

Ram Seshadri: Publications and Patents

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In press, or submitted:

- K. Wyckoff, J. Bienz, M. Saber, A. Zohar, A. K. Cheetham, and R. Seshadri, Relating structural features to electrode performance in Wadsley-Roth anodes.
- A. Reach, M. Wright, A. Mulligan, Z. Fang, K.-T. Tseng, C. Wang, J. Hu, M. Chi, A. K. Cheetham, R. Seshadri, and J. Sakamoto, Enhanced sodium dynamics in biphasic NaSICON solid electrolytes, *Chem. Mater.*
- H. Tian, T. Li, A. Mulligan, J. Tregidga, M. Wright, A. Zohar, A. Chezhayan, M. Preefer, K. Stone, J. Hu, G. Wu, A. Manjón-Sanz, S. Lapidus, J. Harter, A. K. Cheetham, and R. Seshadri, Structural propensities in Cs_2MBiX_6 (M = Na, Ag; X = Cl, Br) bismuth halide double perovskites. *Chem. Mater.*
- K. Brockmeyer, A. Bologna, M. Wright, J. Wong, C. Rodriguez, T. Li, R. A. Segalman, and R. Seshadri, Direct microwave pyrolysis of cellulose to hard carbon anodes for sodium-ion batteries, *Chem. Mater.*
- A. Watkins, A. K. Cheetham, and R. Seshadri, Metallic oxides and the overlooked role of bandwidth, *Chem. Mater.* [DOI: 10.1021/acs.chemmater.5c02578]
- A. Zambotti, K. Thurber, A. Sebastian, K. Liang, R. Chen, J. Li, A. Zohar, Arava; G. Nkala, Y. Li, A. Van der Ven, R. Seshadri, J. Nelson Weker, B. Melot, S. Tolbert, and B. Dunn, Morphological impact on sodium-ion storage in TiO_2 (B) nanostructures, *Chem. Mater.* [DOI: 10.1021/acs.chemmater.5c02317]

Appeared:

449. A. Balvanz, A. Pournara, R. P. Reynolds, P. E. Meza, C. D. Malliakas, J. D. Fletcher, R. Seshadri, V. P. Dravid, and M. G. Kanatzidis, Tuning optical properties and local lone-pair off-centering in “hollow” $\text{FA}_{1-x}\text{en}_x\text{Pb}_{1-y}\text{Sn}_y\text{Br}_3$ perovskites, *Chem. Sci.* **17** (2026) 526–543. [DOI: 10.1039/D5SC01841B]
448. A. Bologna, D. Liu, S. Antall, B. Schmidt, R. Zhang, F. Seeler, K. Schierle-Arndt, and R. Seshadri, Impact of Al and Cu current collectors on Li-ion battery recycling, *ACS Sustainable Resour. Manage.* **3** (2026) 223–232. [DOI: 10.1021/acssusresmg.5c00528]
447. S. J. Gomez Alvarado, J. R. Chamorro, D. Rout, J. Hielscher, S. Schwarz, C. Benyacko, M. B. Stone, V. O. Garlea, A. R. Jackson, G. Pokharel, R. Gomez, B. R. Ortiz, S. Sarker, L. Kautzsch, L. C. Gallington, R. Seshadri, and S. D. Wilson, Interleaved bond frustration in the triangular lattice antiferromagnet LnCd_3P_3 , *Nature Mater.* **25** (2026) 65–72. [DOI: 10.1038/s41563-025-02380-x]
446. M. A. Wright, A. S. Mulligan, D. Rout, J. Hu, J. Liu, R. L. Behrens, J. R. Chamorro, S. D. Wilson, A. K. Cheetham, and R. Seshadri, Strong, yet split hydrogen bonding with ice rules in delafossite (H/D) RhO_2 , *Angew. Chem. Int. Ed.* **64** (2025) e15471. [DOI: 10.1002/anie.202515471]
445. M. A. Wright and R. Seshadri, Linking battery electrode science with correlated and quantum materials, *Phys. Rev. Mater.* **9** (2025) 110302. [DOI: 10.1103/zwkw-zc5n]
444. K. E. Wyckoff, A. Zohar, T. Li, Y. Zhou, L. Kautzsch, W. Wang, A. Kepper, A. Patterson, H. C. Mandujano, K. P. Koirala, A. Kallistova, W. Xu, J. Liu, L. Pilon, A. K. Cheetham, and R. Seshadri, Metallicity, atomic disorder, and Li-ion storage in fast-charging anodes, *J. Am. Chem. Soc.* **147** (2025) 33432–33441. [DOI: 10.1021/jacs.5c06578]
443. A. J. Bologna, R. Vincent, A. Kallistova, J. A. Mayer, M. A. Wright, C. De la Cruz, R. Zhang, F. Seeler, K. Schierle-Arndt, and R. Seshadri, Pyrolyzed “black mass” feedstocks and their synthetic proxies relevant to Li-ion battery recycling, *ACS Omega* **10** (2025) 25546–25554. [DOI: 10.1021/acsomega.5c00995]
442. O. Kuklinski, A. Brumberg, L. Tang, A. S. Mulligan, T. Kodalle, C. M. Sutter-Fella, R. Seshadri, and M. L. Chabiny, Two-step spin-coating of vacancy-ordered double perovskites enables growth of thin films for electronic devices, *J. Mater. Chem. C* **13** (2025) 11402–11412. [DOI: 10.1039/D5TC00502G]

441. A. Reach, A. Zohar, M. Wright, T. Li, and R. Seshadri, Rapid microwave preparation of $\text{AlNb}_{11}\text{O}_{29}$ and $\text{Ti}_2\text{Nb}_{10}\text{O}_{29}$ Wadsley–Roth lithium-ion anode compounds from parent oxides, *ACS Appl. Energy Mater.* **8** (2025) 7714–7721. [DOI: 10.1021/acsaem.5c01005]
440. Y. Li, R. Seshadri, S. D. Wilson, A. K. Cheetham, and R. Valentí, Origins of temperature-dependent magnetism in open-shell 4d and 5d halide perovskites, *Phys. Rev. Res.* **7** (2025) L012083. [DOI: 10.1103/PhysRevResearch.7.L012083]
439. M. J. Brady, J. L. Andrews A. Zambotti, D. Zhang, X. Yuan, K. Thurber, X. Duan, Y. Li, J. Nelson Weker, A. R. Balakrishna, K. See, R. Seshadri, A. Van der Ven, Bruce S. Dunn, S. H. Tolbert, and B. C. Melot, Multiscale approaches for optimizing the impact of strain on Na-ion battery cycle life, *MRS Energy & Sustainability* **12** (2025) 32–45. [DOI: 10.1557/s43581-024-00118-x]
438. A. Zohar, T. Li, Y. Zhou, K. E. Wyckoff, A. Patterson, L. Pilon, and R. Seshadri, Fast charging from low Li-ion migration barriers in Wadsley–Roth $\text{NaNb}_7\text{O}_{18}$ anodes, *Chem. Mater.* **37** (2025) 1523–1530. [DOI: 10.1021/acs.chemmater.4c02980] & [UC-eScholarship]
437. L. Kautzsch, A. Georgescu, L. Yuan, K. Taddei, A. Reilly, R. Seshadri, J. Rondinelli, and S. Wilson, Highly quantum spin chains from strong covalency in Ca_3CrN_3 , *J. Am. Chem. Soc.* **147** (2025) 3092–3101. [DOI: 10.1021/jacs.4c11629] & [UC-eScholarship]
436. A. S. Mulligan, G. T. Kent, J. Zhuang, A. Zohar, K. R. Albanese, E. E. Morgan, G. Wu, A. K. Cheetham, and R. Seshadri, Iodide double perovskites and the limit of their structural stability, *Chem. Eur. J.* **31** (2025) e202404009. [DOI: 10.1002/chem.202404009] & [UC-eScholarship]
435. A. Brumberg, O. Kuklinski, G. Kent, E. Morgan, A. Mikhailovsky, T. Strom, M. L. Chabiny, and R. Seshadri, Optical band gap modulation in vacancy-ordered double perovskites through metal precursor and solvent selection, *Chem. Mater.* **36** (2024) 9625–9635. [DOI: 10.1021/acs.chemmater.4c01701] & [UC-eScholarship]
434. E. E. Morgan, A. Brumberg, S. Panuganti, G. Kent, A. Zohar, A. Mikhailovsky, M. G. Kanatzidis, R. Schaller, M. L. Chabiny, A. K. Cheetham, and R. Seshadri, Molecular origins of near-infrared luminescence in molybdenum and tungsten oxyhalide perovskites, *Chem. Mater.* **36** (2024) 7754–7763. [DOI: 10.1021/acs.chemmater.4c00856] & [UC-eScholarship]
433. A. Balvanz, M. Safdari, M. Zacharias, D. Kim, C. Welton, E. H. Oriel, M. Kepenekian, C. Katan, C. D. Malliakas, J. Even, V. Klepov, G. N. Manjunatha Reddy, R. D. Schaller, L. X. Chen, R. Seshadri, and M. G. Kanatzidis, Structural evolution and photoluminescence quenching across the $\text{FASnI}_{3-x}\text{Br}_x$ ($x = 0 - 3$) perovskites, *J. Am. Chem. Soc.* **146** (2024) 16128–16147. [DOI: 10.1021/jacs.4c03669] & [UC-eScholarship]
432. A. K. Watkins, D. Johrendt, V. Vlcek, S. D. Wilson, and R. Seshadri, Fidelity and variability in the interlayer electronic structure of the kagome superconductor CsV_3Sb_5 , *Phys. Rev. Mater.* **8** (2024) 054204(1–10). [DOI: 10.1103/PhysRevMaterials.8.054204] & [UC-eScholarship]
431. A. K. Cheetham and R. Seshadri, Artificial intelligence driving materials discovery? Perspective on the article: Scaling deep learning for materials discovery, *Chem. Mater.* **36** (2024) 3490–3495. [DOI: 10.1021/acs.chemmater.4c00643]
430. E. Mozur and R. Seshadri, Magnetic tunability in tetragonal Mn–Rh–Ir–Sn inverse Heusler compounds, *J. Phys.: Condens. Matter* **36** (2024) 195802 (open access). [DOI: 10.1088/1361-648X/ad2585]
429. J. Chamorro, J. Zuo, E. Bassey, A. Watkins, G. Zhu, A. Zohar, K. Wyckoff, T. Kinnibrugh, S. Lapidus, S. Stemmer, R. Clément, S. Wilson, R. Seshadri, Soft-chemical synthesis, structure evolution, and insulator-to-metal transition in a prototypical metal oxide, $\lambda\text{-RhO}_2$, *Chem. Mater.* **36** (2024) 1547–1558. [DOI: 10.1021/acs.chemmater.3c02814] & [UC-eScholarship]
428. E. E. Morgan, A. Zohar, S. Lipkin, B. Monserrat, S. Vaidyanathan, D. Loeffler, R. Zhang, K. Schierle-Arndt, A. K. Cheetham, and R. Seshadri, Screening aluminum-based compounds as low- κ dielectrics for high-frequency applications. *Chem. Mater.* **36** (2024) 1228–1237. [DOI: 10.1021/acs.chemmater.3c01975] & [UC-eScholarship]

427. J. A. Mayer, K. V. Vamsi, R. Seshadri, and T. M. Pollock, Antiphase boundaries in B2 intermetallics: Proximate structures, formation energies, and chemical stability, *Phys. Rev. Mater.* **8** (2024) 013610. [DOI: 10.1103/PhysRevMaterials.8.013610] & [UC-eScholarship]
426. G. Kent, J. Huang, K. Albanese, A. Zohar, E. Morgan, A. Kallistova, L. Kautzsch, A. Mikhailovsky, P. Vishnoi, R. Seshadri, and A. K. Cheetham, Hybrid iodide perovskites of divalent alkaline earth and lanthanide elements, *J. Am. Chem. Soc.* **145** (2023) 27850–27856. [DOI: 10.1021/jacs.3c11494] & [UC-eScholarship]
425. L. Kautzsch, A. B. Georgescu, D. Puggioni, G. Kent, K. M. Taddei, A. Reilly, R. Seshadri, J. M. Rondinelli, and S. D. Wilson, Canted antiferromagnetism in polar MnSiN_2 with high Néel temperature, *Phys. Rev. Mater.* **7** (2023) 104406. [DOI: 10.1103/PhysRevMaterials.7.104406] & [UC-eScholarship]
424. E. E. Morgan, G. T. Kent, A. Zohar, A. O'Dea, G. Wu, A. K. Cheetham, and R. Seshadri, Hybrid and inorganic vacancy-ordered double perovskites A_2WCl_6 , *Chem. Mater.* **35** (2023) 7032–7038. [DOI: 10.1021/acs.chemmater.3c01300] & [UC-eScholarship]
423. J. R. Chamorro, A. R. Jackson, A. K. Watkins, R. Seshadri, and S. D. Wilson, Magnetic order in the $S_{eff} = 1/2$ triangular-lattice compound NdCd_3P_3 , *Phys. Rev. Mater.* **7** (2023) 094402. [DOI: 10.1103/PhysRevMaterials.7.094402] & [UC-eScholarship]
422. Y. Zhou, Y. Luo, A. Patterson, S. W. Baek, M. Frajnkovič, R. Seshadri, B. S. Dunn, and L. Pilon, Microcalorimetry electrothermal impedance spectroscopy (ETIS) informs entropy evolution at individual electrodes of $\text{PNb}_9\text{O}_{25}$ or TiNb_2O_7 battery cells, *Electrochim. Acta* **468** (2023) 143072. [DOI: 10.1016/j.electacta.2023.143072] & [UC-eScholarship]
421. A. Patterson, R. Elizalde-Segovia, K. Wyckoff, A. Zohar, P. Ding, W. Turner, K. Poeppelmeier, S. Narayan, R. Clément, R. Seshadri, and K. Griffith, Rapid and reversible lithium insertion in the Wadsley–Roth-derived phase $\text{NaNb}_{13}\text{O}_{33}$, *Chem. Mater.* **35** (2023) 6364–6373. [DOI: 10.1021/acs.chemmater.3c01066] & [UC-eScholarship]
420. G. Kent, E. Morgan, K. R. Albanese, A. Kallistova, A. Brumberg, L. Kautzsch, G. Wu, P. Vishnoi, R. Seshadri, and A. K. Cheetham, Elusive double perovskite iodides: Structural, optical, and magnetic properties, *Angew. Chemie.* **62** (2023) e202306000. [DOI: 10.1002/anie.202306000] & [UC-eScholarship]
419. L. Kautzsch, Y. M. Oey, H. Li, Z. Ren, B. R. Ortiz, R. Seshadri, J. Ruff, Z. Wang, I. Zeljkovic, and S. D. Wilson, Incommensurate charge-stripe correlations in the kagome superconductor $\text{CsV}_3\text{Sb}_{5-x}\text{Sn}_x$, *npj Quantum Mater.* (2023) 37. [DOI: 10.1038/s41535-023-00570-x] & [UC-eScholarship]
418. A. Zohar, K. E. Wyckoff, R. C. Vincent, T. E. Mates, and R. Seshadri, Controlling operating voltages in molybdenum oxide anodes through inductive effects, *Chem. Mater.* **35** (2023) 5009–5016. [DOI: 10.1021/acs.chemmater.3c00354] & [UC-eScholarship]
417. K. E. Wyckoff, L. Kautzsch, J. Kaufman, B. Ortiz, A. Kallistova, G. Pokharel, J. Liu, K. Taddei, K. Wiaderek, S. Lapidus, S. Wilson, A. Van der Ven, and R. Seshadri, Electrochemical control of magnetism on the breathing kagome network of $\text{Li}_x\text{ScMo}_3\text{O}_8$, *Chem. Mater.* **35** (2023) 4945–4954. [DOI: 10.1021/acs.chemmater.3c00202] & [UC-eScholarship]
416. B. R. Ortiz, P. M. Sarte, A. H. Avidor, A. Hay, E. Kenney, A. I. Kolesnikov, D. M. Pajerowski, A. A. Aczel, K. M. Taddei, C. M. Brown, C. Wang, M. J. Graf, R. Seshadri, L. Balents, and S. D. Wilson, Quantum disordered ground state in the triangular-lattice magnet NaRuO_2 , *Nature Phys.* **19** (2023) 943–949. [DOI: 10.1038/s41567-023-02039-x] & [UC-eScholarship]
415. A. D. Ready, A. Irshad, A. Kallistova, M. Carrillo, M. Gembicky, R. Seshadri, S. Narayan, and A. M. Spokoyny, Electrochemical cycling of redox-active boron cluster-based materials in the solid state, *J. Am. Chem. Soc.* **145** (2023) 14345–14353. [DOI: 10.1021/jacs.3c03065] & [UC-eScholarship]
414. B. R. Ortiz, G. Pokharel, M. Gundayao, H. Li, F. Kaboudvand, L. Kautzsch, S. Sarker, J. P. C. Ruff, T. Hogan, S. J. Gomez Alvarado, P. M. Sarte, G. Wu, T. Braden, R. Seshadri, E. S. Toberer, I. Zeljkovic, and S. D. Wilson, YbV_3Sb_4 and EuV_3Sb_4 , vanadium-based kagome metals with Yb^{2+} and Eu^{2+} zig-zag chains, *Phys. Rev. Mater.* **7** (2023) 064201. [DOI: 10.1103/PhysRevMaterials.7.064201] & [UC-eScholarship]

