_4$  solid solutions, *J. Sol. State Chem.* **83** (2010) 1266–1271 [doi]
17. B. C. Melot, B. Paden, R. Seshadri, E. Suard, G. Néner, A. Dixit, and G. Lawes, Magnetic structure and susceptibility of  $\text{CoSe}_2\text{O}_5$ : An antiferromagnetic chain compound, *Phys. Rev. B* **82** (2010) 014411 [doi]
16. S. A. Corr, D. P. Shoemaker, B. C. Melot, R. Seshadri, Real space investigation of structural changes at the metal-insulator transition in  $\text{VO}_2$  *Phys. Rev. Lett* **105** (2010) 056404 [doi]
15. B. C. Melot, K. Page, R. Seshadri, E. M. Stoudenmire, L. Balents, D. L. Bergman, and Th. Proffen, Magnetic frustration on the diamond lattice of the A-site magnetic spinels  $\text{CoAl}_{2-x}\text{Ga}_x\text{O}_4$ : The role of lattice expansion and site disorder, *Phys. Rev. B* **80** (2009) 104420(1-8) [doi]
14. B. C. Melot, R. Tackett, J. O'Brien, A. L. Hector, G. Lawes, R. Seshadri, A. P. Ramirez, Large low temperature specific heat in pyrochlore  $\text{Bi}_2\text{Ti}_2\text{O}_7$ , *Phys. Rev. B* (Editor's Suggestion) **79** (2009) 224111(1-5). [doi]
13. E. E. Rodriguez, A. Llobet, Th. Proffen, B. C. Melot, R. Seshadri, P. B. Littlewood, and A. K. Cheetham, The role of static disorder in negative thermal expansion in  $\text{ReO}_3$ , *J. Appl. Phys.* **105** (2009) 114901. [doi]
12. B. C. Melot, J. E. Drewes, R. Seshadri, and A. P. Ramirez, Magnetic phase evolution in the spinel compounds  $\text{Zn}_{1-x}\text{Co}_x\text{Cr}_2\text{O}_4$ , *J. Phys.: Condens. Matter* **21** (2009) 216007(1–7). [doi]
11. S. A. Corr, M. Grossman, J. D. Furman, B. C. Melot, A. K. Cheetham, K. R. Heier, and R. Seshadri, Controlled reduction of vanadium oxide nanoscrolls: Crystal structure, morphology, and electrical properties. *Chem. Mater.* **20** (2008) 6396–6404. [doi]
10. R. Tackett, G. Lawes, B. C. Melot, M. Grossman, E. S. Toberer, and R. Seshadri, Magnetodielectric coupling in  $\text{Mn}_3\text{O}_4$ , *Phys. Rev. B* **76** (2007) 024409(1-6). [doi]
9. G. Lawes, B. Melot, K. Page, C. Ederer, M. A. Hayward, Th. Proffen, and R. Seshadri, Dielectric anomalies and spiral magnetic order in  $\text{CoCr}_2\text{O}_4$ , *Phys. Rev. B* **74** (2006) 024413(1-6). [doi]
8. B. Melot, E. Rodriguez, Th. Proffen, M. A. Hayward, and R. Seshadri, Displacive disorder in three high- $k$  bismuth oxide pyrochlores, *Mater. Res. Bull.* **41** (2006) 961-966. [doi]

7. J. D. Furman, B. C. Melot, S. J. Treat, A. A. Mikhailovsky, and A. K. Cheetham Towards enhanced ligand-centered photoluminescence in inorganic-organic frameworks for solid state lighting *Phys. Chem. Chem. Phys.* **13** (2010) 7622–7629 [[doi](#)]
6. A. J. Hatt, B. C. Melot, and S. Narasimhan, Harmonic and anharmonic properties of Fe and Ni: Thermal expansion, exchange-correlation errors and magnetism, *Phys. Rev. B.* **82** (2010) 134418 [[doi](#)]
5. Z. Hulvey, B. C. Melot, and A. K. Cheetham, Structure and magnetic field-induced transition in a one-dimensional hybrid inorganic-organic chain system,  $\text{Co}_2(4,4'\text{-bpy})(\text{tfhba})_2 \cdot 4,4'\text{-bpy}$  (4,4'-bpy = 4,4'-bipyridine; tfhba = 2,3,5,6-tetrafluoro-4-hydroxybenzoate) *Inorg. Chem.* **49** (2010) 4594–4598 [[doi](#)]
4. E. S. Toberer, A. F. May, B. C. Melot, E. Flage-Larsen, and G. J. Snyder, Electronic structure and transport in thermoelectric compounds  $A\text{Zn}_2\text{Sb}_2$  ( $A=\text{Sr},\text{Ca},\text{Yb},\text{Eu}$ ), *Dalton Trans.* **39** (2010) 1046–1054 [[doi](#)]
3. S. Fortier, G. Wu, B. C. Melot, and T. W. Hayton, Synthesis and characterization of several homoleptic uranium(IV) alkyl complexes *J. Am. Chem. Soc.* **131** (2009) 15512–15521. [[doi](#)]
2. R. K. Feller, B. C. Melot, P. M. Forster, and A. K. Cheetham, Structure and magnetic properties of a hybrid cobalt disulfonate-hydroxide with a novel inorganic layer architecture, *J. Mater. Chem.* **19** (2009) 2604–2609. [[doi](#)]
1. A. Aravindh, A. Arkundato, S. Barman, S. Baroni, *et al.*,  $\text{Si}_x\text{C}_{1-x}\text{O}_2$  alloys: A possible route to stabilize carbon-based silica-like solids?, *Solid State Commun.* **144** (2007) 273–276. [[doi](#)]

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