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### Submitted or In Press

*Names underlined indicate Bates undergraduate student.*

### Appeared

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35. U Dang, J. O'Hara, H. A. Evans, D. Olds, J. Chamorro, D. Hickox-Young, G. Laurita, and R. T. Macaluso, Vacancy driven disorder and elevated dielectric response in the pyrochlore  $\text{Pb}_{1.5}\text{Nb}_2\text{O}_{6.5}$ . *Inorg. Chem.* (2022) [DOI:10.1021/acs.inorgchem.2c03031]
34. D. Hickox-Young, G. Laurita, Q. N. Meier, D. Olds, N. A. Spaldin, M. R. Norman, and J. M. Rondinelli. Local structure and its implications for the relaxor ferroelectric  $\text{Cd}_2\text{Nb}_2\text{O}_7$ . *Phy. Rev. Res.* **4** (2022) 033187 [DOI:10.1103/PhysRevResearch.4.033187]
33. *Invited contribution to the Emerging Investigators 2022 issue:* O. Bailey, S. Husremovic, M. Murphy, J. Ross, J. Gong, D. Olds, and G. Laurita<sup>†</sup>. Compositional Influence of Local and Long-Range Polarity in the Frustrated Pyrochlore System  $\text{Bi}_{2-x}\text{RE}_x\text{Ti}_2\text{O}_7$  ( $\text{RE} = \text{Y}^{3+}, \text{Ho}^{3+}$ ). *J. Mater. Chem. C.* **10** (2022) 13886 - 13895 (2022) [DOI:10.1039/D2TC01328B]
32. *Invited contribution:* C. Chepkemboi<sup>\*</sup>, K. Jorgensen<sup>\*</sup>, J. Sato<sup>\*</sup>, and G. Laurita<sup>†</sup>. [\*equal contributions] Strategies and considerations for least squares analysis of total scattering data. *ACS Omega* **7** (2022) 14402–14411. [DOI:10.1021/acsomega.2c01285]
31. G. Laurita and R. Seshadri. Chemistry, Structure, and Function of Lone Pairs in Extended Solids. *Acc. Chem. Res.* **55** (2022) 1004–1014 [DOI:10.1021/acs.accounts.1c00741]
30. Q. N. Meier, D. Hickox-Young, G. Laurita, N. A. Spaldin, J. M. Rondinelli, and M. R. Norman. Leggett Modes Accompanying Crystallographic Phase Transitions. *Phys. Rev. X* **12** (2022) 011024 [DOI:10.1103/PhysRevX.12.011024]
29. M. Saber, M. Preefer, S. Kolli, W. Zhang, G. Laurita, B. Dunn, R. Seshadri, and A. Van der Ven. The role of electronic structure on Li-ordering and chemical strain in the fast charging Wadsley-Roth phase  $\text{PNb}_9\text{O}_{25}$ . *Chem. Mater.* **33** (2021) 7755–7766. [DOI:10.1021/acs.chemmater.1c02059]
28. E. Zoghlin, J. Schmehr, C. Holgate, R. Dally, G. Laurita, C. Levi, and S. D. Wilson. Evaluating the Effects of Structural Disorder on the Magnetic Properties of  $\text{Nd}_2\text{Zr}_2\text{O}_7$ . *Phys. Rev. Mater.*, **5** (2021) 084403. [DOI:10.1103/PhysRevMaterials.5.084403]
27. E. Zoghlin, Z. Porter, **S. Britner**, **S. Husremovic**, Y. Choi, D. Haskel, G. Laurita, and S. Wilson, Mapping the structural, magnetic and electronic behaviour of  $(\text{Eu}_{1-x}\text{Ca}_x)_2\text{Ir}_2\text{O}_7$  across a metal-insulator transition, *J. Phys. Condens. Matter*, **33** (2020) 055601. [DOI:10.1088/1361-648X/abbf2b]
26. J. N. Tang, D. M. Crook, G. Laurita, and M. A. Subramanian, Vacancy tuning in Li, V-substituted lyonsites, *Solvent Extr. Ion Exc.* **38**, (2020) 656-680. [DOI:10.1080/07366299.2020.1780705]
25. U. Dang, W. Zaheer, **W. Zhou**, **A. Kandel**, M. Orr, R. Schwenz, G. Laurita, S. Banerjee, R. Macaluso, Lattice Anharmonicity of Stereochemically Active Lone Pairs Controls Thermochromic Band Gap Reduction of  $\text{PbVO}_3\text{Cl}$ . *Chem. Mater.* **32** (2020) 7404–7412. [DOI:10.1021/acs.chemmater.0c02342]
24. **M. L. Robinson**, **E. Whitaker**, L. Jin, M. A. Hayward, and G. Laurita, Evidence of paracrystalline cation order in the Ruddlesden-Popper phase  $\text{LaSr}_3\text{NiRuO}_8$  through total scattering techniques, *Inorg. Chem.* **59** (2020) 3026-3033. [DOI:10.1021/acs.inorgchem.9b03382]