413. E. M. Mozur and R. Seshadri, Methods and protocols: Practical magnetic measurement, *Chem. Mater.* **35** (2023) 3450–3463. [DOI: [10.1021/acs.chemmater.3c00297](https://doi.org/10.1021/acs.chemmater.3c00297)] & [UC-eScholarship]
412. S. A. Meynell, Y. M. Eggeler, J. D. Bocarsly, D. A. Kitchaev, B. E. Rhodes, T. M. Pollock, S. D. Wilson, A. Van der Ven, R. Seshadri, M. De Graef, A. Bleszynski Jayich, and D. S. Gianola, Inducing skyrmion flop transitions in $\text{Co}_8\text{Zn}_8\text{Mn}_4$ at room temperature, *Phys. Rev. Mater.* **7** (2023) 04401. [DOI: [10.1103/PhysRevMaterials.7.044401](https://doi.org/10.1103/PhysRevMaterials.7.044401)] & [UC-eScholarship]
411. L. Kautzsch, B. R. Ortiz, K. Mallayya, J. Plumb, G. Pokharel, J. P. C. Ruff, Z. Islam, E.-A. Kim, R. Seshadri, and S. D. Wilson, Structural evolution of the kagome superconductors AV_3Sb_5 ($A = \text{K}, \text{Rb}, \text{and Cs}$) through charge density wave order, *Phys. Rev. Mater.* **7** (2023) 024806(1–8). [DOI: [10.1103/PhysRevMaterials.7.024806](https://doi.org/10.1103/PhysRevMaterials.7.024806)] & [UC-eScholarship]
410. S. Bhunia, A. Peña-Duarte, H. Li, M. F. Sanad, P. Saha, M. A. Addicoat, K. Sasaki, T. A. Strom, M. José Yacamán, C. R. Cabrera, R. Seshadri, S. Bhattacharya, J.-L. Brédas, and L. Echegoyen, [2,1,3]-Benzothiadiazole-spaced Co-porphyrin-based covalent organic frameworks for O_2 reduction, *ACS Nano* **17** (2023) 3492–3505. [DOI: [10.1021/acsnano.2c09838](https://doi.org/10.1021/acsnano.2c09838)]
409. S. W. Baek, K. E. Wyckoff, D. Robertson, M. Frajnkovič, Y. Zhou, S. Tolbert, R. Seshadri, and L. Pilon, Operando calorimetry investigation of particle size effects on heat generation in Wadsley-Roth $(\text{W}_{0.2}\text{V}_{0.8})_3\text{O}_7$ based electrodes, *ACS Appl. Energ. Mater.* **6** (2023) 1355–1367. [DOI: [10.1021/acsaem.2c03150](https://doi.org/10.1021/acsaem.2c03150)] & [UC-eScholarship]
408. R. C. Vincent, A. K. Cheetham, and R. Seshadri, Structure and lithium insertion in oxides of molybdenum, *APL Mater.* **11** (2023) 010902. [DOI: [10.1063/5.0133518](https://doi.org/10.1063/5.0133518)] & [UC-eScholarship]
407. D. Werhahn, B. R. Ortiz, A. K. Hay, S. D. Wilson, R. Seshadri, and D. Johrendt, The kagomé metals RbTi_3Bi_5 and CsTi_3Bi_5 , *Z. Naturforsch. B* **77(11–12)b** (2022) 757–764. [DOI: [10.1515/znb-2022-0125](https://doi.org/10.1515/znb-2022-0125)] & [UC-eScholarship]
406. C. Chen, E. E. Morgan, Y. Liu, R. Seshadri and L. Mao, “Breathing” organic cation to stabilize multiple structures in low-dimensional Ge-, Sn-, and Pb-based hybrid iodide perovskites, *Inorg. Chem. Frontiers* **9** (2022) 4892–4898. [DOI: [10.1039/D2QI01247B](https://doi.org/10.1039/D2QI01247B)] & [UC-eScholarship]
405. L. Mao, E. E. Morgan, A. Li, R. M. Kennard, M. J. Hong, Y. Liu, C. J. Dahlman, J. G. Labram, M. L. Chabinyc, and R. Seshadri, Layered hybrid lead iodide perovskites with short interlayer distances, *ACS Energy Lett.* **7** (2022) 2801–2806. [DOI: [10.1021/acsenerylett.2c01321](https://doi.org/10.1021/acsenerylett.2c01321)] & [UC-eScholarship]
404. A. K. Cheetham, R. Seshadri, and F. Wudl, Chemical synthesis and materials discovery, *Nature Synth.* **1** (2022) 514–520. [DOI: [10.1038/s44160-022-00096-3](https://doi.org/10.1038/s44160-022-00096-3)] & [UC-eScholarship]
403. Y. M. Oey, F. Kaboudvand, B. R. Ortiz, R. Seshadri, and S. D. Wilson, Tuning charge-density wave order and superconductivity in the kagome metals $\text{KV}_3\text{Sb}_{5-x}\text{Sn}_x$ and $\text{RbV}_3\text{Sb}_{5-x}\text{Sn}_x$, *Phys. Rev. Mater.* **6** (2022) 074802. [DOI: [10.1103/PhysRevMaterials.6.074802](https://doi.org/10.1103/PhysRevMaterials.6.074802)] & [UC-eScholarship]
402. A. D. Ready, S. M. Becwar, D. Jung, A. Kallistova, E. Schueller, K. P. Anderson, R. Kubena, R. Seshadri, B. F. Chmelka, and A. M. Spokoyny, Synthesis and structural properties of a 2D Zn(II) dodecahydroxy-closo-dodecaborate coordination polymer, *Dalton* **51** (2022) 11547–11557. [DOI: [10.1039/D2DT01292H](https://doi.org/10.1039/D2DT01292H)] & [UC-eScholarship]
401. R. M. Kennard, C. J. Dahlman, E. E. Morgan, G. Wu, J. Chung, B. L. Cotts, A. Mikhailovsky, L. Mao, J. R. A. Kincaid, R. A. DeCrescent, K. H. Stone, S. Panuganti, N. R. Venkatesan, Y. Mohtashami, S. Assadi, M. G. Kanatzidis, A. Salleo, J. A. Schuller, R. Seshadri, and M. L. Chabinyc, Enhancing and extinguishing the different emission features of two-dimensional $(\text{EA}_{1-x}\text{FA}_x)_4\text{Pb}_3\text{Br}_{10}$ perovskite films, *Adv. Opt. Mater.* **5** (2022) 2200547. [DOI: [10.1002/adom.202200547](https://doi.org/10.1002/adom.202200547)] & [UC-eScholarship]
400. J. A. Mayer and R. Seshadri, Electron count dictates phase separation in Heusler alloys, *Phys. Rev. Mater.* **6** (2022) 054406(1–13). [DOI: [10.1103/PhysRevMaterials.6.054406](https://doi.org/10.1103/PhysRevMaterials.6.054406)] & [UC-eScholarship]
399. R. Vincent, Y. Luo, J. Andrews, A. Zohar, Y. Zhou, Q. Yan, E. Mozur, M. Preefer, J. Nelson Weker, A. K. Cheetham, J. Luo, L. Pilon, B. Melot, B. Dunn, and R. Seshadri, High-rate lithium cycling and structure evolution in Mo_4O_{11} , *Chem. Mater.* **34** (2022) 4122–4133. [DOI: [10.1021/acs.chemmater.2c00420](https://doi.org/10.1021/acs.chemmater.2c00420)] & [UC-eScholarship]

398. E. Morgan, H. Evans, K. Pilar, C. Brown, R. Clément, R. Maezono, R. Seshadri, B. Monserrat, and A. K. Cheetham, Lattice dynamics in the NASICON $\text{NaZr}_2(\text{PO}_4)_3$ solid electrolyte from temperature-dependent neutron diffraction, NMR, and ab initio computational studies, *Chem. Mater.* **34** (2022) 4029–4038. [DOI: [10.1021/acs.chemmater.2c00212](https://doi.org/10.1021/acs.chemmater.2c00212)] & [UC-eScholarship]
397. P. Vishnoi, J. Pratap; X. Li, D. C. Binwal, K. Wyckoff, L. Mao, L. Kautzsch, G. Wu, S. D. Wilson, M. G. Kanatzidis, R. Seshadri and A. K. Cheetham, Hybrid layered double perovskite halides of transition metals, *J. Am. Chem. Soc.* **144** (2022) 6661–6666. [DOI: [10.1021/jacs.1c12760](https://doi.org/10.1021/jacs.1c12760)] & [UC-eScholarship]
396. S. Wang, E. E. Morgan, S. Panuganti, L. Mao, P. Vishnoi, G. Wu, Q. Liu, M. G. Kanatzidis, R. Schaller, and R. Seshadri, Ligand control of structural diversity in luminescent hybrid copper (I) iodides, *Chem. Mater.* **34** (2022) 3206–3216. [DOI: [10.1021/acs.chemmater.1c04408](https://doi.org/10.1021/acs.chemmater.1c04408)] & [UC-eScholarship]
395. Y. Wang, X.-J. Zhang, F. Xia, E. A. Olivetti, S. D. Wilson, R. Seshadri, and J. M. Rondinelli, Learning the crystal structure genome for property classification, *Phys. Rev. Res.* **4** (2022) 023029. [DOI: [10.1103/PhysRevResearch.4.023029](https://doi.org/10.1103/PhysRevResearch.4.023029)] & [UC-eScholarship]
394. 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](https://doi.org/10.1021/acs.accounts.1c00741)] & [UC-eScholarship]
393. K. E. Wyckoff, J. Kaufman, S. W. Baek, C. Dolle, J. Zak, J. Bienz, L. Kautzsch, R. Vincent, A. Zohar, K. See, Y. Eggeler, L. Pilon, A. Van der Ven, and R. Seshadri, Metal-metal bonding as an electrode design principle in the low-strain cluster compound $\text{LiScMo}_3\text{O}_8$, *J. Am. Chem. Soc.* **144** (2022) 5841–5854. [DOI: [10.1021/jacs.1c12070](https://doi.org/10.1021/jacs.1c12070)] & [UC-eScholarship]
392. Y. M. Oey, B. R. Ortiz, F. Kaboudvand, J. Frassinetti, E. Garcia, S. Sanna, V. Mitrović, R. Seshadri, and S. D. Wilson, Fermi level tuning and double-dome superconductivity in the kagome metals $\text{CsV}_3\text{Sb}_{5-x}\text{Sn}_x$, *Phys. Rev. Mater.* **6** (2022) L041801. [DOI: [10.1103/PhysRevMaterials.6.L041801](https://doi.org/10.1103/PhysRevMaterials.6.L041801)] & [UC-eScholarship]
391. F. Kaboudvand, S. M. L. Teicher, S. D. Wilson, R. Seshadri, and M. D. Johannes, Fermi surface nesting and the Lindhard response function in the kagome superconductor CsV_3Sb_5 , *Appl. Phys. Lett.* **120** (2022) 111901. [DOI: [10.1063/5.0081081](https://doi.org/10.1063/5.0081081)] & [UC-eScholarship]
390. X. Li, M. Kepenekian, L. Li, H. Dong, C. Stoumpos, R. Seshadri, C. Katan, P. Guo, J. Even, and M. Kanatzidis, Tolerance factor for stabilizing 3D hybrid halide perovskitoids using linear diammonium cations, *J. Am. Chem. Soc.* **144** (2022) 3902–3912. [DOI: [10.1021/jacs.1c11803](https://doi.org/10.1021/jacs.1c11803)] & [UC-eScholarship]
389. S. W. Baek, M. B. Preefer, M. Saber, K. Zhai, M. Frajnković, Y. Zhao, B. S. Dunn, A. Van der Ven, R. Seshadri, and L. Pilon, Potentiometric entropy and operando calorimetric measurements reveal fast charging mechanisms in $\text{PNb}_9\text{O}_{25}$, *J. Power Sources* **520** (2022) 230776(1–12). [DOI: [10.1016/j.jpowsour.2021.230776](https://doi.org/10.1016/j.jpowsour.2021.230776)] & [UC-eScholarship]
388. G. Pokharel, S. M. L. Teicher, B. Ortiz, P. Sarte, G. Wu, S. Peng, J. He, R. Seshadri, and S. D. Wilson, Study of the electronic properties of topological kagome metals YV_6Sn_6 and GdV_6Sn_6 , *Phys. Rev. B.* **104** (2021) 235139(1–10). [DOI: [10.1103/PhysRevB.104.235139](https://doi.org/10.1103/PhysRevB.104.235139)] & [UC-eScholarship]
387. M. B. Preefer, J. H. Grebenkemper, C. E. Wilson, M. Everingham, J. A. Cooley, and R. Seshadri, Subtle local structural details influence ion transport in glassy Li^+ thiophosphate solid electrolytes. *ACS Appl. Mater. Interfaces* **13** (2021) 57567–57575. [DOI: [10.1021/acsami.1c16515](https://doi.org/10.1021/acsami.1c16515)] & [UC-eScholarship]
386. B. R. Ortiz, S. M. L. Teicher, L. Kautzsch, P. M. Sarte, N. Ratcliff, J. Harter, J. P. C. Ruff, R. Seshadri, and S. D. Wilson, Fermi surface mapping and the nature of charge density wave order in the kagome superconductor CsV_3Sb_5 , *Phys. Rev. X* **11** (2021) 041030(1–14). [DOI: [10.1103/PhysRevX.11.041030](https://doi.org/10.1103/PhysRevX.11.041030)] & [UC-eScholarship]
385. M. Saber, M. B. 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](https://doi.org/10.1021/acs.chemmater.1c02059)] & [UC-eScholarship]
384. R. Kennard, C. Dahlman, J. Chung, B. Cotts, A. Mikhailovsky, L. Mao, R. DeCrescent, K. Stone, N. Venkatesan, Y. Mohtashami, S. Assadi, A. Salleo, J. Schuller, R. Seshadri, and M. Chabinyc, Growth-controlled broad emission in phase-pure two-dimensional hybrid perovskite films, *Chem. Mater.* **33** (2021) 72900–7300. [DOI: [10.1021/acs.chemmater.1c01641](https://doi.org/10.1021/acs.chemmater.1c01641)] & [UC-eScholarship]

383. D. Rawlings, D. Lee, J. Kim, I.-B. Magdau, G. Pace, P. Richardson, E. Thomas, S. Danielsen, S. Tolbert, T. Miller, R. Seshadri, and R. Segalman, Concurrent Li^+ and oxidant addition to control ionic and electronic conduction in ionic liquid functionalized conjugated polymers, *Chem. Mater.* **33** (2021) 6464–6474. [DOI: 10.1021/acs.chemmater.1c01811] & [UC-eScholarship]
382. H. A. Evans, L. Mao, R. Seshadri, and A. K. Cheetham, Layered double perovskites, *Annu. Rev. Mater. Res.* **51** (2021) 351–380. [DOI: 10.1146/annurev-matsci-092320-102133] & [UC-eScholarship]
381. N. S. Schausser, G. A. Kliegle, P. A. Cooke, R. A. Segalman, and R. Seshadri, Database creation, visualization, and statistical learning for polymer Li^+ electrolyte design, *Chem. Mater.* **33** (2021) 4863–4876. [DOI: 10.1021/acs.chemmater.0c04767] & [UC-eScholarship]
380. E. McCalla, E. E. Levin, J. E. Douglas, J. G. Barker, M. Frontzek, W. Tian, R. M. Fernandes, R. Seshadri, and C. Leighton, Understanding magnetic phase coexistence in $\text{Ru}_2\text{Mn}_{1-x}\text{Fe}_x\text{Sn}$ Heusler alloys: A neutron scattering, thermodynamic, and phenomenological analysis, *Phys. Rev. Mater.* **5** (2021) 064417. [DOI: 10.1103/PhysRevMaterials.5.064417] & [UC-eScholarship]
379. R. Vincent, J.-X. Shen, M. Preefer, J. Lin, F. Seeler, K. Schierle-Arndt, K. Persson, and R. Seshadri, Prospects for employing lithium copper phosphates as high-voltage Li-ion cathodes, *J. Phys. Chem. C* **125** (2021) 13123–13130. [DOI: 10.1021/acs.jpcc.1c01406] & [UC-eScholarship]
378. E. C. Schueller, Y. M. Oey, K. Miller, K. E. Wyckoff, R. Zhang, S. D. Wilson, J. R. Rondinelli, and R. Seshadri, AB_2X_6 compounds and the stabilization of trirutile oxides, *Inorg. Chem.* **60** (2021) 9224–9232. [DOI: 10.1021/acs.inorgchem.1c01366] & [UC-eScholarship]
377. P. Vishnoi, R. Seshadri, A. K. Cheetham, Why are double perovskite iodides so rare? *J. Phys. Chem. C* **125** (2021) 11756–117764. [DOI: 10.1021/acs.jpcc.1c02870] & [UC-eScholarship]
376. J. L. Zuo, D. Kitchaev, E. C. Schueller, J. D. Bocarsly, R. Seshadri, A. Van der Ven, and S. D. Wilson, Magnetoentropic mapping and computational modeling of cycloids and skyrmions in the lacunar spinels GaV_4S_8 and GaV_4Se_8 , *Phys. Rev. Mater.* **5** (2021) 054410 (1–10). [DOI: 10.1103/PhysRevMaterials.5.054410] & [UC-eScholarship]
375. I. Spanopoulos, I. Hadar, W. Ke, P. Guo, E. Mozur, E. Morgan, S. Wang, D. Zheng, S. Padgaonkar, G. N. Manjunatha Reddy, E. Weiss, M. Hersam, R. Seshadri, R. Schaller, and M. Kanatzidis, Tunable broad light emission from 3D “hollow” bromide perovskites through defect engineering, *J. Am. Chem. Soc.* **143** (2021) 7069–7080. [DOI: 10.1021/jacs.1c01727] & [UC-eScholarship]
374. B. R. Ortiz, P. M. Sarte, E. Kenney, M. J. Graf, S. M. L. Teicher, R. Seshadri, and S. D. Wilson, Superconductivity in the $\mathbb{Z}_2$ kagome metal KV_3Sb_5 , *Phys. Rev. Mater.* **5** (2021) 034801(1–7). [DOI: 10.1103/PhysRevMaterials.5.034801] & [UC-eScholarship]
373. P. Vishnoi, J. L. Zuo, J. A. Cooley, L. Kautzsch, A. Gómez-Torres, J. Murillo, S. Fortier, S. D. Wilson, R. Seshadri, and A. K. Cheetham, Chemical control of spin-orbit coupling and charge transfer in vacancy-ordered Ru(IV) halide perovskites, *Angew. Chem.* **60** (2021) 5184–5188. [DOI: 10.1002/anie.202013383] & [UC-eScholarship]
372. S. W. Baek, K. E. Wyckoff, D. M. Butts, J. Bienz, A. Likitchatchawankun, M. B. Preefer, M. Frajkovič, B. S. Dunn, R. Seshadri, and L. Pilon, Operando calorimetry informs the origin of rapid rate performance in microwave-prepared TiNb_2O_7 electrodes, *J. Power Sources* **490** (2021) 229537. [10.1016/j.jpowsour.2021.229537] & [UC-eScholarship]
371. Y. M. Oey, D. A. Kitchaev, J. D. Bocarsly, E. C. Schueller, J. A. Cooley, and R. Seshadri, Magnetocaloric behavior and magnetic ordering in MnPdGa , *Phys. Rev. Mater.* **5** (2021) 014414(1–6). [DOI: 10.1103/PhysRevMaterials.5.014414] & [UC-eScholarship]
370. E. E. Levin, D. A. Kitchaev, Y. M. Eggeler, J. A. Mayer, P. Behera, D. S. Gianola, A. Van der Ven, T. M. Pollock, and R. Seshadri, Influence of plastic deformation on the magnetic properties of Heusler MnAu_2Al , *Phys. Rev. Mater.* **5** (2021) 014408(1–8). [DOI: 10.1103/PhysRevMaterials.5.014408] & [UC-eScholarship]
369. R. M. Kennard, C. J. Dahlman, R. A. DeCrescent, J. A. Schuller, K. Mukherjee, R. Seshadri, and M. L. Chabynyc, Ferroelastic hysteresis in thin films of methylammonium lead iodide, *Chem. Mater.* **33** (2021) 298–309. [DOI: 10.1021/acs.chemmater.0c03776] & [UC-eScholarship]

