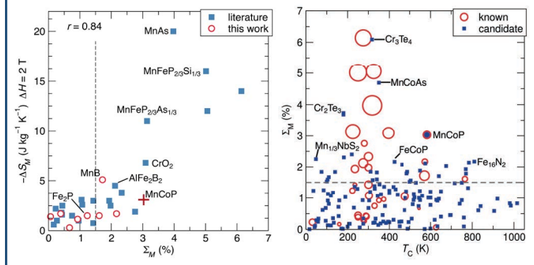
http://www.mrl.ucsb.edu/~seshadri
Ram Seshadri Group
Materials Department,
Department of Chemistry and Biochemistry, and
Materials Research Laboratory
University of California, Santa Barbara CA 93106

"we do many things; none of them very well"

Developing a Simple Computational Proxy for Screening Magnetocaloric Materials

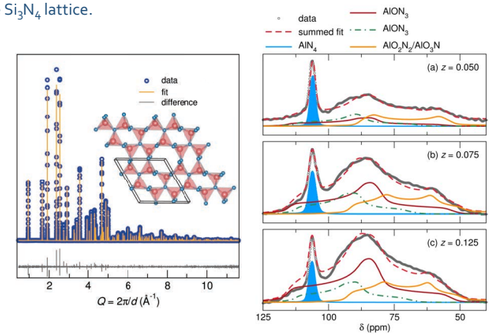
It is widely believed that magnetocaloric refrigeration may prove competitive with vapor-compression technologies, with the advantage that no fluorocarbons are needed. We have developed a simple DFT-based scheme to screen magnetic materials for their magnetocaloric figure of merit.



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.

Using NMR Studies to Understand O/N ordering in SiAlON Phosphor Host Materials

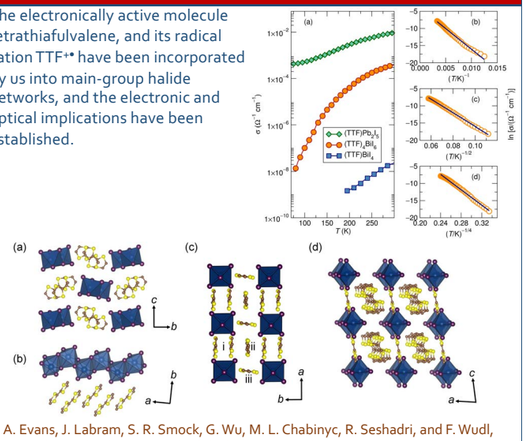
Eu-doped SiAlON phases are effective phosphors for solid-state white lighting applications. We have employed ^{27}Al ssNMR techiques to establish the propensity for O to cluster around the dilute Al impurities in the Si_3N_4 lattice.



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) 2153–2158.

Hybrid Halide Compounds with Electroactive Organic Cations

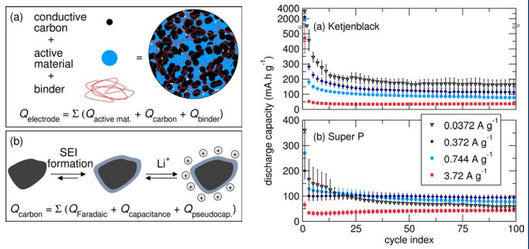
The electronically active molecule tetrathiafulvalene, and its radical cation $TTF^{+\bullet}$ have been incorporated by us into main-group halide networks, and the electronic and optical implications have been established.



H. A. Evans, J. Labram, S. R. Smock, G. Wu, M. L. Chabinyc, R. Seshadri, and F. Wudl, Mono and mixed-valence tetrathiafulvalene semiconductors (TTF)BiI_4 and (TTF)$_4Bi_6$ with 1D and oD bismuth- iodide networks, *Inorg. Chem.* **56** (2017) 395–401.

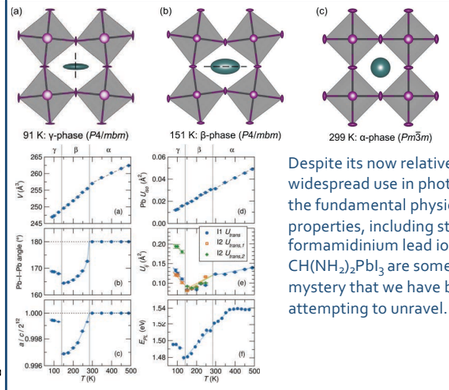
Testing and Understanding Battery Materials Measured at Low Potentials

When conversion materials are tested as anodes (low-voltage electrodes) in lithium batteries, it is standard practice to add conducting carbons to the electrode composite. However, the literature frequently ignores the rather significant capacitive and other contributions that these carbons can make to the estimated charge-storage capacity.



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.

Structural Intricacies and Structure–Property Correlations in the Hybrid Halide Perovskites

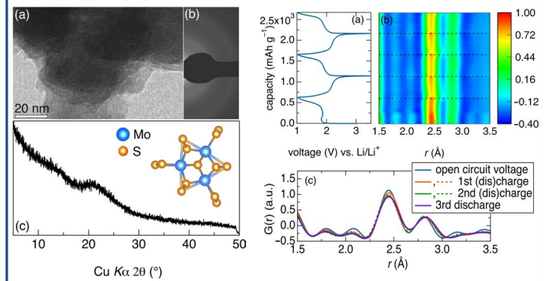


Despite its now relatively widespread use in photovoltaics, the fundamental physical properties, including structure, of formamidinium lead iodide $CH(NH_2)_2PbI_3$ are something of a mystery that we have been attempting to unravel.