23. G. Laurita, D. Puggioni, D. Hickox-Young, M. W. Gaultois, L. K. Lamontagne, K. Page, J. Rondinelli, and R. Seshadri, Uncorrelated Bi off-centering and the insulator-to-metal transition in ruthenium  $A_2Ru_2O_7$  pyrochlores. *Phys. Rev. Mater.* **3** (2019) 095003. [DOI:10.1103/PhysRevMaterials.3.095003]
22. G. Laurita, D. Hickox-Young, S. Husremovic, J. Li, A. W. Sleight, R. T. Macaluso, J. M. Rondinelli, and M. A. Subramanian, Covalency-Driven Structural Evolution in the Polar Pyrochlore Series  $Cd_2Nb_2O_{7-x}S_x$ . *Chem. Mater.* **31** (2019) 7626–7637. [DOI:10.1021/acs.chemmater.9b02466]
21. Z. Porter, E. Zoghlin, S. Britner, S. Husremovic, J. P. C. Ruff, Y. Choi, D. Haskel, G. Laurita, and S. Wilson, Evolution of structure and magnetism across the metal-insulator transition in the pyrochlore iridate  $(Nd_{1-x}Ca_x)_2Ir_2O_7$ , *Phys. Rev. B.* **100** (2019) 054409. [DOI:10.1103/PhysRevB.100.054409]
20. E. Schueller, G. Laurita, D. Fabini, C. Stoumpos, M. Kanatzidis, and R. Seshadri, Crystal structure evolution and notable thermal expansion in hybrid perovskites formamidinium tin iodide and formamidinium lead bromide, *Inorg. Chem.* **57** (2018) 695–701. [DOI:10.1021/acs.inorgchem.7b02576]
19. D. Fabini, T. A. Siaw, C. Stoumpos, G. Laurita, D. Olds, K. Page, J. Hu, M. Kanatzidis, S. Han, and R. Seshadri, Universal dynamics of molecular reorientation in hybrid lead iodide perovskites, *J. Am. Chem. Soc.* **139** (2017) 16875–16884. [DOI:10.1021/jacs.7b09536]
18. C. Cozzan, G. Laurita, M. W. Gaultois, M. Cohen, A. A. Mikhailovsky, M. Balasubramanian, and R. Seshadri, Compositional control of emission color and thermal stability in the green-emitting  $\beta$ -SiAlON:Eu<sup>2+</sup> phosphor, *J. Mater. Chem. C* **5** (2017) 10039–10046. [DOI:10.1039/C7TC03039H]
17. J. Buchanan, D. B. Fast, B. E. Hanken, T. J. Mustard, G. Laurita, T.-H. Chiang, D. Keszler, M. Subramanian, J. F. Wager, M. Dolgos, J. R. Rustad, and P. H. Y. Cheong, Structural convergence properties of amorphous  $InGaZnO_4$  from simulated liquid-quench methods, *Dalton Trans.* **46** (2017) 15311–15316. [DOI:10.1039/C7DT02181J]
16. M. L. C. Buffon, G. Laurita, L. Lamontagne, E. Levin, S. Mooraj, D. L. Lloyd, N. White, T. M. Pollock, and R. Seshadri, Thermoelectric performance and the role of anti-site disorder in the 24-electron Heusler  $TiFe_2Sn$ , *J. Phys. Condensed Matt.* **29** (2017) 405702(1–7). [DOI:10.1088/1361-648X/aa81e7]
15. G. Laurita, D. H. Fabini, C. C. Stoumpos, M. G. Kanatzidis, and R. Seshadri, Chemical tuning of dynamic cation off-centering in the cubic phases of hybrid tin and lead halide perovskites, *Chem. Sci.* **8** (2017) 5628–5635. [doi:10.1039/C7SC01429E]
14. L. Devys, G. Dantelle, G. Laurita, E. Homeyer, I. Gautier-Luneau, C. Dujardin, R. Seshadri, and T. Gacoin, A strategy to increase phosphor brightness: application with  $Ce^{3+}$ -doped  $Gd_3Sc_2Al_3O_{12}$ , *J. Lumin.* **190** (2017) 62–68. [doi:10.1016/j.jlumin.2017.05.035]
13. L. K. Lamontagne, G. Laurita, M. Knight, H. Yusuf, J. Hu, R. Seshadri, and K. Page, The role of structural and compositional heterogeneities in the insulator-to-metal transition in the hole-doped  $A_{1-x}Na_xPd_3O_4$  ( $A = Ca, Sr$ ), (*Inorg. Chem.*), **56** (2017) 5158–5164. [doi:10.1021/acs.inorgchem.7b00307]
12. M. M. Butala, M. Mayo, V. Doan-Nguyen, M. A. Lumley, C. Göbel, K. M. Wiaderek, O. J. Borkiewicz, K. W. Chapman, P. J. Chupas, M. Balasubramanian, G. Laurita, S. Britto, A. Morris, C. P. Grey, and R. Seshadri, Local structure evolution and modes of charge storage in secondary Li–FeS<sub>2</sub> cells, (*Chem. Mater.*), **29** (2017) 3070–3082. [doi:10.1021/acs.chemmater.7b00070]
11. C. Cozzan, K. J. Griffith, G. Laurita, J. G. Hu, C. P. Grey, and Ram Seshadri, Structural evolution and atom clustering in  $\beta$ -SiAlON: $\beta$ -Si<sub>6-z</sub>Al<sub>z</sub>O<sub>z</sub>N<sub>8-z</sub>, *Inorg. Chem.*, **56** (2017) 2153. [doi:10.1021/acs.inorgchem.6b02780]
10. D. H. Fabini, C. C. Stoumpos, G. Laurita, A. Kaltzoglou, A. G. Kontos, P. Falaras, M. G. Kanatzidis, and R. Seshadri, Large positive thermal expansion and re-entrant structural and optical properties in perovskite formamidinium lead iodide, *Angew. Chem.* **55** (2016) 15392. [doi:10.1002/anie.201609538/pdf]