368. N. S. Schauser, A. Nikolaev, P. M. Richardson, S. Xie, K. Johnson, E. M. Susca, H. Wang, R. Seshadri, R. J. Clément, J. Read de Alaniz, and R. A. Segalman, Glass transition temperature and ion binding determine conductivity and lithium-ion transport in polymer electrolytes, *ACS Macro. Lett.* **10** (2021) 104–109. [DOI: [10.1021/acsmacrolett.0c00788](https://doi.org/10.1021/acsmacrolett.0c00788)] & [UC-eScholarship]
367. J. D. Bocarsly, M. D. Johannes, S. D. Wilson, and R. Seshadri, Magnetostructural coupling from competing magnetic and chemical bonding effects, *Phys. Rev. Research* **2** (2020) 042048(R) (1–7). [DOI: [10.1103/PhysRevResearch.2.042048](https://doi.org/10.1103/PhysRevResearch.2.042048)] & [UC-eScholarship]
366. W. Cai, J. D. Bocarsly, A. Gomez, R. J. Letona Lee, A. Metta-Magaña, R. Seshadri, and L. Echegoyen, High blocking temperatures for DyScS endohedral fullerene single-molecule magnets, *Chem. Sci.* **11** (2020) 13129–13136. [DOI: [10.1039/D0SC05265E](https://doi.org/10.1039/D0SC05265E)] & [UC-eScholarship]
365. B. R. Ortiz, S. M. L. Teicher, Y. Hu, J. L. Zuo, P. M. Sarte, E. C. Schueller, M. Krogstad, S. Rosenkranz, R. Osborn, R. Seshadri, L. Balents, J. He, and S. D. Wilson, CsV₃Sb₅: a $\mathbb{Z}_2$ topological kagome metal with a superconducting ground state, *Phys. Rev. Lett.* **125** (2020) 247002(1–6). [DOI: [10.1103/PhysRevLett.125.247002](https://doi.org/10.1103/PhysRevLett.125.247002)] & [UC-eScholarship]
364. C. E. Reilly, G. Lheureux, C. Cozzan, E. Zeitz, T. Margalith, S. Nakamura, R. Seshadri, C. Weisbuch, and S. P. DenBaars, Transmission geometry laser lighting with a compact emitter, *Phys. Status Solidi A* **217** (2020) 2000391(1–9). [DOI: [10.1002/pssa.202000391](https://doi.org/10.1002/pssa.202000391)] & [UC-eScholarship]
363. K. E. Wyckoff, D. D. Robertson, M. B. Preefer, S. M. L. Teicher, J. Bienz, L. Kautzsch, T. E. Mates, J. A. Cooley, S. H. Tolbert, and R. Seshadri, High capacity Li⁺ storage through multielectron redox in the fast-charging Wadsley–Roth phase (W_{0.2}V_{0.8})₃O₇, *Chem. Mater.* **32** (2020) 9415–9424. [DOI: [10.1021/acs.chemmater.0c03496](https://doi.org/10.1021/acs.chemmater.0c03496)] & [UC-eScholarship]
362. R. Vincent, P. Vishnoi, M. B. Preefer, J. Shen, F. Seeler, K. Persson, and R. Seshadri, Li₅VF₄(SO₄)₂: A prototype high voltage Li-ion cathode, *ACS Appl. Mater. Interfaces* **12** (2020) 48662–48668. [DOI: [10.1021/acsaami.0c14781](https://doi.org/10.1021/acsaami.0c14781)] & [UC-eScholarship]
361. S. Wang, E. E. Morgan, P. Vishnoi, L. Mao, S. M. L. Teicher, G. Wu, Q. Liu, A. K. Cheetham, and R. Seshadri, Tunable luminescence in hybrid Cu(I) and Ag(I) iodides, *Inorg. Chem.* **59** (2020) 15487–15494. [DOI: [10.1021/acs.inorgchem.0c02517](https://doi.org/10.1021/acs.inorgchem.0c02517)] & [UC-eScholarship]
360. E. C. Schueller, K. D. Miller, W. Zhang, J. L. Zuo, J. M. Rondinelli, S. D. Wilson, and R. Seshadri, Structural signatures of the insulator-to-metal transition in BaCo_{1-x}Ni_xS₂, *Phys. Rev. Mater.* **4** (2020) 104401(1–9). [DOI: [10.1103/PhysRevMaterials.4.104401](https://doi.org/10.1103/PhysRevMaterials.4.104401)] & [UC-eScholarship]
359. C. J. Dahlman, N. R. Venkatesan, P. T. Corona, R. M. Kennard, L. Mao, N. C. Smith, J. Zhang, R. Seshadri, M. E. Helgeson, and M. L. Chabiniy, Structural evolution of layered hybrid lead iodide perovskites – Colloidal nanocrystals or Ruddlesden-Popper phases? *ACS Nano* **14** (2020) 11294–11308. [DOI: [10.1021/acsnano.0c03219](https://doi.org/10.1021/acsnano.0c03219)] & [UC-eScholarship]
358. Y. M. Eggeler, E. E. Levin, F. Wang, D. A. Kitchaev, A. Van der Ven, R. Seshadri, T. M. Pollock, and D. S. Gianola, Interfacial structure and strain accommodation in two-phase NbCo_{1.2}Sn Heusler intermetallics, *Phys. Rev. Mater.* **4** (2020) 093601(1–9). [DOI: [10.1103/PhysRevMaterials.4.093601](https://doi.org/10.1103/PhysRevMaterials.4.093601)] & [UC-eScholarship]
357. L. Mao, P. Guo, S. Wang, A. K. Cheetham, and R. Seshadri, Design principles for enhancing photoluminescence quantum yield in hybrid manganese bromides, *J. Am. Chem. Soc.* **142** (2020) 13582–13589. [DOI: [10.1021/jacs.0c06039](https://doi.org/10.1021/jacs.0c06039)] & [UC-eScholarship]
356. N. H. Bashian, M. B. Preefer, J. Milam-Guerrero, J. Zak, C. Sendi, S. Ahsan, R. Vincent, R. Haiges, K. A. See, R. Seshadri, and B. C. Melot, Understanding the role of crystallographic shear planes on the electrochemical behavior of niobium oxyfluorides, *J. Mater. Chem. A* **8** (2020) 12623–12632. [DOI: [10.1039/D0TA01406K](https://doi.org/10.1039/D0TA01406K)] & [UC-eScholarship]
355. D. H. Fabini, R. Seshadri, and M. G. Kanatzidis, The underappreciated lone pair in halide perovskites underpins their unusual properties. *MRS Bulletin* **45** (2020) 467–477. [DOI: [10.1557/mrs.2020.142](https://doi.org/10.1557/mrs.2020.142)] & [UC-eScholarship]

354. M. B. Preefer, M. Saber, Q. Wei, N. H. Bashian, J. D. Bocarsly, W. Zhang, G. Lee, J. Milam-Guerrero, E. S. Howard, R. C. Vincent, B. C. Melot, A. Van der Ven, R. Seshadri, and B. Dunn, Multielectron redox and insulator-to-metal transition upon lithium insertion in the fast-charging, Wadsley-Roth phase $\text{PNb}_9\text{O}_{25}$, *Chem. Mater.* **32** (2020) 4553–4563. [DOI: [10.1021/acs.chemmater.0c00560](https://doi.org/10.1021/acs.chemmater.0c00560)] & [UC-eScholarship]
353. E. C. Schueller, D. A. Kitchaev, J. L. Zuo, J. D. Bocarsly, J. A. Cooley, A. Van der Ven, S. D. Wilson, and R. Seshadri, Structural evolution and skyrmionic phase diagram of the lacunar spinel GaMo_4Se_8 , *Phys. Rev. Mater.* **4** (2020) 064402(1–9). [DOI: [10.1103/PhysRevMaterials.4.064402](https://doi.org/10.1103/PhysRevMaterials.4.064402)] & [UC-eScholarship]
352. Y. M. Oey, J. D. Bocarsly, D. Mann, E. E. Levin, M. Shatruk, and R. Seshadri, Structural changes upon magnetic ordering in magnetocaloric AlFe_2B_2 , *Appl. Phys. Lett.* **116** (2020) 212403(1–5) [DOI: [10.1063/5.0007266](https://doi.org/10.1063/5.0007266)] & [UC-eScholarship]
351. P. Vishnoi, J. L. Zuo, T. A. Strom, G. Wu, S. D. Wilson, R. Seshadri, and A. K. Cheetham, Hybrid ruthenium halide perovskites and related compounds, *Angew. Chem.* **59** (2020) 8974–8981. [DOI: [10.1002/anie.202003095](https://doi.org/10.1002/anie.202003095)] & [UC-eScholarship]
350. L. Mao, P. Guo, M. Kepenekian, I. Spanopoulos, Y. He, C. Katan, J. Even, R. D. Schaller, R. Seshadri, C. C. Stoumpos, and M. G. Kanatzidis, Organic cation alloying on intralayer A and interlayer A' Sites in 2D hybrid Dion–Jacobson lead bromide perovskites (A')(A) Pb_2Br_7 , *J. Am. Chem. Soc.* **142** (2020) 8342–8351. [DOI: [10.1021/jacs.0c01625](https://doi.org/10.1021/jacs.0c01625)] & [UC-eScholarship]
349. D. Sengupta, C. Sandoval-Pauker, E. Schueller, A. M. Encerrado-Manriquez, A. Metta-Magaña, W.-Y. Lee, R. Seshadri, B. Pinter, and S. Fortier, Isolation of a bimetallic cobalt(III) nitride and examination of its hydrogen atom abstraction chemistry and reactivity towards H_2 , *J. Am. Chem. Soc.* **142** (2020) 8233–8242. [DOI: [10.1021/jacs.0c00291](https://doi.org/10.1021/jacs.0c00291)] & [UC-eScholarship]
348. N. S. Schausser, D. J. Grzetic, T. Tabassum, G. A. Kliegle, M. L. Le, E. M. Susca, S. Antoine, T. J. Keller, K. T. Delaney, S. Han, R. Seshadri, G. H. Fredrickson, and R. A. Segalman, Impact of ion aggregation on conductivity in polymer electrolytes, *J. Am. Chem. Soc.* **142** (2020) 7055–7065. [DOI: [10.1021/jacs.0c00587](https://doi.org/10.1021/jacs.0c00587)] & [UC-eScholarship]
347. J. A. Cooley, J. D. Bocarsly, E. C. Schueller, E. E. Levin, E. E. Rodriguez, A. Huq, S. H. Lapidus, S. D. Wilson, and R. Seshadri, Evolution of non-collinear magnetism in magnetocaloric MnPtGa , *Phys. Rev. Mater.* **4** (2020) 044405(1–10). [DOI: [10.1103/PhysRevMaterials.4.044405](https://doi.org/10.1103/PhysRevMaterials.4.044405)] & [UC-eScholarship]
346. E. E. Levin, J. D. Bocarsly, J. H. Grebenkemper, R. Issa, S. D. Wilson, T. M. Pollock, and R. Seshadri, Structural coupling and magnetic tuning in $\text{Mn}_{2-x}\text{Co}_x\text{P}$ magnetocalorics for thermomagnetic power generation, *APL Mater.* **8** (2020) 041106. [DOI: [10.1063/1.5142000](https://doi.org/10.1063/1.5142000)] & [UC-eScholarship]
345. E. E. Morgan, S. M. L. Teicher, G. Wu, L. Mao, and R. Seshadri, Tunable perovskite-derived bismuth halides: $\text{Cs}_3\text{Bi}_2(\text{Cl}_{1-x}\text{I}_x)_9$, *Inorg. Chem.* **59** (2020) 3387–3393. [DOI: [10.1021/acs.inorgchem.9b03415](https://doi.org/10.1021/acs.inorgchem.9b03415)] & [UC-eScholarship]
344. Z. Deng, F. Wei, Y. Wu, R. Seshadri, A. K. Cheetham, and P. Canepa, Understanding structural and electronic properties of bismuth trihalides and related compounds, *Inorg. Chem.* **59** (2020) 3377–3386. [DOI: [10.1021/acs.inorgchem.9b03214](https://doi.org/10.1021/acs.inorgchem.9b03214)] & [UC-eScholarship]
343. H. A. Evans, Y. Wu, R. Seshadri, and A. K. Cheetham, Perovskite-related ReO_3 structures, *Nat. Rev. Mater.* **5** (2020) 196–213. [DOI: [10.1038/s41578-019-0160-x](https://doi.org/10.1038/s41578-019-0160-x)] & [UC-eScholarship]
342. L. Kautzsch, J. D. Bocarsly, C. Felser, S. D. Wilson, and R. Seshadri, Controlling Dzyaloshinskii–Moriya interactions in the skyrmion host candidates $\text{FePd}_{1-x}\text{Pt}_x\text{Mo}_3\text{N}$, *Phys. Rev. Mater.* **4** (2020) 024412(1–8). [DOI: [10.1103/PhysRevMaterials.4.024412](https://doi.org/10.1103/PhysRevMaterials.4.024412)] & [UC-eScholarship]
341. J. A. Cooley, M. K. Horton, E. E. Levin, S. H. Lapidus, K. A. Persson, R. Seshadri, From waste-heat recovery to refrigeration: Compositional tuning of magnetocaloric Mn_{1+x}Sb , *Chem. Mater.* **32** (2020) 1243–1249. [DOI: [10.1021/acs.chemmater.9b04643](https://doi.org/10.1021/acs.chemmater.9b04643)] & [UC-eScholarship]
340. C. A. C. Garcia, J. D. Bocarsly, and R. Seshadri, Computational screening of magnetocaloric alloys, *Phys. Rev. Mater.* **4** (2020) 024402(1–9). [DOI: [10.1103/PhysRevMaterials.4.024402](https://doi.org/10.1103/PhysRevMaterials.4.024402)] & [UC-eScholarship]

339. A. M. Zieschang, J. Bocarsly, J. Schuch, C. Reichel, B. Kaiser, W. Jaegermann, R. Seshadri, and B. Albert, Magnetic and electrocatalytic properties of nanoscale cobalt boride, Co_3B , *Inorg. Chem.* **58** (2019) 16609–16617. [DOI: [10.1021/acs.inorgchem.9b02617](https://doi.org/10.1021/acs.inorgchem.9b02617)] & [UC-eScholarship]
338. S. M. L. Teicher, I. K. Svenningsson, L. M. Schoop, and R. Seshadri, Weyl nodes and magnetostructural instability in antiperovskite Mn_3ZnC , *APL Materials*. **7** (2019) 121104(1–9). [DOI: [10.1063/1.5129689](https://doi.org/10.1063/1.5129689)] & [UC-eScholarship]
337. L. Mao, S. Teicher, C. Stoumpos, R. Kennard, R. DeCrescent, G. Wu, J. Schuller, M. L. Chabiny, A. K. Cheetham, and R. Seshadri, Chemical and structural diversity of hybrid layered double perovskite halides, *J. Am. Chem. Soc.* **141** (2019) 19099–19109. [DOI: [10.1021/jacs.9b09945](https://doi.org/10.1021/jacs.9b09945)] & [UC-eScholarship]
336. M. Preefer, J. Grebenkemper, F. Schroeder, J. Bocarsly, K. Pilar, J. Cooley, W. Zhang, J. Hu, S. Misra, F. Seeler, K. Schierle-Arndt, and R. Seshadri, Rapid and tunable assisted-microwave preparation of glass and glass-ceramic thiophosphate “ $\text{Li}_7\text{P}_3\text{S}_{11}$ ” Li-ion conductors, *ACS Appl. Mater. Interfaces* **11** (2019) 42280–42287. [DOI: [10.1021/acsami.9b15688](https://doi.org/10.1021/acsami.9b15688)] & [UC-eScholarship]
335. E. Decolvenaere, E. Levin, R. Seshadri, A. Van der Ven, Modeling magnetic evolution and exchange hardening in disordered magnets: The example of $\text{Mn}_{1-x}\text{Fe}_x\text{Ru}_2\text{Sn}$ Heusler alloys, *Phys. Rev. Mater.* **3** (2019) 104411(1–6). [DOI: [10.1103/PhysRevMaterials.3.104411](https://doi.org/10.1103/PhysRevMaterials.3.104411)] & [UC-eScholarship]
334. N. Venkatesan, A. Mahdi, B. Barraza, G. Wu, M. L. Chabiny, and R. Seshadri, Enhanced yield-mobility products in hybrid halide Ruddlesden-Popper compounds with aromatic ammonium spacers, *Dalton* **48** (2019) 14019–14026. [DOI: [10.1039/C9DT03074C](https://doi.org/10.1039/C9DT03074C)] & [UC-eScholarship]
333. E. E. Levin, J. H. Grebenkemper, T. M. Pollock, and R. Seshadri, Protocols for high temperature assisted-microwave preparation of inorganic compounds, *Chem. Mater.* **31** (2019) 7151–7159. [DOI: [10.1021/acs.chemmater.9b02594](https://doi.org/10.1021/acs.chemmater.9b02594)] & [UC-eScholarship]
332. G. Laurita, D. Puggioni, D. Hickox-Young, J. M. Rondinelli, M. W. Gaultois, K. Page, L. K. Lamontagne and R. 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** (2019) 095003(1–9). [DOI: [10.1103/PhysRevMaterials.3.095003](https://doi.org/10.1103/PhysRevMaterials.3.095003)] & [UC-eScholarship]
331. M. D. Radin, J. Vinkeviciute, R. Seshadri, and A. Van der Ven, Mn oxidation as the origin of the anomalous capacity of Mn-containing Li-excess cathode materials, *Nature Energy* **4** (2019) 639–646. [DOI: [10.1038/s41560-019-0439-6](https://doi.org/10.1038/s41560-019-0439-6)] & [UC-eScholarship]
330. E. C. Schueller, J. L. Zuo, J. D. Bocarsly, D. A. Kitchaev, S. D. Wilson, and R. Seshadri, Modeling the structural distortion and magnetic ground state of the polar lacunar spinel GaV_4Se_8 , *Phys. Rev. B* **100** (2019) 045131(1–5). [DOI: [10.1103/PhysRevB.100.045131](https://doi.org/10.1103/PhysRevB.100.045131)] & [UC-eScholarship]
329. N. Wagner, R. Seshadri, and J. M. Rondinelli, Property control from polyhedral connectivity in ABO_3 oxides, *Phys. Rev. B*. **100** (2019) 064101(1–12). [DOI: [10.1103/PhysRevB.100.064101](https://doi.org/10.1103/PhysRevB.100.064101)] & [UC-eScholarship]
328. R. Kennard, C. Dahlman, H. Nakayama, R. DeCrescent, J. Schuller, R. Seshadri, K. Mukherjee, and M. Chabiny, Phase stability and diffusion in lateral heterostructures of methylammonium lead halides, *ACS Appl. Mater. Interfaces* **11** (2019) 25313–25321. [DOI: [10.1021/acsami.9b06069](https://doi.org/10.1021/acsami.9b06069)] & [UC-eScholarship]
327. J. D. Bocarsly, E. E. Levin, S. A. Humphrey, T. Faske, W. Donner, S. D. Wilson, R. Seshadri, Magnetostructural coupling drives magnetocaloric behavior: The case of MnB versus FeB , *Chem. Mater.* **31** (2019) 4873–4881. [DOI: [10.1021/acs.chemmater.9b01476](https://doi.org/10.1021/acs.chemmater.9b01476)] & [UC-eScholarship]
326. S. M. L. Teicher, L. K. Lamontagne, L. M. Schoop, and R. Seshadri, Fermi-level Dirac crossings in $4d$ and $5d$ cubic metal oxides: NaPd_3O_4 and NaPt_3O_4 *Phys. Rev. B* **99** (2019) 195148(1–8). [DOI: [10.1103/PhysRevB.99.195148](https://doi.org/10.1103/PhysRevB.99.195148)] & [UC-eScholarship]
325. K. Pilar, Z. Deng, M. B. Preefer, J. A. Cooley, R. Clément, R. Seshadri, and A. K. Cheetham, *Ab initio* computation for solid-state ^{31}P NMR of inorganic phosphates: Revisiting X-ray structures, *Phys. Chem. Chem. Phys.* **21** (2019) 10070–10074. [DOI: [10.1039/c9cp01420a](https://doi.org/10.1039/c9cp01420a)] & [UC-eScholarship]
324. N. S. Schausser, R. Seshadri, and R. A. Segalman, Multivalent ion conduction in solid polymer systems, *Mol. Syst. Des. Eng.* **4** (2019) 263–279. [DOI: [10.1039/c8me00096d](https://doi.org/10.1039/c8me00096d)] & [UC-eScholarship]