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.

Amorphous Metal Chalcogel Strategies for Li–Battery Conversion Electrodes

Conversion reaction cells based on crystalline electrode materials frequently result in electrode amorphization upon cycling. By employing amorphous metal chalcogels as electrodes we eliminate these issues of (further) amorphization. In this system, we also establish that all of the redox is anion-based.



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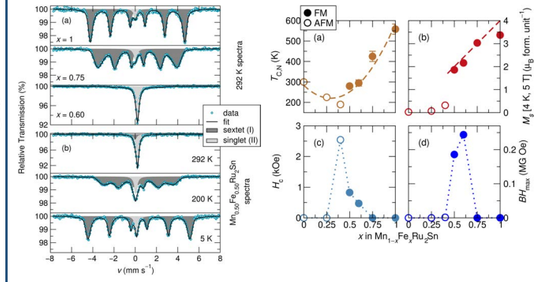
Magnetic Interactions and Magnetic Hardening in Heusler Solid Solutions

The Heusler compound $MnRu_2Sn$ is an antiferromagnet (AF), while $MnFe_2Sn$ is a ferromagnet (FM). Complete, homogeneous, solid-solutions are formed between these two compounds that to our surprise, display behavior attributable to the presence of AF/FM interfaces.



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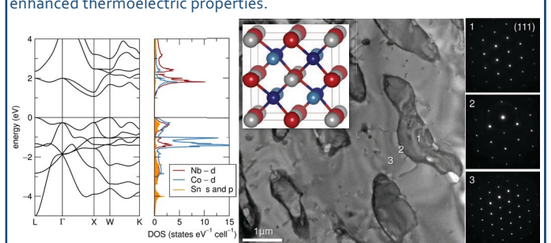
Heusler Thermoelectrics with Spontaneously Formed Coherent Precipitates

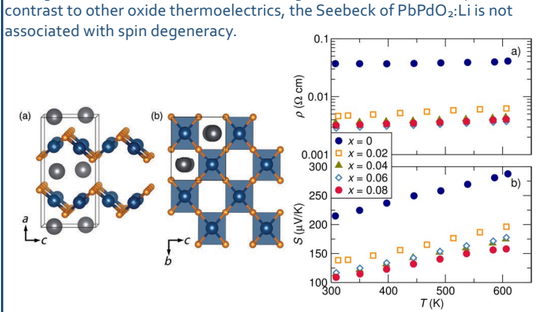
18-electron half-Heulser compounds such as NbCoSn can be effective semiconductors and thermoelectric materials, but suffer from relatively large lattice thermal conductivities. We find that adding excess Co in the preparation of these materials leads to spontaneously formed precipitates of the full Heusler phase, $NbCo_2Sn$, that act as scattering sites for phonons. The results are reduced thermal conductivity, and enhanced thermoelectric properties.



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).

A Hole-Doped Complex Palladium Oxide Thermoelectric

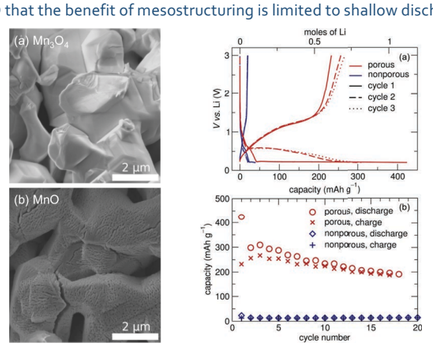
$PbPdO_2$ is a layered palladium oxide that is readily hole doped by substitution of Li for Pd, into a metallic state. Interestingly, we have established $PbPdO_2$:Li as a rare example of an oxide thermoelectric that has significant Seebeck coefficient and high electrical conductivity. In contrast to other oxide thermoelectrics, the Seebeck of $PbPdO_2$:Li is not associated with spin degeneracy.



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.

Mesostructuring and Morphology Retention/Destruction in MnO Conversion

Mesostructuring of electrodes is frequently proposed as a means of enhancing the kinetics associated with conversion reaction electrodes. We have demonstrated in the case of spontaneously mesostructured MnO that the benefit of mesostructuring is limited to shallow discharge.



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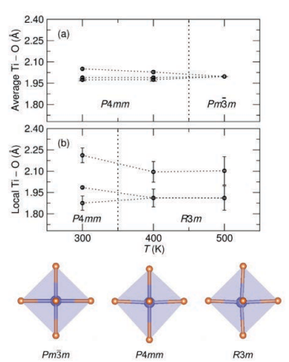
Local Structure Studies of Some Pb–free Lone-Pair-Driven Ferroelectrics

The lone-pair on the Pb^{2+} ion is an important driver in the polar properties of Pb^{2+}–based materials, and makes lead so difficult to replace in polar materials.

Perovskite titanates can be prepared with small amounts of Sn^{2+} substituted on the *A*–site. Our local structure studies from analysis of neutron total scattering suggest that despite low substitution rates, the perovskites are very sensitive to lone-pair induced distortions.



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