9. D. H. Fabini,\* G. Laurita,\* J. S. Bechtel, C. C. Stoumpos, H. A. Evans, A. Van der Ven, M. G. Kanatzidis, and R. Seshadri. [\* equal contributions] Dynamic stereochemical activity of the Sn<sup>2+</sup> lone pair in perovskite CsSnBr<sub>3</sub>, *J. Am. Chem. Soc.* **138** (2016) 11820. [[doi:10.1021/jacs.6b06287](https://doi.org/10.1021/jacs.6b06287)]
8. M. L. C. Buffon, G. Laurita, N. Verma, L. Lamontagne, L. Ghadbeigi, D. L. Lloyd, T. D. Sparks, C. M. Brown, T. M. Pollock, and R. Seshadri, Enhancement of thermoelectric properties in the Nb–Co–Sn half-Heusler/Heusler system through spontaneous inclusion of a coherent second phase, *J. Appl. Phys.* **120** (2016) 075104. [[doi:10.1063/1.4961215](https://doi.org/10.1063/1.4961215)].
7. L. K. Lamontagne, G. Laurita, M. Gaultois, M. Knight, L. Ghadbeigi, T. D. Sparks, M. E. Gruner, R. Pentcheva, C. Brown, and R. Seshadri, High thermopower with metallic conductivity in p-type Li-substituted PbPdO<sub>2</sub>, *Chem. Mater.* **28** (2016) 3367. [[doi:10.1021/acs.chemmater.6b00447](https://doi.org/10.1021/acs.chemmater.6b00447)]
6. G. Laurita, R. Grajczyk, M. Stolt, I. Coutinho, A. W. Sleight, and M. A. Subramanian, Influence of structural disorder on hollandites A<sub>x</sub>Ru<sub>4</sub>O<sub>8</sub> (A<sup>+</sup> = K, Rb, Rb<sub>1-x</sub>Na<sub>x</sub>), *Inorg. Chem.* **55** (2016) 3462. [[doi:10.1021/acs.inorgchem.5b02897](https://doi.org/10.1021/acs.inorgchem.5b02897)]
5. G. Laurita, K. Page, S. Suzuki, and R. Seshadri, Average and local structure of the Pb-free ferroelectric perovskites (Sr,Sn)TiO<sub>3</sub> and (Ba,Ca,Sn)TiO<sub>3</sub>, *Phys. Rev. B.* **92** (2015) 214209. [[doi:10.1103/PhysRevB.92.214109](https://doi.org/10.1103/PhysRevB.92.214109)]
4. J. Heo, G. Laurita, S. Muir, M. A. Subramanian, and D. A. Keszler, Enhanced thermoelectric performance of synthetic tetrahedrites, *Chem. Mater.* **26** (2014) 2047. [[doi:10.1021/cm404026k](https://doi.org/10.1021/cm404026k)]
3. G. Laurita, J. Vielma, R. Berthelot, F. Winter, R. Pöttgen, G. Schneider and M. A. Subramanian, From Ag<sub>2</sub>Sb<sub>2</sub>O<sub>6</sub> to Cd<sub>2</sub>Sb<sub>2</sub>O<sub>7</sub>: investigations on an anion-deficient to ideal pyrochlore solid solution, *J. Solid State Chem.* **210** (2014) 65. [[doi:10.1021/cm404026k](https://doi.org/10.1021/cm404026k)]
2. G. Laurita, K. Page, A. W. Sleight and M. A. Subramanian, Investigation of the anion-deficient pyrochlore AgSbO<sub>3</sub> through total scattering techniques, *Inorg. Chem.* **52** (2013) 11530. [[doi:10.1021/ic401860j](https://doi.org/10.1021/ic401860j)]
1. T. Siritanon, G. Laurita, R. T. Macaluso, J. Millican, A. W. Sleight and M. A. Subramanian, First observation of electronic conductivity in mixed valent tellurium oxides, *Chem. Mater.* **21** (2009) 5572. [[doi:10.1021/cm9029769](https://doi.org/10.1021/cm9029769)]