323. D. H. Fabini, M. Koerner, and R. Seshadri, Candidate inorganic photovoltaic materials from electronic structure-based optical absorption and charge transport proxies, *Chem. Mater.* **31** (2019) 1561–1574. [DOI: [10.1021/acs.chemmater.8b04542](https://doi.org/10.1021/acs.chemmater.8b04542)] & [UC-eScholarship]
322. H. A. Evans, Z. Deng, I. E. Collings, Y. Wu, J. L. Andrews, K. Pilar, J. M. Tuffnell, G. Wu, J. Wang, S. E. Dutton, P. D. Bristowe, R. Seshadri, and A. K. Cheetham, Polymorphism in $M(\text{H}_2\text{PO}_2)_3$ ($M = \text{V}, \text{Al}, \text{Ga}$) compounds with the perovskite-related ReO_3 structure, *Chem. Comm.* **55** (2019) 2964–2967. [DOI: [10.1039/c9cc00118b](https://doi.org/10.1039/c9cc00118b)] & [UC-eScholarship]
321. H. A. Evans, J. L. Andrews, D. H. Fabini, M. B. Preefer, G. Wu, A. K. Cheetham, F. Wudl, and R. Seshadri, The capricious nature of iodine catenation in I_2 excess, perovskite-derived hybrid Pt(IV) compounds, *Chem. Comm.* **55** (2019) 588–591. [DOI: [10.1039/c8cc07536k](https://doi.org/10.1039/c8cc07536k)] & [UC-eScholarship]
320. J. D. Bocarsly, C. Heikes, C. M. Brown, S. D. Wilson, and R. Seshadri, Deciphering structural and magnetic disorder in the chiral skyrmion host materials $\text{Co}_x\text{Zn}_y\text{Mn}_z$ ($x + y + z = 20$), *Phys. Rev. Mater.* **3** (2019) 014402(1–16), Editor's Suggestion. [DOI: [10.1103/PhysRevMaterials.3.014402](https://doi.org/10.1103/PhysRevMaterials.3.014402)] & [UC-eScholarship]
319. M. M. Butala, V. V. T. Doan-Nguyen, A. Lehner, C. Göbel, M. A. Lumley, S. Arnon, K. Wiaderek, O. Borkiewicz, K. Chapman, P. Chupas, M. Balasubramanian, and R. Seshadri, Operando studies reveal structural evolution with electrochemical cycling in Li-CoS_2 , *J. Phys. Chem. C.* **122** (2018) 24559–24569. [DOI: [10.1021/acs.jpcc.8b07828](https://doi.org/10.1021/acs.jpcc.8b07828)] & [UC-eScholarship]
318. N. Schauer, G. Sanoja, J. Bartels, S. Jain, J. Hu, S. Han, L. Walker, M. Helgeson, R. Seshadri, and R. Segalman, Decoupling bulk mechanics and mono- and multivalent ion transport in polymers based on metal-ligand coordination, *Chem. Mater.* **30** (2018) 5759–5769. [DOI: [10.1021/acs.chemmater.8b02633](https://doi.org/10.1021/acs.chemmater.8b02633)] & [UC-eScholarship]
317. H. A. Evans, D. H. Fabini, J. L. Andrews, M. Koerner, M. B. Preefer, G. Wu, F. Wudl, A. K. Cheetham, and R. Seshadri, Hydrogen bonding controls the structural evolution in perovskite-related hybrid platinum (IV) iodides, *Inorg. Chem.* **57** (2018) 10375–10382. [DOI: [10.1021/acs.inorgchem.8b01597](https://doi.org/10.1021/acs.inorgchem.8b01597)] & [UC-eScholarship]
316. E. E. Levin, F. Long, J. E. Douglas, M. L. C. Buffon, L. K. Lamontagne, T. M. Pollock, and R. Seshadri, Enhancing thermoelectric properties through control of nickel interstitials and phase separation in Heusler/half-Heusler $\text{TiNi}_{1.1}\text{Sn}$ composites, *Materials* **11** (2018) 903(1–12). [DOI: [10.3390/ma11060903](https://doi.org/10.3390/ma11060903)] & [UC-eScholarship]
315. I. Spanopoulos, W. Ke, C. Stoumpos, E. C. Schueller, O. Kontsevoi, R. Seshadri, and M. Kanatzidis, Unraveling the chemical nature of the 3D “hollow” hybrid halide perovskites, *J. Am. Chem. Soc.* **140** (2018) 5728–5742. [DOI: [10.1021/jacs.8b01034](https://doi.org/10.1021/jacs.8b01034)] & [UC-eScholarship]
314. J. D. Bocarsly, R. F. Need, R. Seshadri, and S. D. Wilson, Magnetoentropic signatures of skyrmionic phase behavior in FeGe , *Phys. Rev. B.* **97** (2018) 100404(R). [DOI: [10.1103/PhysRevB.97.100404](https://doi.org/10.1103/PhysRevB.97.100404)] & [UC-eScholarship]
313. G. Sanoja, N. Schauer, J. Bartels, C. Evans, M. Helgeson, R. Seshadri, R. Segalman, Ion transport in dynamic polymer networks based on metal–ligand coordination: Effect of cross-linker concentration, *Macromolecules* **51** (2018) 2017–2026. [DOI: [10.1021/acs.macromol.7b02141](https://doi.org/10.1021/acs.macromol.7b02141)] & [UC-eScholarship]
312. A. M. Zieschang, J. Bocarsly, M. Duerrschabel, H.-J. Kleebe, R. Seshadri, and B. Albert, Low-temperature synthesis and magnetostructural transition in antiferromagnetic, refractory nanoparticles: Chromium nitride, CrN , *Chem. Mater.* **30** (2018) 1610–1616. [DOI: [10.1021/acs.chemmater.7b04815](https://doi.org/10.1021/acs.chemmater.7b04815)] & [UC-eScholarship]
311. J. Grebenkemper, J. Bocarsly, E. Levin, G. Seward, C. Heikes, C. Brown, S. Misra, F. Seeler, K. Schierle-Arndt, S. Wilson, and R. Seshadri, Rapid microwave preparation and composition tuning of the high-performance magnetocalorics $(\text{Mn}, \text{Fe})_2(\text{P}, \text{Si})$, *ACS Appl. Mater. Interfaces* **10** (2018) 7208–7213. [DOI: [10.1021/acsami.7b16988](https://doi.org/10.1021/acsami.7b16988)] & [UC-eScholarship]
310. C. Cozzan, G. Lheureux, N. O'Dea, E. Levin, J. Graser, T. Sparks, S. Nakamura, S. DenBaars, C. Weisbuch, and R. Seshadri, Stable, heat conducting phosphor composites for high-power laser lighting, *ACS Appl. Mater. Interfaces* **10** (2018) 5673–5681. [DOI: [10.1021/acsami.8b00074](https://doi.org/10.1021/acsami.8b00074)] & [UC-eScholarship]

309. G. C. B. Alexander, D. H. Fabini, R. Seshadri, and M. G. Kanatzidis, AuPb₂I₇: A narrow bandgap Au³⁺ iodide semiconductor, *Inorg. Chem.* **57** (2018) 804–810. [DOI: [10.1021/acs.inorgchem.7b02723](https://doi.org/10.1021/acs.inorgchem.7b02723)] & [UC-eScholarship]
308. 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](https://doi.org/10.1021/acs.inorgchem.7b02576)] & [UC-eScholarship]
307. E. E. Levin, J. D. Bocarsly, K. E. Wyckoff, T. M. Pollock, and R. Seshadri, Tuning the magnetocaloric response in half-Heusler/Heusler MnNi_{1+x}Sb solid solutions, *Phys. Rev. Mater.* **1** (2017) 075003(1–8). [DOI: [10.1103/PhysRevMaterials.1.075003](https://doi.org/10.1103/PhysRevMaterials.1.075003)] & [UC-eScholarship]
306. 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](https://doi.org/10.1021/jacs.7b09536)] & [UC-eScholarship]
305. S. Soe, C. Stoumpos, M. Kepenekian, B. Traoré, H. Tsai, W. Nie, B. Wang, C. Katan, R. Seshadri, A. Mohite, J. Even, T. Marks, and M. Kanatzidis, New type of 2D perovskites with alternating cations in the interlayer space, (C(NH₂)₃)(CH₃NH₃)_nPb_nI_{3n+1}: Structure, properties and photovoltaic performance. *J. Am. Chem. Soc.* **39** (2017) 16297–16309. [DOI: [10.1021/jacs.7b09096](https://doi.org/10.1021/jacs.7b09096)] & [UC-eScholarship]
304. M. B. Preefer, B. Oschmann, C. J. Hawker, R. Seshadri, and F. Wudl, High sulfur content material with stable cycling in lithium–sulfur batteries, *Angew. Chemie.* **56** (2017) 15118–15122. [DOI: [10.1002/anie.201708746](https://doi.org/10.1002/anie.201708746)] & [UC-eScholarship]
303. H. A. Evans, E. C. Schueller, S. R. Smock, G. Wu, R. Seshadri, and F. Wudl, Perovskite-related hybrid noble metal iodides: Formamidinium platinum iodide [(FA)₂Pt^{IV}I₆] and mixed-valence methylammonium gold iodide [(MA)₂Au^IAu^{III}I₆], *Inorg. Chim. Acta* **68** (2017) 280–284. [DOI: [10.1016/j.ica.2017.04.060](https://doi.org/10.1016/j.ica.2017.04.060)] & [UC-eScholarship] & [Corrigendum, DOI: [10.1016/j.ica.2018.06.036](https://doi.org/10.1016/j.ica.2018.06.036)]
302. M. Butala, M. Perez, C. Göbel, M. Preefer, S. Arnon, and R. Seshadri, Rapid microwave-assisted preparation of binary and ternary transition metal sulfide compounds, *Solid State Sci.* **74** (2017) 8–12. [DOI: [10.1016/j.solidstatesciences.2017.09.010](https://doi.org/10.1016/j.solidstatesciences.2017.09.010)] & [UC-eScholarship]
301. E. Decolvenaere, M. Gordon, R. Seshadri, and A. Van der Ven, First-principles investigation of competing magnetic interactions in (Mn,Fe)Ru₂Sn Heusler solid solutions, *Phys. Rev. B.* **96** (2017) 165109(1–12). [DOI: [10.1103/PhysRevB.96.165109](https://doi.org/10.1103/PhysRevB.96.165109)] & [UC-eScholarship]
300. C. Cozzan, G. Laurita, M. W. Gaultois, M. Cohen, A. A. Mikhailovsky, M. Balasubramanian, and R. Seshadri, Understanding the links between composition, polyhedral distortion, and luminescence properties in green-emitting β-Si_{6–z}Al_zO_zN_{8–z}:Eu²⁺ phosphor, *J. Mater. Chem. C* **5** (2017) 10039–10046. [DOI: [10.1039/C7TC03039H](https://doi.org/10.1039/C7TC03039H)] & [UC-eScholarship]
299. M. Buffon, G. Laurita, L. Lamontagne, E. Levin, S. Mooraj, D. Lloyd, N. White, T. Pollock, and R. Seshadri, Thermoelectric performance and the role of anti-site disorder in the 24-electron Heusler TiFe₂Sn, *J. Phys. Condensed Matter* **29** (2017) 405702(1–7). [DOI: [10.1088/1361-648X/aa81e7](https://doi.org/10.1088/1361-648X/aa81e7)] & [UC-eScholarship]
298. G. Laurita, D. H. Fabini, 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](https://doi.org/10.1039/C7SC01429E)] & [UC-eScholarship]
297. 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 Ce³⁺-doped Gd₃Sc₂Al₃O₁₂, *J. Lumin.* **190** (2017) 62–68. [DOI: [10.1016/j.jlumin.2017.05.035](https://doi.org/10.1016/j.jlumin.2017.05.035)] & [UC-eScholarship]
296. L. Lamontagne, M. Knight, G. Laurita, H. Yusuf, J. Hu, R. Seshadri, and K. Page, The role of structural and compositional heterogeneities in the insulator-to-metal transition in hole-doped APd₃O₄ (A = Ca, Sr), *Inorg. Chem.* **56** (2017) 5158–5164. [DOI: [10.1021/acs.inorgchem.7b00307](https://doi.org/10.1021/acs.inorgchem.7b00307)] & [UC-eScholarship]
295. N. George, J. Brgoch, A. Pell, C. Cozzan, A. Jaffe, G. Dantelle, A. Llobet, G. Pintacuda, R. Seshadri, and B. Chmelka, Correlating local compositions and structures with the macroscopic optical properties of Ce³⁺-doped CaSc₂O₄, an efficient green-emitting phosphor, *Chem. Mater.* **29** (2017) 3538–3546. [DOI: [10.1021/acs.chemmater.6b0539](https://doi.org/10.1021/acs.chemmater.6b0539)] & [UC-eScholarship]

294. M. M. Butala, M. Mayo, V. V. T. 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. J. Morris, C. P. Grey, and R. Seshadri, Local structure evolution and modes of charge storage in secondary Li-FeS₂ cells, *Chem. Mater.* **29** (2017) 3070–3082. [DOI: [10.1021/acs.chemmater.7b00070](https://doi.org/10.1021/acs.chemmater.7b00070)] & [UC-eScholarship]
293. J. D. Bocarsly, E. E. Levin, C. A. C. Garcia, K. Schwennicke, S. D. Wilson, and R. Seshadri, A simple computational proxy for screening magnetocaloric compounds, *Chem. Mater.* **29** (2017) 1613–1622. [DOI: [10.1021/acs.chemmater.6b04729](https://doi.org/10.1021/acs.chemmater.6b04729)] & [UC-eScholarship]
292. C. Cozzan, K. J. Griffith, G. Laurita, J. G. Hu, C. P. Grey, and R. Seshadri, Structural evolution and atom clustering in β -SiAlON: β -Si_{6-z}Al_zO_zN_{8-z}, *Inorg. Chem.* **56** (2017) pp 2153–2158. [DOI: [10.1021/acs.inorgchem.6b02780](https://doi.org/10.1021/acs.inorgchem.6b02780)] & [UC-eScholarship]
291. A.-M. Zieschang, J. Bocarsly, M. Duerrschabel, L. Molina-Luna, H.-J. Kleebe, R. Seshadri, and B. Albert, Nanoscale iron nitride, ϵ -Fe₃N: Preparation from liquid ammonia and magnetic properties, *Chem. Mater.* **29** (2017) 621–628. [DOI: [10.1021/acs.chemmater.6b04088](https://doi.org/10.1021/acs.chemmater.6b04088)] & [UC-eScholarship]
290. H. A. Evans, J. Labram, S. R. Smock, G. Wu, M. L. Chabiny, R. Seshadri, and F. Wudl, Mono and mixed-valence tetrathiafulvalene semiconductors (TTF)BiI₄ and (TTF)₄BiI₆ with 1D and 0D bismuth-iodide networks, *Inorg. Chem.* **56** (2017) 395–401. [DOI: [10.1021/acs.inorgchem.6b02287](https://doi.org/10.1021/acs.inorgchem.6b02287)] & [UC-eScholarship]
289. D. H. Fabini, J. Labram, A. J. Lehner, J. Bechtel, H. Evans, A. Van der Ven, F. Wudl, M. Chabiny, and R. Seshadri, Main-group halide semiconductors derived from perovskite: Distinguishing chemical, structural, and electronic aspects, *Inorg. Chem. (Forum)* **56** (2017) 11–25. [DOI: [10.1021/acs.inorgchem.6b01539](https://doi.org/10.1021/acs.inorgchem.6b01539)] & [UC-eScholarship]
288. K. A. See, M. Lumley, G. D. Stucky, C. P. Grey, and R. Seshadri, Reversible capacity of conductive carbon additives at low potentials: Caveats for testing alternative anode materials for Li-ion batteries, *J. Electrochem. Soc.* **164** (2017) A327–A333. [DOI: [10.1149/2.0971702jes](https://doi.org/10.1149/2.0971702jes)] & [UC-eScholarship]
287. D. H. Fabini, C. C. Stoumpos, G. Laurita, A. Kaltzoglou, A. G. Kontos, P. Falaras, M. G. Kanatzidis, and R. Seshadri, Reentrant structural and optical properties and large positive thermal expansion in perovskite formamidinium lead iodide, *Angew. Chem.* **55** (2016) 15392–15396. [DOI: [10.1002/anie.201609538](https://doi.org/10.1002/anie.201609538)] & [UC-eScholarship]
286. V. Doan-Nguyen, K. Subrahmanyam, M. Butala, J. Gerbec, S. Islam, K. Kanipe, C. Wilson, M. Balasubramanian, K. Wiaderek, O. Borkiewicz, K. Chapman, P. Chupas, M. Moskovits, B. Dunn, M. Kanatzidis, and R. Seshadri, Molybdenum polysulfide chalcogels as high-capacity, anion-redox-driven electrode materials for Li-ion batteries, *Chem. Mater.* **28** (2016) 8357–8365. [DOI: [10.1021/acs.chemmater.6b03656](https://doi.org/10.1021/acs.chemmater.6b03656)] & [UC-eScholarship]
285. C. Cozzan, M. Brady, N. O'Dea, E. Levin, S. Nakamura, S. DenBaars, and R. Seshadri, Monolithic translucent BaMgAl₁₀O₁₇:Eu²⁺ phosphors for laser-driven solid state lighting, *AIP Advances* **6** (2016) 105005(1–6). [DOI: [10.1063/1.4964925](https://doi.org/10.1063/1.4964925)] & [UC-eScholarship]
284. J. E. Douglas, E. E. Levin, T. M. Pollock, J. C. Castillo, P. Adler, C. Felser, S. Krämer, K. L. Page, and R. Seshadri, Magnetic hardening and antiferromagnetic/ferromagnetic phase coexistence in Mn_{1-x}Fe_xRu₂Sn Heusler solid solutions, *Phys. Rev. B* **94** (2016) 094412(1–9). [doi] & [UC-eScholarship]
283. D. Fabini, G. Laurita, J. Bechtel, C. Stoumpos, H. Evans, A. Kontos, Y. Raptis, P. Falaras, A. Van der Ven, M. Kanatzidis, and R. Seshadri, Dynamic stereochemical activity of the Sn²⁺ lone pair in perovskite CsSnBr₃, *J. Am. Chem. Soc.* **138** (2016) 11820–11832. [doi] & [UC-eScholarship]
282. M. L. C. Buffon, G. Laurita, N. Verma, L. Lamontagne, L. Ghadbeigi, D. L. Lloyd, T. D. Sparks, 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(1–8). [doi] & [UC-eScholarship]
281. S. Madhu, H. A. Evans, V. Doan-Nguyen, J. Labram, G. Wu, M. L. Chabiny, R. Seshadri, and F. Wudl, Infinite polyiodide chains in the pyrroloperylene–iodine complex: Insights into the starch-iodine and perylene-iodine complexes, *Angew. Chem. Int. Ed.* **55** (2016) 8032–8035. [doi] & [UC-eScholarship]

280. N. Verma, J. Douglas, S. Krämer, T. M. Pollock, R. Seshadri, and C. G. Levi, Microstructure evolution of biphasic $\text{TiNi}_{1+x}\text{Sn}$ thermoelectric materials, *Metal. Mater. Trans. A* **47** (2016) 4116–4127. [doi] & [UC-eScholarship]
279. J. S. Bechtel, R. Seshadri, and A. Van der Ven, Energy landscape of molecular motion in cubic methylammonium lead iodide from first principles, *J. Phys. Chem. C* **120** (2016) 12403–12410. [doi] & [UC-eScholarship]
278. H. Evans, A. Lehner, J. Labram, D. Fabini, O. Barreda, S. Smock, G. Wu, M. Chabiny, R. Seshadri, and F. Wudl, $(\text{TTF})\text{Pb}_2\text{I}_5$: A radical cation-stabilized hybrid lead iodide with synergistic optoelectronic signatures. *Chem. Mater.* **28** (2016) 3607–3611. [doi] & [UC-eScholarship]
277. L. K. Lamontagne, G. Laurita, M. W. Gaultois, M. Knight, L. Ghadbeigi, T. D. Sparks, M. E. Gruner, R. Pentcheva, C. M. Brown, and R. Seshadri, High thermopower with metallic conductivity in *p*-type Li-substituted PbPdO_2 , *Chem. Mater.* **28** (2016) 3367–3373. [doi] & [UC-eScholarship]
276. J. Hill, G. Mulholland, K. Persson, R. Seshadri, C. Wolverton, and B. Meredig, Unlocking new opportunities in materials science with large-scale data and informatics, *MRS Bulletin* **41** (2016) 399–409. [doi]
275. R. Seshadri and T. D. Sparks, Interactive materials properties databases through aggregation of literature data, *APL Materials* **4** (2016) 053206(1–8). [doi] & [UC-eScholarship]
274. 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 mesostructuring. *ACS Appl. Mater. Interfaces*, **8** (2016) 6496–6503. [doi] & [UC-eScholarship]
273. J. K. Harada, L. Balhorn, J. Hazi, M. C. Kemei, and R. Seshadri, Magnetodielectric coupling in the ilmenites MTiO_3 ($M = \text{Co}, \text{Ni}$), *Phys. Rev. B* **93** (2016) 104404(1–6). [doi] & [UC-eScholarship]
272. D. Fabini, T. Hogan, H. Evans, C. Stoumpos, M. Kanatzidis, and R. Seshadri, Dielectric and thermodynamic signatures of low temperature glassy dynamics in the hybrid perovskites $\text{CH}_3\text{NH}_3\text{PbI}_3$ and $\text{HC}(\text{NH}_2)_2\text{PbI}_3$, *J. Phys. Chem. Lett.* **7** (2016) 376–381. [doi] & [UC-eScholarship]
271. G. Laurita, K. Page, S. Suzuki, and R. Seshadri, Average and local structure of the Pb-free ferroelectric perovskites $(\text{Sr},\text{Sn})\text{TiO}_3$ and $(\text{Ba},\text{Ca},\text{Sn})\text{TiO}_3$, *Phys. Rev. B* **92** (2015) 214109(1–9). [doi] & [UC-eScholarship]
270. K. Hofmann, N. Kalyon, C. Kapfenberger, L. Lamontagne, S. Zarrini, R. Berger, R. Seshadri, and B. Albert, Metastable Ni_7B_3 – a new paramagnetic boride from solution chemistry, and its crystal structure, *Inorg. Chem.* **54** (2015) 10873–10877. [doi] & [UC-eScholarship]
269. A. P. Black, K. A. Denault, C. Frontera, R. Seshadri, A. R. Goñi, and A. Fuertes, Emission colour tuning through coupled N/La introduction in $\text{Sr}_2\text{SiO}_4\text{:Eu}^{2+}$, *J. Mater. Chem. C* **3** (2015) 11471–11477. [doi] & [UC-eScholarship]
268. A. J. Lehner, D. H. Fabini, H. A. Evans, C.-A. Hébert, S. R. Smock, J. Hu, H. Wang, J. W. Zwanziger, M. L. Chabiny, and R. Seshadri, Crystal and electronic structures of complex bismuth iodides $\text{A}_3\text{Bi}_2\text{I}_9$ ($A = \text{K}, \text{Rb}, \text{Cs}$) related to perovskite: Aiding the rational design of photovoltaics, *Chem. Mater.* **27** (2015) 7137–7148. [doi] & [UC-eScholarship]
267. J. E. Douglas, M. P. Echlin, W. C. Lenthe, R. Seshadri, and T. M. Pollock, Three-dimensional multimodal imaging and analysis of biphasic microstructure in a Ti–Ni–Sn thermoelectric material, *APL Mater.* **3** (2015) 096107(1–8). [doi] & [UC-eScholarship]
266. A. J. Lehner, H. Wang, D. Fabini, C. D. Liman, C.-A. Hébert, E. E. Perry, M. Wang, G. C. Bazan, M. L. Chabiny, and R. Seshadri, Electronic structure and photovoltaic application of BiI_3 , *Appl. Phys. Lett.* **107** (2015) 131109(1–4). [doi] & [UC-eScholarship]
265. M. W. Gaultois, J. E. Douglas, T. E. Sparks, and R. Seshadri, Single-step preparation and consolidation of reduced early-transition-metal oxide/metal *n*-type thermoelectric composites, *AIP Advances* **5** (2015) 097144(1–8). [doi] & [UC-eScholarship]

264. J. G. Labram, D. H. Fabini, E. E. Perry, A. J. Lehner, H. Wang, A. M. Glaudell, G. Wu, H. Evans, D. Buck, R. Cotta, L. Echegoyen, F. Wudl, R. Seshadri, and M. L. Chabiny, Temperature-dependent polarization in field-effect transport and photovoltaic measurements of methylammonium lead iodide, *J. Phys. Chem. Lett.* **6** (2015) 3565–3571. [doi] & [UC-eScholarship]
263. A. Birkel, N. A. DeCino, C. Cozzan, A. A. Mikhailovsky, B.-C. Hong, and R. Seshadri, A single-phase full-color phosphor based on $\text{Ba}_3\text{MgSi}_2\text{O}_8$ co-activated with Eu^{2+} , Tb^{3+} , and Mn^{2+} , *Solid State Sci.* **48** (2015) 82–89. [doi] & [UC-eScholarship]
262. S. Britto, M. Leskes, X. Hua, C.-A. Hébert, H. S. Shin, S. Clarke, O. Borkiewicz, K. Chapman, R. Seshadri, J. Cho, and C. Grey, Multiple redox modes in the reversible lithiation of high-capacity, Peierls-distorted vanadium sulfide, *J. Am. Chem. Soc.* **137** (2015) 8499–8508. [doi] & [UC-eScholarship]
261. K. See, S. Hug, K. Schwinghammer, M. Lumley, Y. Zheng, J. Nolt, G. Stucky, F. Wudl, B. Lotsch, and R. Seshadri, Lithium charge storage mechanisms of cross-linked triazine networks and their porous carbon derivatives, *Chem. Mater.* **27** (2015) 3821–3829. [doi] & [UC-eScholarship]
260. A. Knappschneider, C. Litterscheid, J. Brgoch, N. C. George, S. Henke, J. G. Hu, A. K. Cheetham, R. Seshadri, and B. Albert, Manganese tetraboride, MnB_4 : high-temperature crystal structure, $p - n$ transition, ^{55}Mn NMR, solid solutions and mechanical properties, *Chem. Eur. J.* **21** (2015) 8177–8181. [doi]
259. K. A. Denault, J. R. Brgoch, S. Klotz, M. W. Gaultois, J. Siewenie, K. Page, and R. Seshadri, Average and local structure, Debye temperature, and structural rigidity in some oxide phosphor host compounds, *ACS Appl. Mater. Interfaces* **13** (2015) 7264–7272. [doi] & [UC-eScholarship]
258. M. Gaultois, M. C. Kemei, J. K. Harada, and R. Seshadri, Rapid preparation and magnetodielectric properties of trirutile Cr_2WO_6 , *J. Appl. Phys.* **117** (2015) 014105(1–5). [doi]
257. J. Brgoch, K. Hasz, K. A. Denault, C. K. H. Borg, A. A. Mikhailovsky, and R. Seshadri, Data-driven discovery of energy materials: Efficient $\text{BaM}_2\text{Si}_3\text{O}_{10}:\text{Eu}^{2+}$ ($M = \text{Sc}, \text{Lu}$) phosphors for application in solid state white lighting, *Faraday Discussions* **176** (2014) 333–347. [doi]
256. J. Brgoch, A. Lehner, M. Chabiny, and R. Seshadri, Ab initio calculations of band gaps and absolute band positions of polymorphs of RbPbI_3 and CsPbI_3 : Implications for main-group halide perovskite photovoltaics, *J. Phys. Chem. C* **118** (2014) 27721–27727. [doi]
255. K. A. See, M. Leskes, J. Griffin, S. Britto, P. Matthews, A. Emly, A. Van der Ven, D. Wright, A. Morris, C. P. Grey, and R. Seshadri, Ab initio structure search and in situ ^7Li NMR studies of discharge products in the Li-S battery system, *J. Am. Chem. Soc.* **136** (2014) 16368–16377. [doi]
254. J. Brgoch, M. W. Gaultois, M. Balasubramanian, K. Page, B.-C. Hong, and R. Seshadri, Local structure and structural rigidity of the green phosphor $\beta\text{-SiAlON}:\text{Eu}^{2+}$, *Appl. Phys. Lett.* **105** (2014) 181904(1–4). [doi]
253. J. E. Douglas, P. A. Chater, C. M. Brown, T. M. Pollock, and R. Seshadri, Nanoscale structural heterogeneity in Ni-rich half-Heusler TiNiSn , *J. Appl. Phys.* **116** (2014) 163514(1–7). [doi]
252. C. Lermer, M. M. Butala, B. R. Lettiere, and R. Seshadri, Mesoporous materials from template-free vapor-phase reductive leaching of Zn from $\text{Zn}-M-\text{O}$ compounds ($M = \text{Nb}, \text{Mo}, \text{W}$), *Cryst. Growth Des.* **14** (2014) 4526–4530. [doi]
251. M. C. Kemei, J. Harada, R. Seshadri, and M. R. Suchomel, Structural change and phase coexistence upon magnetic ordering in the magnetodielectric spinel Mn_3O_4 , *Phys. Rev. B* **90** (2014) 064418(1–8). [doi]
250. P. T. Barton, M. C. Kemei, M. W. Gaultois, S. L. Moffitt, L. E. Darago, R. Seshadri, M. R. Suchomel, and B. C. Melot, Structural distortion below the Néel temperature in spinel GeCo_2O_4 , *Phys. Rev. B* **90** (2014) 064105(1–7). [doi]
249. G. Kieslich, U. Burkhardt, C. S. Birkel, I. Veremchuk, J. E. Douglas, M. W. Gaultois, I. Lieberwirth, R. Seshadri, G. D. Stucky, Y. Grin, and W. Tremel, Enhanced thermoelectric properties of the n -type Magnéli phase $\text{WO}_{2.90}$: reduced thermal conductivity through microstructure engineering, *J. Mater. Chem. A* **2** (2014) 13492–13497. [doi]

248. K. See, Y.-S. Jun, J. Gerbec, J. Sprafke, F. Wudl, G. Stucky, and R. Seshadri, Sulfur-functionalized mesoporous carbons as sulfur hosts in Li–S batteries: Increasing the affinity of sulfur intermediates to enhance performance, *ACS Appl. Mater. Interfaces* **6** (2014) 10908–10916. [doi]
247. Y. Zheng, M. Miao, M. C. Kemei, R. Seshadri, and F. Wudl, The pyreno-triazinyl radical – magnetic and sensor properties, *Israel J. Chem.* **54** (2014) 774–778. [doi]
246. J. Brgoch, S. D. Kloss, K. A. Denault, and R. Seshadri, Accessing $(\text{Ba}_{1-x}\text{Sr}_x)\text{Al}_2\text{Si}_2\text{O}_8\text{:Eu}^{2+}$ phosphors for solid state white lighting via microwave assisted preparation: Tuning emission color through coordination environment, *Z. Anorg. Allg. Chem. (C. N. R. Rao Festschrift)* **640** (2014) 1182–1189. [doi]
245. M. C. Kemei, S. L. Moffitt, L. E. Darago, R. Seshadri, M. R. Suchomel, D. P. Shoemaker, K. Page, and J. Siewenie, Structural ground states of $(A, A')\text{Cr}_2\text{O}_4$ ($A = \text{Mg, Zn}$; $A' = \text{Co, Cu}$) spinel solid solutions: Spin-Jahn-Teller and Jahn-Teller effects, *Phys. Rev. B* **89** (2014) 174410(1–15). [doi]
244. J. R. Neilson, N. C. George, M. M. Murr, R. Seshadri, and D. E. Morse, Mesostructure from hydration gradients in demop sponge biosilica, *Chem. Eur. J.* **20** (2014) 4956–4965. [doi]
243. K. A. Denault, J. Brgoch, M. Gaultois, A. Mikhailovsky, R. Petry, H. Winkler, S. DenBaars, and R. Seshadri, Consequences of optimal bond valence on structural rigidity and improved luminescence properties in $\text{Sr}_x\text{Ba}_{2-x}\text{SiO}_4\text{:Eu}^{2+}$ orthosilicate phosphors, *Chem. Mater.* **26** (2014) 2275–2282. [doi]
242. A. Krishnapriyan, P. T. Barton, M. Miao, and R. Seshadri, First-principles study of band alignments in the p -type hosts BaM_2X_2 ($M = \text{Cu, Ag}$; $X = \text{S, Se}$), *J. Phys. Condens. Matter* **26** (2014) 155802(1–6). [doi]
241. L. Misch, J. R. Brgoch, A. Birkel, T. Mates, G. D. Stucky, and R. Seshadri, Rapid microwave preparation, and *ab-initio* studies of the stable complex noble metal oxides $\text{La}_2\text{BaPdO}_5$ and $\text{La}_2\text{BaPtO}_5$, *Inorg. Chem.* **53** (2014) 2628–2634. [doi]
240. S. Rades, S. Krämer, R. Seshadri, and B. Albert, Size and crystallinity dependence of magnetism in nanoscale iron boride, α -FeB, *Chem. Mater.* **26** (2014) 1549–1552. [doi]
239. A. Knappschneider, C. Litterscheid, N. C. George, J. Brgoch, N. Wagner, J. Beck, J. A. Kurzman, R. Seshadri, and B. Albert, Peierls-distorted monoclinic MnB_4 with a Mn–Mn bond, *Angew. Chem. Int. Ed.* **53** (2014) 1684–1688. [doi]
238. J. E. Douglas, C. S. Birkel, N. Verma, V. M. Miller, M.-S. Miao, G. D. Stucky, T. M. Pollock, and R. Seshadri, Phase stability and property evolution of biphasic Ti–Ni–Sn alloys for use in thermoelectric applications, *J. Appl. Phys.* **115** (2014) 043720(1–11). [doi]
237. M.-S. Miao, S. Yarbrough, P. T. Barton, and R. Seshadri, Electron affinities and ionization energies of Cu and Ag delafossite compounds: A hybrid functional study, *Phys. Rev. B.* **89** (2014) 045306(1–8). [doi]
236. T. D. Sparks, M. C. Kemei, P. T. Barton, R. Seshadri, E.-D. Mun, and V. Zapf, Magnetocapacitance as a sensitive probe of magnetostructural changes in NiCr_2O_4 , *Phys. Rev. B.* **89** (2014) 024405(1–6). [doi]
235. L. M. Misch, A. Birkel, C. A. Figg, B. P. Fors, C. J. Hawker, G. D. Stucky, and R. Seshadri, Rapid microwave-assisted sol-gel preparation of Pd-substituted LnFeO_3 ($\text{Ln} = \text{Y, La}$): Phase formation and catalytic activity, *Dalton Trans.* **43** (2014) 2079–2087. [doi]
234. N. C. George, A. Birkel, J. Brgoch, B.-C. Hong, A. Mikhailovsky, K. Page, A. Llobet, and R. Seshadri, Average and local structural origins of the optical properties of the nitride phosphor $\text{La}_{3-x}\text{Ce}_x\text{Si}_6\text{N}_{11}$ ($0 < x \leq 3$), *Inorg. Chem.* **52** (2013) 13730–13741. [doi]
233. J. Brgoch, C. K. H. Borg, K. A. Denault, J. R. Douglas, T. A. Strom, S. P. DenBaars, and R. Seshadri, Rapid microwave preparation of cerium-substituted sodium yttrium silicate phosphors for solid state white lighting, *Solid State Sci.* **26C** (2013) 115–120. [doi]
232. K. A. Denault, Z. Cheng, J. Brgoch, S. P. DenBaars, and R. Seshadri, Structure–composition relationships and optical properties in cerium-substituted $(\text{Sr,Ba})_3(\text{Y,Lu})(\text{BO}_3)_3$ borate phosphors, *J. Mater. Chem. C* **1** (2013) 7339–7345. [doi]

-
231. N. George, A. Pell, G. Dantelle, K. Page, A. Llobet, M. Balasubramanian, G. Pintacuda, B. Chmelka, and R. Seshadri, Local environments of dilute activator ions in the solid-state lighting phosphor $\text{Y}_{3-x}\text{Ce}_x\text{Al}_5\text{O}_{12}$, *Chem. Mater.* **25** (2013) 3979–3995. [doi]
230. C. S. Birkel, J. E. Douglas, B. R. Lettiere, G. Seward, Y. Zhang, T. M. Pollock, R. Seshadri, and G. D. Stucky, Influence of Ni nanoparticle addition and spark plasma sintering on the TiNiSn –Ni system: Structure, microstructure, and thermoelectric properties, *Solid State Sci.* **26** (2013) 16–22. [doi]
229. G. Kieslich, C. S. Birkel, J. E. Douglas, M. Gaultois, R. Seshadri, Y. Grin, G. D. Stucky, and W. Tremel, SPS-assisted preparation of the Magnéli phase $\text{WO}_{2.90}$ for thermoelectric applications, *J. Mater. Chem. A* **1** (2013) 13050–13054. [doi]
228. P. T. Barton, Y. D. Premchand, P. A. Chater, R. Seshadri, and M. J. Rosseinsky, Chemical inhomogeneity, short-range order, and magnetism in the LiNiO_2 – NiO solid solution, *Chem. Eur. J.* **43** (2013) 14521–14531. [doi]
227. J. A. Kurzman, L. M. Misch, and R. Seshadri, Chemistry of precious metal oxides relevant to heterogeneous catalysis, *Dalton Trans.* **42** (2013) 14653–14667. [doi]
226. J. Brgoch, S. P. DenBaars, and R. Seshadri, Proxies from *Ab-initio* calculations for screening efficient Ce^{3+} phosphor hosts, *J. Phys. Chem. C* **117** (2013) 17955–17959. [doi]
225. S. A. Corr and R. Seshadri, Synthetic Methodologies, Comprehensive Inorganic Chemistry II (Second Edition). From Elements to Applications. Volume 4: Solid-State Materials, Including Ceramics and Minerals (2013) 1–15. [doi]
224. K. A. See, J. A. Gerbec, Y.-S. Jun, F. Wudl, G. D. Stucky, and R. Seshadri, A high capacity calcium primary cell based on the Ca–S system, *Adv. Ener. Mater.* **3** (2013) 1056–1061. [doi]
223. M. W. Gaultois, T. D. Sparks, C. K. H. Borg, R. Seshadri, W. D. Bonificio, and D. R. Clarke, A data-driven review of thermoelectric materials: Performance and resource considerations, *Chem. Mater.* **25** (2013) 2911–2920. [doi]
222. M.-S. Miao, J. Brgoch, A. Krishnapriyan, A. Goldman, J. A. Kurzman, and R. Seshadri, On the stereochemical inertness of the auride lone-pair: *Ab-initio* studies of AAu ($A = \text{K}, \text{Rb}, \text{Cs}$), *Inorg. Chem.* **52** (2013) 8183–8189. [doi]
221. J. Brgoch, C. K. H. Borg, K. A. Denault, A. A. Mikhailovsky, S. P. DenBaars, and R. Seshadri, An efficient, thermally stable cerium-based silicate phosphor for solid state white lighting, *Inorg. Chem.* **52** (2013) 8010–8016. [doi]
220. M. C. Kemei, P. T. Barton, S. L. Moffitt, M. W. Gaultois, J. A. Kurzman, R. Seshadri, M. R. Suchomel, and Y.-I. Kim, Crystal structures of spin-Jahn-Teller-ordered MgCr_2O_4 and ZnCr_2O_4 , *J. Phys.: Condens. Matter* **25** (2013) 326001(1–7). [doi]
219. K. A. Denault, M. Cantore, S. Nakamura, S. P. DenBaars, and R. Seshadri, Efficient and stable laser-driven white lighting, *AIP Advances* **3** (2013) 072107(1–6). [doi] [Physics Today] [Laser Focus World]
218. P. T. Barton, R. Seshadri, A. Llobet, and M. R. Suchomel, Magnetostructural transition, metamagnetism, and magnetic phase coexistence in $\text{Co}_{10}\text{Ge}_3\text{O}_{16}$, *Phys. Rev. B* **88** (2013) 024403(1–7). [doi]
217. N. C. George, K. A. Denault, and R. Seshadri, Phosphors for solid-state white lighting, *Annu. Rev. Mater. Res.* **43** (2013) 481–501. [doi]
216. C. S. Birkel, J. E. Douglas, B. R. Lettiere, G. Seward, N. Verma, Y. Zhang, T. M. Pollock, R. Seshadri, and G. D. Stucky, Improving the thermoelectric properties of half-Heusler TiNiSn through inclusion of a second full-Heusler phase: Microwave preparation and spark plasma sintering of $\text{TiNi}_{1+x}\text{Sn}$, *Phys. Chem. Chem. Phys.* **15** (2013) 6990–6997. [doi]
215. M. W. Gaultois, P. T. Barton, C. S. Birkel, L. M. Misch, E. E. Rodriguez, G. D. Stucky, and R. Seshadri, Structural disorder, magnetism, and electrical and thermoelectric properties of pyrochlore $\text{Nd}_2\text{Ru}_2\text{O}_7$, *J. Phys.: Condens. Matter* **25** (2013) 186004(1–10). [doi]

214. A. Birkel, N. A. DeCino, N. C. George, K. A. Hazelton, B.-C. Hong, and R. Seshadri, Eu²⁺-doped $M_2\text{SiO}_4$ ($M = \text{Ca}, \text{Ba}$) phosphors prepared by a rapid microwave-assisted sol-gel method: Phase formation and optical properties, *Solid State Sci.* **19** (2013) 51–57. [doi]
213. J. Brgoch, C. K. H. Borg, K. A. Denault, S. P. DenBaars, and R. Seshadri, Tuning luminescent properties through solid-solution in $(\text{Ba}_{1-x}\text{Sr}_x)_9\text{Sc}_2\text{Si}_6\text{O}_{24}:\text{Ce}^{3+}, \text{Li}^+$, *Solid State Sci.* **18** (2013) 149–154. [doi]
212. K. A. Denault, A. A. Mikhailovsky, S. Brinkley, S. P. DenBaars, and R. Seshadri, Improving color rendition in solid state white lighting through the use of quantum dots, *J. Mater. Chem. C* **1** (2013) 1461–1466. [doi]
211. A. Knappschneider, C. Litterscheid, D. Dzivenko, J. Kurzman, R. Seshadri, N. Wagner, J. Beck, R. Riedel, and B. Albert, Possible superhardness of CrB_4 , *Inorg. Chem.* **52** (2013) 540–542. [doi]
210. T. V. Pho, J. D. Yuen, J. A. Kurzman, B. G. Smith, M.-S. Miao, W. T. Walker, R. Seshadri, and F. Wudl, *N*-alkyldinaphthocarbazoles, azaheptacenes, for solution-processed organic field-effect transistors, *J. Am. Chem. Soc.* **134** (2012) 18185–18188. [doi]
209. J. E. Douglas, C. S. Birkel, M. Miao, C. J. Torbet, G. D. Stucky, T. M. Pollock, and R. Seshadri, Enhanced thermoelectric properties of bulk TiNiSn via formation of a TiNi_2Sn second phase, *Appl. Phys. Lett.* **101** (2012) 183902(1–4). [doi]
208. K. A. Denault, N. C. George, S. R. Paden, S. Brinkley, A. A. Mikhailovsky, J. Neuefeind, S. P. DenBaars, and R. Seshadri, A green-yellow emitting oxyfluoride solid solution phosphor $\text{Sr}_2\text{Ba}(\text{AlO}_4\text{F})_{1-x}(\text{SiO}_5)_x:\text{Ce}^{3+}$ for thermally stable, high color rendition solid state white lighting, *J. Mater. Chem.* **22** (2012) 18204–18213 [ORNL Highlight]
207. M. R. Suchomel, D. P. Shoemaker, L. Ribaud, M. C. Kemei, and R. Seshadri, Spin-induced symmetry breaking in orbitally ordered NiCr_2O_4 and CuCr_2O_4 , *Phys. Rev. B* **86** (2012) 054406(1–9). [doi]
206. M.-S. Miao, J. A. Kurzman, N. Mammen, S. Narasimhan, and R. Seshadri, Trends in the electronic structure of extended gold compounds: Implications for use of gold in heterogeneous catalysis, *Inorg. Chem.* **51** (2012) 7569–7578. [doi]
205. R. Seshadri, S. L. Brock, A. Ramirez, M. A. Subramanian, and M. E. Thompson, Advances in the development and growth of functional materials: Toward the paradigm of materials by design, *MRS Bulletin* **37** (2012) 682–690. [doi]
204. C. S. Birkel, W. G. Zeier, J. E. Douglas, B. R. Lettiere, C. E. Mills, G. Seward, A. Birkel, M. L. Snedaker, Y. Zhang, G. J. Snyder, T. M. Pollock, R. Seshadri, and G. D. Stucky, Rapid microwave preparation of thermoelectric TiNiSn and TiCoSb half-Heusler compounds, *Chem. Mater.* **24** (2012) 2558–2565. [doi]
203. M.-S. Miao and R. Seshadri, Rh_2O_3 versus IrO_2 : Relativistic effects and the stability of Ir^{4+} , *J. Phys.: Condens. Matter* **24** (2012) 215503(1–9). [doi]
202. A. Birkel, L. E. Darago, A. Morrison, L. Lory, N. C. George, A. A. Mikhailovsky, C. S. Birkel, and R. Seshadri, Microwave assisted preparation of Eu²⁺-doped Åkermanite $\text{Ca}_2\text{MgSi}_2\text{O}_7$, *Solid State Sci.* **14** (2012) 739–745. [doi]
201. A. Birkel, K. A. Denault, N. C. George, C. E. Doll, B. Héry, A. A. Mikhailovsky, C. S. Birkel, B.-C. Hong, and R. Seshadri, Rapid microwave preparation of highly efficient Ce^{3+} -substituted garnet phosphors for solid state white lighting, *Chem. Mater.* **24** (2012) 1198–1204. [doi]
200. M. C. Kemei, S. L. Moffitt, D. P. Shoemaker, and R. Seshadri, Evolution of magnetic properties in the normal spinel solid solution $\text{Mg}_{1-x}\text{Cu}_x\text{Cr}_2\text{O}_4$, *J. Phys.: Condens. Matter* **24** (2012) 046003(1–8). [doi]
199. P. T. Barton, R. Seshadri, A. Knöller, and M. J. Rosseinsky, Structural and magnetic characterization of the complete delafossite solid solution $(\text{CuAlO}_2)_{1-x}(\text{CuCrO}_2)_x$, *J. Phys.: Condens. Matter* **24** (2012) 016002(1–6). [doi]
198. L. M. Misch, J. A. Kurzman, A. R. Derk, Y.-I. Kim, R. Seshadri, H. Metiu, E. W. McFarland, and G. D. Stucky, C-H bond activation by Pd-substituted CeO_2 : Substituted ions versus reduced species, *Chem. Mater.* **23** (2011) 5432–5439. [doi]

-
197. S. E. Brinkley, N. Pfaff, K. A. Denault, Z. Zhang, H. T. (Bert) Hintzen, R. Seshadri, S. Nakamura, and S. P. DenBaars, Robust thermal performance of $\text{Sr}_2\text{Si}_5\text{N}_8\text{:Eu}^{2+}$: An efficient red emitting phosphor for light emitting diode based white lighting, *Appl. Phys. Lett.* **99** (2011) 241106(1–3). [doi]
196. R. M. Shayib, N. C. George, R. Seshadri, A. W. Burton, S. I. Zones, B. F. Chmelka, Structure-directing roles and interactions of fluoride and organocations with siliceous zeolite frameworks, *J. Am. Chem. Soc.* **133** (2011) 18728–18741. [doi]
195. A. Knappschneider, C. Litterscheid, J. A. Kurzman, R. Seshadri, and B. Albert, Crystal structure refinement and bonding patterns of CrB_4 : A boron-rich boride with a framework of tetrahedrally coordinated B atoms, *Inorg. Chem.* **50** (2011) 10540–10542. [doi]
194. J. A. Kurzman, M.-S. Miao, and R. Seshadri, Hybrid functional electronic structure of PbPdO_2 , a small-gap semiconductor, *J. Phys.: Condens. Matter* **23** (2011) 465501(1–7). [doi]
193. J. A. Kurzman, J. Li, T. D. Schladt, C. R. Parra, X. Ouyang, R. Davis, J. T. Miller, S. L. Scott, and R. Seshadri, $\text{Pd}^{2+}/\text{Pd}^0$ redox cycling in hexagonal $\text{YMn}_{0.5}\text{Fe}_{0.5}\text{O}_3$: Implications for catalysis by PGM-substituted complex oxides, *Inorg. Chem.* **50** (2011) 8073–8084. [doi]
192. D. P. Shoemaker, R. Seshadri, M. Tachibana, and A. L. Hector, Incoherent Bi off-centering in $\text{Bi}_2\text{Ti}_2\text{O}_6\text{O}'$ and $\text{Bi}_2\text{Ru}_2\text{O}_6\text{O}'$: Insulator versus metal, *Phys. Rev. B* **84** (2011) 064117(1–6). [doi]
191. D. P. Shoemaker, A. Llobet, M. Tachibana, and R. Seshadri, Reverse Monte Carlo neutron scattering study of the “ordered-ice” oxide pyrochlore $\text{Pb}_2\text{Ru}_2\text{O}_{6.5}$, *J. Phys.: Condens. Matter* **23** (2011) 315404(1–6). [doi]
190. T. Z. Forbes, J. A. Kurzman, R. Seshadri, and A. Navrotsky, The energetics of $\text{La}_4\text{LiAuO}_8$, *J. Mater. Res.* **26** (2011) 1188–1192. [doi]
189. W. B. Im, N. George, J. Kurzman, S. Brinkley, A. Mikhailovsky, J. Hu, B. F. Chmelka, S. P. DenBaars, and R. Seshadri, Efficient and color-tunable oxyfluoride solid solution phosphors for solid-state white lighting, *Adv. Mater.* **23** (2011) 2300–2305. [doi]
188. J. A. Kurzman, S. L. Moffitt, A. Llobet, and R. Seshadri, Neutron diffraction study of $\text{La}_4\text{LiAuO}_8$: Understanding Au^{3+} in an oxide environment, *J. Solid State Chem.* **184** (2011) 1439–1444. [doi]
187. A. Révaux, G. Dantelle, N. George, R. Seshadri, T. Gacoin, and J.-P. Boilot, A protected annealing strategy to enhanced light emission and photostability of YAG:Ce nanoparticle-based films, *Nanoscale* **3** (2011) 2015–2022. [doi]
186. J. R. Neilson, J. A. Kurzman, R. Seshadri, and D. E. Morse, Ordering double perovskite hydroxides by kinetically controlled aqueous hydrolysis. *Inorg. Chem.* **50** (2011) 3003–3009. [doi]
185. P. Moetakef, J. Y. Zhang, A. Kozhanov, B. Jalan, R. Seshadri, S. J. Allen, and S. Stemmer, Transport in ferromagnetic $\text{GdTiO}_3/\text{SrTiO}_3$ heterostructures, *Appl. Phys. Lett.* **98** (2011) 112110(1–3). [doi]
184. J. R. Neilson, D. E. Morse, B. C. Melot, D. P. Shoemaker, J. A. Kurzman, and R. Seshadri, Understanding complex magnetic order in disordered cobalt hydroxides through analysis of the local structure, *Phys. Rev. B* **83** (2011) 094418(1–7). [doi]
183. P. T. Barton, R. Seshadri, and M. J. Rosseinsky, Electrical and magnetic properties of the complete solid solution series between SrRuO_3 and LaRhO_3 : Filling t_{2g} versus tilting, *Phys. Rev. B* **83** (2011) 064417(1–8). [doi]
182. E. E. Rodriguez, F. Poineau, A. Llobet, B. J. Kennedy, M. Avdeev, G. J. Thorogood, M. L. Carter, R. Seshadri, D. J. Singh, and A. K. Cheetham, High temperature magnetic ordering in the 4d perovskite SrTcO_3 , *Phys. Rev. Lett.* **106** (2011) 067201(1–4). [doi]
181. E. E. Rodriguez, F. Poineau, A. Llobet, J. D. Thompson, R. Seshadri, and A. K. Cheetham, Preparation, magnetism and electronic structures of cadmium technetates, *J. Mater. Chem.* **21** (2011) 1496–1502. [doi]
180. Y.-I. Kim, J. Li, J.-P. Zhang, and R. Seshadri, GaN powders from ammonolysis: Preparation, structure, morphology, and optical properties, *Solid State Sci.* **13** (2011) 216–223. [doi]

179. D. P. Shoemaker and R. Seshadri, Total-scattering descriptions of local and cooperative distortions in the oxide spinel $\text{Mg}_{1-x}\text{Cu}_x\text{Cr}_2\text{O}_4$ with dilute Jahn-Teller ions, *Phys. Rev. B* **82** (2010) 214107(1–9). [[doi](#)]
178. B. C. Melot, A. Goldman, L. E. Darago, J. D. Furman, E. E. Rodriguez, and R. Seshadri, Magnetic ordering and magnetodielectric phenomena in CoSeO_4 , *J. Phys.: Condens. Matter* **22** (2010) 506003(1–7). [[doi](#)]
177. S.-H. Kim, P. S. Halasyamani, B. C. Melot, R. Seshadri, M. A. Green, A. S. Sefat, and D. Mandrus, Experimental and computational investigation of the polar ferrimagnet VOSe_2O_5 , *Chem. Mater.* **22** (2010) 5074–50083. [[doi](#)]
176. J. Neilson, J. Kurzman, R. Seshadri, and D. E. Morse, Cobalt coordination and clustering in $\alpha\text{-Co(OH)}_2$ revealed by synchrotron X-ray total scattering, *Chem. Eur. J.* **16** (2010) 9998–10006. [[doi](#)]
175. K. Page, Th. Proffen, M. Niederberger, and R. Seshadri, Probing local dipoles and ligand structure in BaTiO_3 nanoparticles, *Chem. Mater.* **22** (2010) 4386–4391. [[doi](#)]
174. S. A. Corr, D. P. Shoemaker, B. C. Melot, and R. Seshadri, Real-space investigation of structural changes at the metal-insulator transition in VO_2 , *Phys. Rev. Lett.* **105** (2010) 056404(1–4). [[doi](#)]
173. B. C. Melot, B. Paden, R. Seshadri, E. Suard, G. Nénert, A. Dixit, and G. Lawes, Magnetic structure and susceptibility of CoSe_2O_5 : An antiferromagnetic chain compound, *Phys. Rev. B* **82** (2010) 014411(1–6). [[doi](#)]
172. P. J. Saines, B. C. Melot, R. 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.* **25** (2010) 7579–7585. [[doi](#)]
171. 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. Solid State Chem.* **183** (2010) 1266–1271. [[doi](#)]
170. J. A. Kurzman, X. Ouyang, W. B. Im, J. Li, J. Hu, S. L. Scott, and R. Seshadri, $\text{La}_4\text{LiAuO}_8$ and $\text{La}_2\text{BaPdO}_5$: Comparing two highly stable d^8 square-planar oxides, *Inorg. Chem.* **49** (2010) 4670–4680. [[doi](#)]
169. W. B. Im, S. Brinkley, A. Mikhailovsky, J. Hu, S. P. DenBaars, and R. Seshadri, $\text{Sr}_{2.975-x}\text{Ba}_x\text{Ce}_{0.025}\text{AlO}_4\text{F}$: A highly efficient green-emitting oxyfluoride phosphor for solid state white lighting, *Chem. Mater.* **22** (2010) 2842–2849. [[doi](#)]
168. D. P. Shoemaker, R. Seshadri, A. L. Hector, A. Llobet, Th. Proffen, and C. J. Fennie, Atomic displacements in the “charge-ice” pyrochlore $\text{Bi}_2\text{Ti}_2\text{O}_6\text{O}'$ studied by neutron total scattering, *Phys. Rev. B.* **81** (2010) 144113(1–9). [[doi](#)]
167. S. A. Corr, D. P. Shoemaker, E. S. Toberer, and R. Seshadri, Spontaneously formed porous and composite materials, *J. Mater. Chem. (Feature)* **20** (2010) 1413–1422. [[doi](#)]
166. Y. Shi, G. Guo, S. A. Corr, Q. Shi, Y. Hu, K. Heier, L. Chen, R. Seshadri, and G. D. Stucky, Ordered mesoporous metallic MoO_2 materials with highly reversible lithium storage capacity, *Nano Lett.* **9** (2009) 4215–4220. [[doi](#)]
165. J. R. Neilson, B. Schwenzer, R. Seshadri, and D. E. Morse, Kinetic control of intralayer cobalt coordination in layered hydroxides: $\text{Co}_{1-0.5x}^{\text{oct}}\text{Co}_x^{\text{tet}}(\text{OH})_2(\text{Cl})_x(\text{H}_2\text{O})_n$, *Inorg. Chem.* **48** (2009) 11017–11023. [[doi](#)]
164. W. B. Im, Y. Fourré, S. Brinkley, J. Sonoda, S. Nakamura, S. P. DenBaars, and R. Seshadri, Substitution of oxygen by fluorine in the $\text{GdSr}_2\text{AlO}_5\text{:Ce}^{3+}$ phosphors: $\text{Gd}_{1-x}\text{Sr}_{2+x}\text{AlO}_{5-x}\text{F}_x$ solid solutions for solid state white lighting, *Optics Express* **17** (2009) 22673–22679. [[doi](#)]
163. W. B. Im, K. Page, N. N. Fellows, S. P. DenBaars, and R. Seshadri, Probing local structure in the yellow phosphor $\text{LaSrAl}_2\text{O}_5\text{:Ce}^{3+}$, by the maximum entropy method and pair distribution function analysis, *J. Mater. Chem.* **19** (2009) 8761–8766. [[doi](#)]
162. D. P. Shoemaker, E. E. Rodriguez, R. Seshadri, I. S. Abumohor, and Th. Proffen, Intrinsic exchange bias in $\text{Zn}_x\text{Mn}_{3-x}\text{O}_4$ ($x \leq 1$) solid solutions, *Phys. Rev. B* **80** (2009) 144422(1–9). [[doi](#)]
161. 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](#)]

-
160. J. Erlebacher and R. Seshadri (Guest Editors), Hard materials with tunable porosity, *MRS Bulletin*, **34** (2009) No. 8, 561–566. [[link](#)]
159. D. P. Shoemaker, J. Li, and R. Seshadri, Unraveling atomic positions in an oxide spinel with two Jahn-Teller ions: Local structure investigation of CuMn_2O_4 , *J. Am. Chem. Soc.* **131** (2009) 11450–11457. [[doi](#)]
158. W. B. Im, N. N. Fellows, S. P. DenBaars, R. Seshadri, and Y.-I. Kim, $\text{LaSr}_2\text{AlO}_5$, a versatile host compound for Ce^{3+} -based yellow phosphors: Structural tuning of optical properties and use in solid state white lighting, *Chem. Mater.* **21** (2009) 2957–2966. [[doi](#)]
157. S. A. Corr, M. Grossman, Y. Shi, K. R. Heier, G. D. Stucky, and R. Seshadri, $\text{VO}_2(\text{B})$ nanorods: solvothermal preparation, electrical properties, and conversion to rutile VO_2 and V_2O_3 , *J. Mater. Chem.* **19** (2009) 4362–4367. [[doi](#)]
156. 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* **79** (2009) 224111(1–5). [[doi](#)]
155. 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 ReO_3 , *J. Appl. Phys.* **105** (2009) 114901(1–6). [[doi](#)]
154. B. C. Melot, J. E. Drewes, R. Seshadri, E. M. Stoudenmire, 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](#)]
153. F. Casper, R. Seshadri, and C. Felser, Semiconducting half-Heusler and LiGaGe structure type compounds, *Physica Stat. Sol. A* **206** (2009) 1090–1095. [[doi](#)]
152. W. B. Im, N. N. Fellows, S. P. DenBaars, and R. Seshadri, $\text{La}_{1-x-0.025}\text{Ce}_{0.025}\text{Sr}_{2+x}\text{Al}_{1-x}\text{Si}_x\text{O}_5$ solid solutions as tunable yellow phosphors for solid state white lighting, *J. Mater. Chem.* **19** (2009) 1325–1330. [[doi](#)]
151. K. Page, T. Kolodiazny, Th. Proffen, A. K. Cheetham, and R. Seshadri, Local structural origins of the distinct electronic properties of Nb-substituted SrTiO_3 and BaTiO_3 , *Phys. Rev. Lett* **101** (2008) 205502(1–4). [[doi](#)]
150. Y.-I. Kim and R. Seshadri, Microstrain and defects in polycrystalline $\text{Zn}_{1-x}\text{Mg}_x\text{O}$ ($0 \leq x \leq 0.15$) studied by X-ray diffraction, and optical and Raman spectroscopies, *J. Korean Phys. Soc.* **53** (2008) 2835–2839. [[link](#)]
149. Y.-I. Kim, S. Cadars, R. Shayib, Th. Proffen, C. S. Feigerle, B. F. Chmelka, and R. Seshadri, Local structures of polar wurtzites $\text{Zn}_{1-x}\text{Mg}_x\text{O}$ studied by Raman and $^{25}\text{Mg}/^{67}\text{Zn}$ NMR spectroscopies, and by total neutron scattering, *Phys. Rev. B* **78** (2008) 195205(1–12). [[doi](#)]
148. K. Page, J. Li, R. Savinelli, H. N. Szumila, J. Zhang, J. K. Stalick, Th. Proffen, S. L. Scott, and R. Seshadri, Reciprocal-space and real-space neutron investigation of nanostructured Mo_2C and WC , *Solid State Sci.* **10** (2008) 1499–1510. [[doi](#)]
147. J. Li, U. G. Singh, T. D. Schladt, J. K. Stalick, S. L. Scott, and R. Seshadri, Hexagonal $\text{YFe}_{1-x}\text{Pd}_x\text{O}_{3-\delta}$: Non-perovskite host compounds for Pd^{2+} and their catalytic activity for CO oxidation, *Chem. Mater.* **20** (2008) 6567–6576. [[doi](#)]
146. 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](#)]
145. Y.-I. Kim and R. Seshadri, Optical properties of cation-substituted zinc oxide. *Inorg. Chem. (forum article)* **47** (2008) 8437–8443. [[doi](#)]
144. W. B. Im, Y.-I. Kim, N. N. Fellows, H. Masui, G. A. Hirata, S. P. DenBaars, and R. Seshadri, A yellow-emitting Ce^{3+} phosphor, $\text{La}_{1-x}\text{Ce}_x\text{Sr}_2\text{AlO}_5$, for white light-emitting diodes. *Appl. Phys. Lett.* **93** (2008) 091905(1–3). [[doi](#)]
143. E. E. Rodriguez, F. Poineau, A. Llobet, K. Czerwinski, R. Seshadri and A. K. Cheetham, Preparation and crystal structures of bismuth technetates: A new metal oxide system, *Inorg. Chem.* **47** (2008) 62810–6288. [[doi](#)]
142. M. B. Smith, K. Page, T. Siegrist, P. L. Redmond, E. C. Walter, R. Seshadri, L. E. Brus, and M. L. Steigerwald, Crystal structure and the paraelectric-to-ferroelectric phase transition of nanoscale BaTiO_3 , *J. Am. Chem. Soc.* **130** (2008) 6955–6963. [[doi](#)]

141. D. P. Shoemaker, M. Grossman, and R. Seshadri, Exchange biasing of single-domain Ni nanoparticles spontaneously grown in an antiferromagnetic MnO matrix, *J. Phys.: Condens. Matter* **20** (2008) 195219(1–9). [doi]
140. F. Casper, C. Felser, R. Seshadri, C. P. Sebastian, and R. Pöttgen, Searching for hexagonal analogues of the half-metallic half-Heusler XYZ compounds, *J. Phys. D: Applied Physics* **41** (2008) 035002(1–7). [doi]
139. K. Page, C. S. Schade, J. Zhang, P. J. Chupas, K. Chapman, Th. Proffen, A. K. Cheetham, and R. Seshadri, Preparation and characterization of Pd₂Sn nanoparticles, *Mater. Res. Bull.* **42** (2007) 1969–1975. [doi]
138. E. S. Toberer, M. Grossman, T. Schladt, F. F. Lange, and R. Seshadri, Epitaxial manganese oxide thin films with connected porosity: Topotactic induction of crystallographic pore alignment, *Chem. Mater.* **19** (2007) 4833–4838. [doi]
137. Y.-I. Kim, K. Page, A. M. Limarga, D. R. Clarke, and R. Seshadri, Evolution of local structures in polycrystalline Zn_{1-x}Mg_xO ($0 \leq x \leq 0.15$) studied by Raman spectroscopy and synchrotron x-ray pair distribution function analysis, *Phys. Rev. B* **76** (2007) 115204(1–10). [doi]
136. P. Baettig, R. Seshadri, and N. A. Spaldin, Anti-polarity in ideal BiMnO₃, *J. Am. Chem. Soc.* **129** (2007) 9854–9855. [doi]
135. K. Page, M. W. Stoltzfus, Y.-I. Kim, Th. Proffen, P. M. Woodward, A. K. Cheetham, and R. Seshadri, Local atomic ordering in BaTaO₂N studied by neutron pair distribution function analysis and density functional theory, *Chem. Mater.* **19** (2007) 4037–4042. [doi]
134. R. Tackett, G. Lawes, B. C. Melot, M. Grossman, E. S. Toberer, and R. Seshadri, Magnetodielectric coupling in Mn₃O₄, *Phys. Rev. B* **76** (2007) 024409(1–6). [doi]
133. U. G. Singh, J. Li, J. W. Bennett, A. M. Rappe, R. Seshadri, and S. L. Scott, A Pd-doped Perovskite Catalyst, BaCe_{1-x}Pd_xO_{3-δ}, for CO Oxidation, *J. Catal.* **249** (2007) 349–358. [doi]
132. S. Thimmaiah, C. Felser, and R. Seshadri, Crystal structure, magnetism, and bonding of the hexagonal compounds Pd_{1.63}Mn_{0.37}Si and Pd_{1.82}Mn_{0.18}Ge related to the Fe₂P structure, *J. Phys. D.* **40** (2007) 3915–3920. [doi]
131. M. W. Stoltzfus, P. M. Woodward, R. Seshadri, J.-H. Park-Kleipsis, and B. Bursten, Structure and bonding in SnWO₄, PbWO₄ and BiVO₄: Lone pairs vs. inert pairs, *Inorg. Chem.* **46** (2007) 3839–3850. [doi]
130. J. Li, U. G. Singh, J. W. Bennett, K. Page, J. Weaver, J.-P. Zhang, Th. Proffen, A. M. Rappe, S. Scott, and R. Seshadri, BaCe_{1-x}Pd_xO_{3-δ} ($0 \leq x \leq 0.1$): Redox controlled ingress and egress of palladium in a perovskite, *Chem. Mater.* **19** (2007) 1418–1426. [doi]
129. Y.-I. Kim, K. Page, and R. Seshadri, Synchrotron x-ray study of polycrystalline wurtzite Zn_{1-x}Mg_xO ($0 \leq x \leq 0.15$): Evolution of crystal structure and polarization, *Appl. Phys. Lett.* **90** (2007) 101904(1–3). [doi]
128. H. C. Kandpal, V. Ksenofontov, M. Wojcik, R. Seshadri, and C. Felser, Electronic structure, magnetism, and disorder in the Heusler compound Co₂TiSn, *J. Phys. D.* **40** (2007) 1587–1592. [doi]
127. E. S. Toberer, J.-D. Epping, B. F. Chmelka, and R. Seshadri, Hierarchically porous rutile titania: Harnessing spontaneous compositional change in mixed metal oxides, *Chem. Mater.* **18** (2006) 6345–6351. [doi]
126. O. Masala, D. Hoffman, N. Sundaram, K. Page, Th. Proffen, G. Lawes, and R. Seshadri, Preparation of magnetic spinel ferrite core/shell nanoparticles: Soft ferrites on hard ferrites and vice-versa, *Solid State Sci.* **8** (2006) 1015–1022. [doi]
125. G. Lawes, B. Melot, K. Page, C. Ederer, M. A. Hayward, Th. Proffen, and R. Seshadri, Dielectric anomalies and spiral magnetic order in CoCr₂O₄, *Phys. Rev. B* **74** (2006) 024413(1–6). [doi]
124. E. S. Toberer and R. Seshadri, Template-free routes to porous inorganic materials, *Chem. Commun.* (2006) 3159–3165. [doi]
123. G. Lawes, R. Tackett, O. Masala, B. Adhikary, R. Naik, and R. Seshadri, Positive and negative magnetocapacitance in magnetic nanoparticle systems, *Appl. Phys. Lett.* **88** (2006) 242903(1–3). [doi]

-
122. R. Seshadri, Zinc oxide-based diluted magnetic semiconductors, *Current Opin. Solid State Mater. Sci.* **9** (2006) 1–7. [doi]
121. 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]
120. R. Seshadri, Lone pairs in insulating pyrochlores: Ice rules and high-*k* behavior, *Solid State Sci.* **8** (2006) 259–266. [doi]
119. H. C. Kandpal, C. Felser, and R. Seshadri, Covalent bonding and the nature of band gaps in some half-Heusler compounds, *J. Phys. D.* **39** (2006) 776–785. [doi]
118. E. S. Toberer, J. P. Löfvander, and R. Seshadri, Topochemical formation of mesoporous MnO crystals, *Chem. Mater.* **18** (2006) 1047–1053. [doi]
117. E. S. Toberer, T. Schladt, and R. Seshadri, Macroporous manganese oxides with regenerative mesopores, *J. Am. Chem. Soc.* **128** (2006) 1462–1463. [doi]
116. L. P. Snedeker, A. S. Risbud, O. Masala, J. P. Zhang, and R. Seshadri, Organic phase conversion of bulk (wurtzite) ZnO to nanophase (wurtzite and zinc blende) ZnO, *Solid State Sci.* **7** (2005) 1500–1505. [doi]
115. E. S. Toberer and R. Seshadri, Spontaneous formation of macroporous monoliths of mesoporous manganese oxide crystals, *Adv. Mater.* **17** (2005) 2244–2246. [doi]
114. O. Masala and R. Seshadri, Spinel ferrite/MnO core/shell nanoparticles: Chemical synthesis of all-oxide exchange biased architectures, *J. Am. Chem. Soc.* **127** (2005) 9354–9355. [doi]
113. B. Schwenzer, C. Meier, O. Masala, R. Seshadri, S. P. DenBaars, and U. K. Mishra, Synthesis of luminescing (In,Ga)N nanoparticles from an inorganic ammonium fluoride precursor, *J. Mater. Chem.* **15** (2005) 1891–1895. [doi]
112. E. S. Toberer, A. Joshi, and R. Seshadri, Template-free routes to macroporous monoliths of nickel and iron oxides: Toward porous metals and conformally coated pore walls, *Chem. Mater.* **17** (2005) 2142–2147. [doi]
111. A. S. Risbud, L. P. Snedeker, M. M. Elcombe, A. K. Cheetham, and R. Seshadri, Wurtzite CoO, *Chem. Mater.* **17** (2005) 834–838. [doi]
110. A. S. Risbud, R. Seshadri, J. Ensling, and C. Felser, Dilute ferrimagnetic semiconductors in Fe-substituted spinel ZnGa_2O_4 , *J. Phys.: Condens. Matter* **17** (2005) 1003–1010. [doi]
109. G. Lawes, A. S. Risbud, A. P. Ramirez, and R. Seshadri, Absence of ferromagnetism in Co and Mn substituted polycrystalline ZnO, *Phys. Rev. B* **71** (2005) 045201(1–5). [doi]
108. O. Masala and R. Seshadri, Magnetic properties of capped, soluble MnFe_2O_4 nanoparticles, *Chem. Phys. Lett.* **402** (2005) 160–164. [doi]
107. K. Ramesha, R. Seshadri, C. Ederer, T. He, and M. A. Subramanian Experimental and computational investigation of structure and magnetism in pyrite $\text{Co}_{1-x}\text{Fe}_x\text{S}_2$: Chemical bonding and half-metallicity, *Phys. Rev. B* **70** (2004) 214409(1–8). [doi]
106. B. Schwenzer, J. Hu, R. Seshadri, S. Keller, S. P. DenBaars, and U. K. Mishra, Gallium nitride powders from ammonolysis: Influence of reaction parameters on structure and properties, *Chem. Mater.* **16** (2004) 5088–5095. [doi]
105. A. K. Kundu, K. Ramesha, R. Seshadri, and C. N. R. Rao, Magnetic and electron transport properties of the rare-earth cobaltates, $\text{La}_{0.7-x}\text{Ln}_x\text{Ca}_{0.3}\text{CoO}_3$ (Ln = Pr, Nd, Gd and Dy): A case of phase separation, *J. Phys.: Condens. Matter* **16** (2004) 7955–7966. [doi]
104. R. P. Haggerty and R. Seshadri, Oxygen stoichiometry, crystal structure, and magnetism in $\text{La}_{0.5}\text{Sr}_{0.5}\text{CoO}_{3-\delta}$, *J. Phys.: Condens. Matter* **16** (2004) 6477–6484. [doi]
103. K. Ramesha and R. Seshadri, Solvothermal preparation of ferromagnetic sub-micron spinel CuCr_2Se_4 particles, *Solid State Sci.* **6** (2004) 841–845. [doi]

-
102. K. Page, Th. Proffen, H. Terrones, M. Terrones, L. Lee, Y. Yang, S. Stemmer, R. Seshadri, and A. K. Cheetham, Direct observation of the structure of gold nanoparticles by total scattering powder neutron diffraction, *Chem. Phys. Lett.* **393** (2004) 385–388. [doi]
101. O. Masala and R. Seshadri, Synthesis routes for large volumes of nanoparticles, *Annu. Rev. Mater. Res.* **34** (2004) 41–81. [doi]
100. E. S. Toberer, J. C. Weaver, K. Ramesha, and R. Seshadri, Macroporous monoliths of functional perovskite materials through assisted metathesis, *Chem. Mater.* **16** (2004) 2194–2200. [doi]
99. M. Lauer, R. Valentí, H. C. Kandpal, and R. Seshadri, First-principles electronic structure of spinel LiCr_2O_4 : A possible half metal, *Phys. Rev. B* **69** (2004) 075117(1–8). [doi]
98. R. Seshadri, Oxide Nanoparticles, Review in, The chemistry of nanomaterials (vol. 1): Synthesis, properties and applications, C. N. R. Rao, Achim Müller, Anthony K. Cheetham (Eds.) Wiley-VCH, ISBN: 3-527-30686-2, (2004).
97. U. K. Gautam and R. Seshadri, Preparation of PbS and PbSe nanocrystals by a new solvothermal route, *Mater. Res. Bull.* **39** (2004) 669–676. [doi]
96. B. Schwenzer, L. Loeffler, R. Seshadri, S. Keller, F. F. Lange, S. P. DenBaars, and U. K. Mishra, Preparation of indium nitride micro- and nanostructures by ammonolysis of indium oxide, *J. Mater. Chem.* **14** (2004) 637–641. [doi]
95. M. Ghosh, G. Lawes, A. Gayen, G. N. Subbanna, W. M. Reiff, M. A. Subramanian, A. P. Ramirez, J.-P. Zhang, and R. Seshadri, A novel route to toluene soluble magnetic oxide nanoparticles: Aqueous hydrolysis followed by surfactant exchange, *Chem. Mater.* **16** (2004) 118–124. [doi]
94. A. S. Risbud, N. A. Spaldin, Z. Q. Chen, S. Stemmer, and R. Seshadri, Magnetism in polycrystalline cobalt-substituted zinc oxide, *Phys. Rev. B* **68** (2003) 205202(1–7). [doi]
93. N. Berntsen, T. Gutjahr, L. Loeffler, J. R. Gomm, R. Seshadri, and W. Tremel, A solvothermal route to high-surface-area nanostructured MoS_2 , *Chem. Mater.* **15** (2003) 4498–4502. [doi]
92. U. K. Gautam, R. Seshadri, and C. N. R. Rao, A solvothermal route to CdS nanocrystals, *Chem. Phys. Lett.* **375** (2003) 560–564. [doi]
91. M. Dinamani, P. Vishnu Kamath, and R. Seshadri, Deposition of oriented SrSO_4 coatings by electrogeneration of acid, *Solid State Sci.* **5** (2003) 805–810. [doi]
90. E. Loste, R. M. Wilson, R. Seshadri, and F. C. Meldrum, The role of magnesium in stabilising amorphous calcium carbonate and controlling calcite morphologies, *J. Cryst. Growth.* **254** (2003) 206–218. [doi]
89. M. Dinamani, P. Vishnu Kamath, and R. Seshadri, Electrodeposition of BaCO_3 on stainless steel substrates, *Crystal Growth & Design* **3** (2003) 417–423. [doi]
88. M. Panda, R. Seshadri and J. Gopalakrishnan, Preparation of $\text{PbZrO}_3/\text{ASO}_4$ composites (A = Ca, Sr, Ba) and PbZrO_3 by metathetic reactions in the solid state: Metathetic exchange of divalent species, *Chem. Mater.* **15** (2003) 1554–1559. [doi]
87. U. V. Waghmare, N. A. Spaldin, H. C. Kandpal, and R. Seshadri, First principles indicators of metallicity and cation off-centricity in the IV–VI rock-salt chalcogenides of divalent Ge, Sn and Pb, *Phys. Rev. B* **67** (2003) 125111(1–10). [doi]
86. S. Barman, N. V. Venkatraman, S. Vasudevan, and R. Seshadri, Phase transitions in the anchored organic bilayers of long-chain alkylammonium lead iodides $(\text{C}_n\text{H}_{2n+1}\text{NH}_3)_2\text{PbI}_4$; $n = 12, 16, 18$, *J. Phys. Chem. B* **107** (2003) 1875–1883. [doi]
85. M. Rajamathi and R. Seshadri, Oxide and chalcogenide nanoparticles from hydrothermal/solvothermal reactions, *Curr. Opinion Solid State Mater. Sci.* **6** (2002) 337–345. [doi]
84. M. Panda, M. Rajamathi, and R. Seshadri, A template free, combustion-chemical route to macroporous nickel monoliths displaying a hierarchy of pore sizes, *Chem. Mater.* **14** (2002) 4762–4767. [doi]

-
83. U. K. Gautam, M. Ghosh, M. Rajamathi, and R. Seshadri, Solvothermal routes to capped oxide and chalcogenide nanoparticles, *Pure Appl. Chem.* **74** (2002) 1643–1649.
82. N. V. Venkatraman, S. Bhagyalakshmi, S. Vasudevan, and R. Seshadri, Conformation and orientation of alkyl chains in the layered inorganic-organic hybrids: $(C_nH_{2n+1}NH_3)_2PbI_4$ ($n = 12, 16, 18$), *Phys. Chem. Chem. Phys.* **4** (2002) 4533–4538. [doi]
81. H. C. Kandpal and R. Seshadri, First-principles electronic structure of the delafossites ABO_2 ($A = Cu, Ag, Au$; $B = Al, Ga, Sc, In, Y$): Evolution of d^{10} – d^{10} interactions, *Solid State Sci.* **4** (2002) 1045–1052. [doi]
80. U. K. Gautam, R. Seshadri, S. Vasudevan, and A. Maignan, Magnetic and transport properties, and electronic structure of the layered chalcogenide $AgCrSe_2$, *Solid State Commun.* **122** (2002) 607–612. [doi]
79. N. V. Venkatraman, S. Barman, S. Vasudevan and R. Seshadri, Structural analysis of alkyl chain conformation in the layered organic-inorganic hybrids $(C_nH_{2n+1}NH_3)_2PbI_4$ ($n = 12, 16, 18$) by IR spectroscopy, *Chem. Phys. Lett.* **358** (2002) 139–143. [doi]
78. M. Rajamathi, M. Ghosh, and R. Seshadri, Hydrolysis and amine-capping in a glycol solvent as a route to soluble maghemite γ - Fe_2O_3 nanoparticles, *Chem. Commun.* (2002) 1152–1153. [doi]
77. G. Baldinozzi, J.-M. Raulot, and R. Seshadri, Lead stereochemistry in incommensurate ferroelectric perovskites and in incommensurate lead monoxide, *Mater. Res. Soc. Symp. Proc.* **718** (2002) D12.7.1
76. J.-M. Raulot, G. Baldinozzi, R. Seshadri, and P. Cortona, An *ab-initio* study of the rôle of lone pairs in the structure and insulator-metal transition in SnO and PbO , *Solid State Sci.* **4** (2002) 467–474. [doi]
75. M. Dinamani, P. Vishnu Kamath, and R. Seshadri, Electrochemical synthesis of calcium carbonate coatings on stainless steel substrates, *Mater. Res. Bull.* **37** (2002) 661–669. [doi]
74. R. Seshadri, Visualizing lone pairs in compounds containing heavier congeners of the carbon and nitrogen group elements, *Proc. Indian Acad. Sci. (Chem. Sci.)* **113** (2001) 487–496.
73. S. Thimmaiah, M. Rajamathi, N. Singh, P. Bera, F. C. Meldrum, N. Chandrasekhar, and R. Seshadri, A solvothermal route to capped nanoparticles of γ - Fe_2O_3 and $CoFe_2O_4$, *J. Mater. Chem.* **11** (2001) 3215–3221. [doi]
72. M. Dinamani, P. Vishnu Kamath, and R. Seshadri, Electrochemical deposition of $BaSO_4$ coatings on stainless steel substrates, *Chem. Mater.* **13** (2001) 3981–3985. [doi]
71. T. Sivakumar, R. Seshadri, and J. Gopalakrishnan, Bridging the Ruddlesden-Popper and Aurivillius phases: Synthesis and structure of a novel series of layered perovskite oxides, $(BiO)LnTiO_4$ (Ln -La, Nd, Sm), *J. Am. Chem. Soc.* **123** (2001) 11496–11497. [doi]
70. R. Seshadri and N. A. Hill, Visualizing the role of Bi 6s “lone pairs” in the off-center distortion in ferromagnetic $BiMnO_3$, *Chem. Mater.* **13** (2001) 2892–2899. [doi]
69. M. Rajamathi, S. Thimmaiah, P. E. D. Morgan, and R. Seshadri, Macroporous materials from crystalline single-source precursors through decomposition followed by selective leaching, *J. Mater. Chem.* **11** (2001) 2489–2492. [doi]
68. U. K. Gautam, M. Rajamathi, F. Meldrum, P. Morgan, and R. Seshadri, A solvothermal route to capped $CdSe$ nanoparticles, *Chem. Commun.* (2001) 629–630. [doi]
67. K. Vijaya Sarathy, P. V. Vanitha, R. Seshadri, A. K. Cheetham, and C. N. R. Rao, Electron-hole asymmetry in the rare-earth manganates: A comparative study of the hole- and the electron-doped materials, *Chem. Mater.* **13** (2001) 787–795. [doi]
66. J. Küther, M. Bartz, R. Seshadri, G. Vaughan, and W. Tremel, Crystallization of $SrCO_3$ on a self-assembled monolayer substrate: An *in-situ* synchrotron x-ray study, *J. Mater. Chem.* **11** (2001) 503–506. [doi]
65. C. Felser and R. Seshadri, Conduction band polarization in some CMR materials: Evolving guidelines for new systems, *Intl. J. Inorg. Mater.* **2** (2000) 677–685. [doi]

-
64. R. Seshadri and F. Meldrum, Bioskeletons as templates for ordered, macroporous structures, *Adv. Mater.* **12** (2000) 1149–1151. [doi]
63. R. Basu, C. Felser, A. Maignan, and R. Seshadri, Magnetization and magnetoresistive response of LiMn_2O_4 near the charge-ordering transition, *J. Mater. Chem.* **10** (2000) 1921–1924. [doi]
62. K. Ahn, C. Felser, R. Seshadri, R. K. Kremer, and A. Simon, Giant negative magnetoresistance in GdI_2 , *J. Alloys. Compounds.* **303–304** (2000) 252–256. [doi]
61. M. Rajamathi, P. Vishnu Kamath, and R. Seshadri, Chemical synthesis of alpha-cobalt hydroxide, *Mater. Res. Bull.* **35** (2000) 271–278. [doi]
60. R. Basu and R. Seshadri, Suppressing the charge-ordering transition in LiMn_2O_4 through substitution of Li by Mg, *J. Mater. Chem.* **10** (2000) 507–510. [doi]
59. M. Rajamathi, P. Vishnu Kamath, and R. Seshadri, Polymorphism in nickel hydroxide: Role of interstratification, *J. Mater. Chem.* **10** (2000) 503–506. [doi]
58. F. C. Meldrum and R. Seshadri, Porous gold structures through templating by echinoid skeletal plates, *Chem. Commun.* (2000) 29–30. [doi]
57. O. Lang, C. Felser, R. Seshadri, F. Renz, J.-M. Kiat, J. Ensling, P. Gütlich, and W. Tremel, Magnetic and electronic structure of the CMR chalcospinel $\text{Fe}_{0.5}\text{Cu}_{0.5}\text{Cr}_2\text{S}_4$, *Adv. Mater.* **12** (2000) 65–69. [doi]
56. M. Bartz, N. Weber, J. Küther, R. Seshadri, and W. Tremel, “Sticky” gold colloids through protection-deprotection and their use in complex metal-organic-inorganic architectures, *Chem. Commun.* (1999) 2085–2086. [doi]
55. M. Goga, R. Seshadri, V. Ksenofontov, P. Gütlich, and W. Tremel, $\text{Ln}_2\text{Ti}_2\text{S}_2\text{O}_5$ (Ln = Nd, Pr, Sm): A novel series of defective Ruddlesden-Popper phases, *Chem. Commun.* (1999) 979–980. [doi]
54. R. Seshadri, G. Baldinozzi, C. Felser, and W. Tremel Visualizing electronic structure changes across an antiferroelectric phase transition: Pb_2MgWO_6 , *J. Mater. Chem.* **9** (1999) 2463–2466. [doi]
53. C. Felser, K. Ahn, R. K. Kremer, R. Seshadri, and A. Simon, Giant negative magnetoresistance in GdI_2 : Prediction and realization, *J. Solid. State Chem.* **147** (1999) 19–25. [doi]
52. M. Bartz, J. Küther, G. Nelles, N. Weber, R. Seshadri, and W. Tremel, Monothiols derived from glycols as agents for stabilizing gold colloids in water: Preparation, self-assembly and use as crystallization templates, *J. Mater. Chem.* **9** (1999) 1121–1125. [doi]
51. J. Küther, R. Seshadri, G. Nelles, W. Assenmacher, H.-J. Butt, W. Mader, and W. Tremel, Mercaptophenol-protected gold colloids as nuclei for the crystallization of inorganic minerals: Templated crystallization on curved surfaces, *Chem. Mater.* **11** (1999) 1317–1325. [doi]
50. C. Felser and R. Seshadri, Electronic structures and instabilities of ZrNCl and HfNCl : Implications for superconductivity in the doped compounds, *J. Mater. Chem.* **9** (1999) 459–464. [doi]
49. C. Felser, K. Thieme, and R. Seshadri, Electronic instabilities in compounds with hexagonal nets, *J. Mater. Chem.* **9** (1999) 451–457. [doi]
48. R. Seshadri, E. Suard, C. Felser, E. W. Finckh, A. Maignan, and W. Tremel, The 63 K phase transition in ZrTe_3 : A neutron diffraction study, *J. Mater. Chem.* **8** (1998) 2869–2874. [doi]
47. M. Nagtegaal, R. Seshadri, and W. Tremel, Colloid-roughened surfaces as templates for the heterogeneous nucleation of lepidocrocite $\gamma\text{-FeO}(\text{OH})$ nanoparticles, *Chem. Commun.* (1998) 2139–2140. [doi]
46. J. Küther, R. Seshadri, and W. Tremel, Crystallization of calcite spherules around designer nuclei, *Angew. Chem. Intl. Edn. Engl.* **37** (1998) 3044–3047. [doi]
45. M. Bartz, J. Küther, R. Seshadri, and W. Tremel, Colloid-bound catalysts for ring-opening metathesis polymerization: A combination of homogenous and heterogeneous properties, *Angew. Chem. Intl. Edn. Engl.* **37** (1998) 2466–2468. [doi]

44. J. Küther, G. Nelles, R. Seshadri, M. Schaub, H.-J. Butt, and W. Tremel, Templated crystallization of calcium and strontium carbonates on centered rectangular self-assembled monolayer substrates, *Chem. Eur. J.* **4** (1998) 1834–1842. [doi]
43. R. Seshadri, C. Felser, K. Thieme, and W. Tremel, Metal-metal bonding and metallic behaviour in some ABO₂ delafossites, *Chem. Mater.* **10** (1998) 2189–2196. [doi]
42. C. Felser, R. Seshadri, A. Leist, and W. Tremel, Bonding patterns and instabilities in the $m=2$ Ruddlesden-Popper Phases: LaSr₂Mn₂O₇ and La₂CaCu₂O₆, *J. Mater. Chem.* **8** (1998) 787–795. [doi]
41. J. Küther, R. Seshadri, G. Nelles, H.-J. Butt, W. Knoll, and W. Tremel, Rough surfaces by design: gold colloids tethered to gold surfaces as substrates for CaCO₃ crystallization, *Adv. Mater.* **10** (1998) 401–404. [doi]
40. J. Küther, R. Seshadri, W. Knoll, and W. Tremel, Templated growth of calcite, vaterite and aragonite crystals on self-assembled monolayers of substituted alkylthiols on gold, *J. Mater. Chem.* **8** (1998) 641–650. [doi]
39. P. Boullay, R. Seshadri, M. Hervieu, F. Studer, D. Groult, and B. Raveau, Chemical and physical aspects of the misfit layer oxides Tl_α[(Sr_{1-y}Ca_y)O]_{1+x}(CoO₂) *Chem. Mater.* **10** (1998) 92–102. [doi]
38. R. Seshadri, A. Maignan, C. Martin, F. Letouzé, and B. Raveau, Magnetic and transport properties of the “1201” phase Tl_{0.94}Sr₂Cu_{0.4}Co_{0.6}O_{5-δ}, *Phys. Rev. B* **56** (1997) 5504–5511. [doi]
37. A. Maignan, R. Seshadri, C. Martin, F. Letouzé, and B. Raveau, Giant negative magnetoresistance in the spin glass insulator Tl_{0.94}Sr₂Cu_{0.4}Co_{0.6}O_{5-δ}, *Solid State Commun.* **102** (1997) 551–554. [doi]
36. R. Seshadri, M. Hervieu, C. Martin, A. Maignan, B. Domenges, B. Raveau, and A. Fitch, A study of the layered magnetoresistive perovskite La_{1.2}Sr_{1.8}Mn₂O₇, by high resolution electron microscopy and synchrotron x-ray powder diffraction, *Chem. Mater.* **9** (1997) 1778–1787. [doi]
35. R. Seshadri, C. Martin, M. Hervieu, B. Raveau, and C. N. R. Rao, Structural evolution and electronic properties of La_{1+x}Sr_{2-x}Mn₂O₇, *Chem. Mater.* **9** (1997) 270–277. [doi]
34. R. Seshadri, A. Maignan, M. Hervieu, N. Nguyen, and B. Raveau, Complex magnetotransport in LaSr₂Mn₂O₇, *Solid State Commun.* **101** (1997) 453–457. [doi]
33. C. N. R. Rao and R. Seshadri in W. Jones (ed.), *Organic Molecular Solids: Properties and Applications*, CRC Press, Boca Raton, Florida (1997) pages 1–26.
32. P. Laffez, G. van Tendeloo, R. Seshadri, M. Hervieu, C. Martin, A. Maignan, and B. Raveau, Microstructural and physical properties of the layered manganites related to the magneto-resistive perovskites, *J. Appl. Phys.* **80** (1996) 5850–5856. [doi]
31. R. Seshadri, C. Martin, A. Maignan, M. Hervieu, B. Raveau, and C. N. R. Rao, Structure and magnetotransport properties of the layered manganites RE_{1.2}Sr_{1.8}Mn₂O₇ (RE = La, Pr, Nd), *J. Mater. Chem.* **6** (1996) 1585–1590. [doi]
30. R. Seshadri, A. Maignan, C. Martin, M. Hervieu, B. Raveau, and C. N. R. Rao, Substitution of chromium for univalent copper in superconducting Pb₂Sr₂(Ca,Y)Cu₃O_{8+δ}, *J. Solid State Chem.* **127** (1996) 64–71. [doi]
29. C. Martin, F. Letouzé, A. Maignan, R. Seshadri, C. Michel, M. Hervieu, and B. Raveau, The superconducting copper oxychromate Tl₃(CrO₄)Sr₈Cu₄O₁₆: Long range ordering between thallium and chromium, *Chem. Mater.* **8** (1996) 865–873. [doi]
28. R. Seshadri, G. N. Subbanna, V. Vijayakrishnan, G. U. Kulkarni, G. Ananthakrishna, and C. N. R. Rao, Growth of nanometric gold particles in the solution phase, *J. Phys. Chem.* **99** (1995) 5639–5644. [acs]
27. C. N. R. Rao, A. Govindaraj, H. N. Aiyer, and R. Seshadri, Polymerization and pressure-induced amorphization of C₆₀ and C₇₀, *J. Phys. Chem.* **99** (1995) 16814–16814. [acs]
26. H. N. Aiyer, R. Seshadri, G. Raina, R. Sen, and C. N. R. Rao, Study of carbon nanocapsules (onions) and spherulitic graphite by STM and other techniques, *Fullerene Sci. Technol.* **3** (1995) 765–777.
25. C. N. R. Rao, R. Seshadri, R. Sen, and A. Govindaraj, Fullerenes, nanotubes, onions and related carbon structures, *Mater. Sci. Eng. R* **15** (1995) 209–262. [doi]

-
24. R. Seshadri, R. Sen, G. N. Subbanna, K. R. Kannan, and C. N. R. Rao, Iron, cobalt and nickel nanoparticles encapsulated in carbon obtained by the arc-evaporation of graphite with the metals, *Chem. Phys. Lett.* **231** (1994) 308–313. [[doi](#)]
 23. S. K. Ramasesha, A. K. Singh, A. K. Sood, R. Seshadri, and C. N. R. Rao, Orientational ordering in C₇₀: Evidence for three phase transitions, *Chem. Phys. Lett.* **220** (1994) 203–206. [[doi](#)]
 22. D. V. S. Muthu, M. N. Shashikala, A. K. Sood, R. Seshadri, and C. N. R. Rao, Raman study of the doped fullerene C₆₀-TDAE, *Chem. Phys. Lett.* **217** (1994) 146–151. [[doi](#)]
 21. R. Seshadri, A. Govindaraj, H. N. Aiyer, R. Sen, G. N. Subbanna, A. R. Raju, and C. N. R. Rao, Investigations of carbon nanotubes, *Current Sci. (India)* **66** (1994) 839.
 20. R. Seshadri, H. N. Aiyer, A. Govindaraj, and C. N. R. Rao, Electron transport properties of carbon nanotubes, *Solid State Commun.* **91** (1994) 195–199. [[doi](#)]
 19. R. Seshadri and C. N. R. Rao, Preparation of monodispersed submicron gold particles, *Mater. Res. Bull.* **29** (1994) 795–799. [[doi](#)]
 18. R. Seshadri and C. N. R. Rao, Phase transitions, superconductivity and ferromagnetism in fullerene systems, *MRS Bulletin* **19** (1994) 28–32. [[PDF](#)]
 17. R. Seshadri, H. Pal, T. Mukherjee, J. P. Mittal, and C. N. R. Rao, Interaction of C₆₀ and C₇₀ with aromatic amines in the ground and excited states: Evidence for fullerene-benzene interaction in the ground state, *Chem. Phys. Lett.* **205** (1993) 395–398. [[doi](#)]
 16. V. Varma, R. Seshadri, A. Govindaraj, A. K. Sood, and C. N. R. Rao, An infrared spectroscopic study of the orientational phase transitions in C₇₀, *Chem. Phys. Lett.* **203** (1993) 545–548. [[doi](#)]
 15. R. Seshadri, F. D'Souza, V. Krishnan, and C. N. R. Rao, Electron donor-acceptor complexes of the fullerenes C₆₀ and C₇₀ with amine, *Chem. Lett.* (1993) 217–220.
 14. R. Seshadri, A. Govindaraj, and C. N. R. Rao, A study of the addition of alkylamines and hydrazine to fullerenes, *Fullerene Sci. Technol.* **1** (1993) 544.
 13. R. Seshadri, V. Vijayakrishnan, A. K. Santra, A. Govindaraj, and C. N. R. Rao, Investigations of the interaction of nickel and carbon monoxide with solid films of C₆₀ and C₇₀ by UV and x-ray photoelectron spectroscopy, *Fullerene Sci. Technol.* **1** (1993) 75.
 12. R. Seshadri, A. Rastogi, S. V. Bhat, S. Ramasesha, and C. N. R. Rao, Molecular ferromagnetism in C₆₀-TDAE, *Solid State Commun.* **85** (1993) 971–974. [[doi](#)]
 11. C. N. R. Rao, R. Seshadri, A. Govindaraj, J. P. Mittal, H. Pal, and T. Mukherjee, Electronic absorption and emission spectroscopic investigations of the interaction of the fullerenes, C₆₀ and C₇₀, with amines and aromatic molecules, *J. Mol. Struct.* **300** (1993) 289–301. [[doi](#)]
 10. A. K. Santra, R. Seshadri, V. Vijayakrishnan, and C. N. R. Rao, Interaction of solid films of C₆₀ and C₇₀ with nickel, *Solid State Commun.* **85** (1993) 77–79. [[doi](#)]
 9. N. Chandrabhas, K. Jayaram, D. V. S. Muthu, A. K. Sood, R. Seshadri, and C. N. R. Rao, Orientational phase transitions in C₇₀: A Raman spectroscopic study, *Phys. Rev. B* **47** (1993) 10963–10966. [[doi](#)]
 8. V. Vijayakrishnan, A. K. Santra, R. Seshadri, R. Nagarajan, T. Pradeep, and C. N. R. Rao, A comparative-study of the interaction of nickel clusters with Buckminsterfullerene, C₆₀, and graphite, *Surface Sci. Lett.* **262** (1992) L87-L90. [[doi](#)]
 7. V. Vijayakrishnan, A. K. Santra, T. Pradeep, R. Seshadri, R. Nagarajan, and C. N. R. Rao, Interaction of nitrogen and oxygen with C₆₀, *Chem. Commun.* (1992) 198–199. [[doi](#)]
 6. C. N. R. Rao, T. Pradeep, R. Seshadri, R. Nagarajan, V. N. Murthy, G. N. Subbanna, F. D'Souza, V. Krishnan, G. A. Nagannagowda, N. R. Suryaprakash, C. L. Khetrpal, and S. V. Bhat, Preparation, characterization and properties of C₆₀ and C₇₀ – Spectroscopy, structure, anions, interaction with electron-donors and superconductivity, *Indian J. Chem. Sec A* **31** (1992) F5-F16.

5. R. Seshadri, A. Govindaraj, R. Nagarajan, and C. N. R. Rao, Addition of amines and halogens to fullerenes C₆₀ and C₇₀, *Tetrahedron Lett.* **33** (1992) 2069–2070. [doi]
4. D. K. Palit, H. N. Ghosh, A. V. Sapre, J. P. Mittal, R. Seshadri, and C. N. R. Rao, Dynamics of charge-transfer in the excited amine complex of the fullerenes C₆₀ and C₇₀: A picosecond laser flash-photolysis study, *Chem. Phys. Lett.* **198** (1992) 113–117. [doi]
3. R. Seshadri, V. Manivannan, K. P. Rajeev, J. Gopalakrishnan, and C. N. R. Rao, Superconductivity in Ba_{1-y}Sr_yBi_{1-x}Pb_xO₃, *J. Solid State Chem.* **89** (1991) 389–391. [doi]
2. G. U. Kulkarni, V. Vijayakrishnan, G. Ranga Rao, R. Seshadri, and C. N. R. Rao, State of bismuth in Ba_{0.6}K_{0.4}BiO₃ and BaPb_{0.75}Bi_{0.25}O₃: Bi 4f Photoemission and Bi L₃ absorption spectroscopic studies, *Appl. Phys. Lett.* **57** (1990) 1823–1824. [doi]
1. P. Somasundaram, R. Vijayaraghavan, R. Nagarajan, R. Seshadri, A. M. Umarji, and C. N. R. Rao, Occurrence of maximum T_C at an optimal carrier concentration in superconducting bismuth and thallium cuprates, *Appl. Phys. Lett.* **56** (1990) 487–489. [doi]

Not peer-reviewed:

4. E. S. Sciaky, L. A. Lenaburg, R. Seshadri, and D. K. Pak, Interdisciplinary research center programs positively impact graduate and postdoctoral training, *MRS Bulletin* **49** (2024) 1300–1304 (2024). [DOI: 10.1557/s43577-024-00800-y]
3. Book Review: The Visual Elements – Photography: A Handbook for Communicating Science and Engineering by Felice C. Frankel, *Am. J. Phys.* **92** (2024) 479–480. [DOI: 10.1119/5.0216761]
2. N. A. Spaldin and R. Seshadri, History of ferroelectrics – a crystallography perspective, *IUCr Newsletter* **29** (2021), Feature. [IUCr Newsletter Link]
1. T. A. Strom, G. Haugstad, J. Shu, and R. Seshadri, Shared instrumentation facilities: Benefiting researchers and universities, sustaining research excellence, *MRS Bulletin* **45** (2020) 331–335. [DOI: 10.1557/mrs.2020.130]

Awarded US Patents:

9. C. J. Cozzan, S. P. DenBaars, and R. Seshadri, Ce:YAG/Al₂O₃ composites for laser-excited solid-state white lighting, United State Patent 0,264,100 (August 29, 2019).
8. K. A. Denault, S. P. DenBaars, and R. Seshadri, Laser-driven white lighting system for high-brightness applications, United State Patent 9,927,076 (March 27, 2018).
7. C. J. Cozzan, S. P. DenBaars, and R. Seshadri, Monolithic translucent BaMgAl₁₀O₁₇:Eu²⁺ phosphors for laser-driven solid state lighting, International Publication Number WO 2018/049050 A1 (March 15, 2018).
6. K. A. Denault, S. P. DenBaars, and R. Seshadri, Laser-driven white lighting system for high-brightness applications, United State Patent 9,574,728 (February 21, 2017).
5. H. Wang, R. Seshadri, M. Chabiny, A. Lehner, C. Liman, Complex pnictide metal halides for optoelectronic applications, US 0,155,974 (June 2, 2016).
4. R. Seshadri, A. Birkel, B. Hong, and J. A. Gerbec, Single phase and full-color phosphor, United State Patent 9,228,125 B2 (January 5, 2016).
3. W.-B. Im, R. Seshadri, and S. P. DenBaars, Solid solution phosphors based on oxyfluoride and white light emitting diodes including the phosphors for solid state white lighting applications, United State Patent 8,535,565 (September 17, 2013).
2. W.-B. Im, R. Seshadri, and S. P. DenBaars, Oxyfluoride phosphors and white light emitting diodes including the oxyfluoride phosphor for solid-state lighting applications, United State Patent 8,344,611 B2 (January 1, 2013).
1. W.-B. Im, R. Seshadri, and S. P. DenBaars, Yellow emitting phosphors based on Ce³⁺-doped aluminate and via solid solution for solid-state lighting applications, United States Patent 8,163,203 (April 24, 2012).