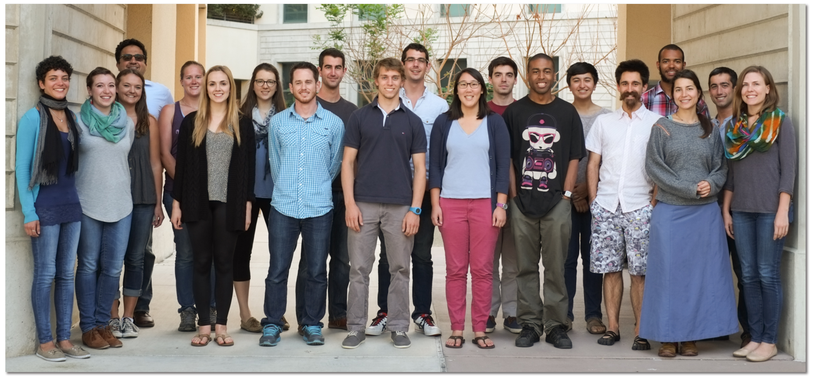
Ram Seshadri Group: Functional Inorganic Materials – Recent Products [April 2015]

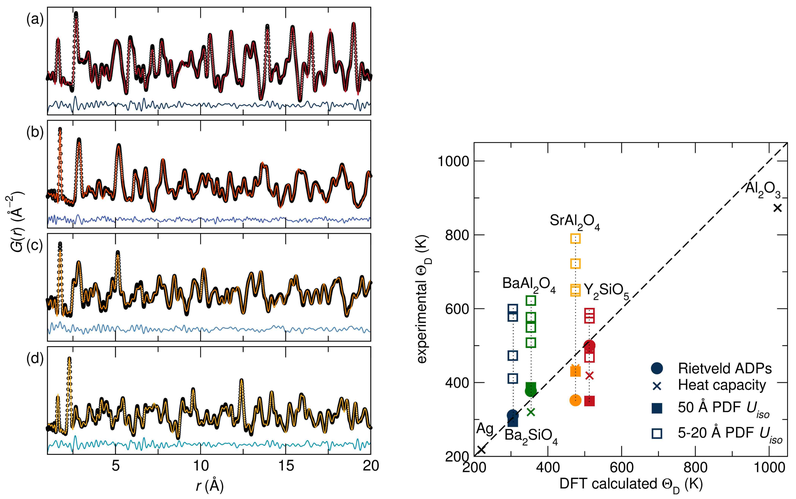
Materials Department, Department of Chemistry and Biochemistry, Materials Research Laboratory, Mitsubishi Chemical Center for Advanced Materials

The group, April 2015



L–R: Claudia Göbel (visiting from LMU, Munich), Dr. Geneva Laurita-Planckis, *Margaret Lumley*, Ram, Mandi Buffon (Materials, NSF Fellow), *Sara Smock*, *Claire-Alice Hébert*, *Michael Knight*, Douglas Fabini (Materials, UCSB Chancellors Fellow), Clayton Cozzan (Materials, NSF Fellow), Hayden Evans (DCB), Jaye Harada (Junior Specialist), Jonathon Bechtel (Materials, joint with Van der Ven), Jason Douglas (Materials, NSF Fellow, joint with Pollock), *Christina Garcia*, Michael Gaultois (DCB, FullBright/NSERC Fellow), Demetrious Lloyd, Dr. Anna Lehner, Leo Lamontagne (Materials), and Megan Butala (Materials). [DCB = Department of Chemistry and Biochemistry. *Undergraduates in italics*]

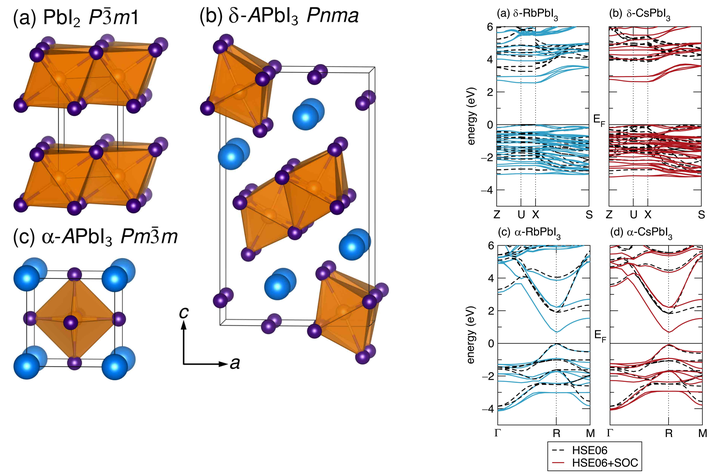
Phosphors for solid–state lighting: The structural origins of efficiency



Neutron pair distribution function analysis of some oxide host compounds (left panel), analyzed as a function of *r*-range permits the nature of correlated motion in the structure, and the structural rigidity as indicated by the proxy of the Debye temperature, to be examined, compared with DFT calculations and heat-capacity measurements (right panel), and correlated with the efficiency (quantum yield) of the phosphors obtained upon appropriate doping of the host.

Denault, Brgoch, Kloß, Gaultois, Siewenie, Page, Seshadri, Average and local structure, Debye temperature, and structural rigidity in some oxide phosphor host compounds, *ACS Appl. Mater. Interfaces.* (2015)

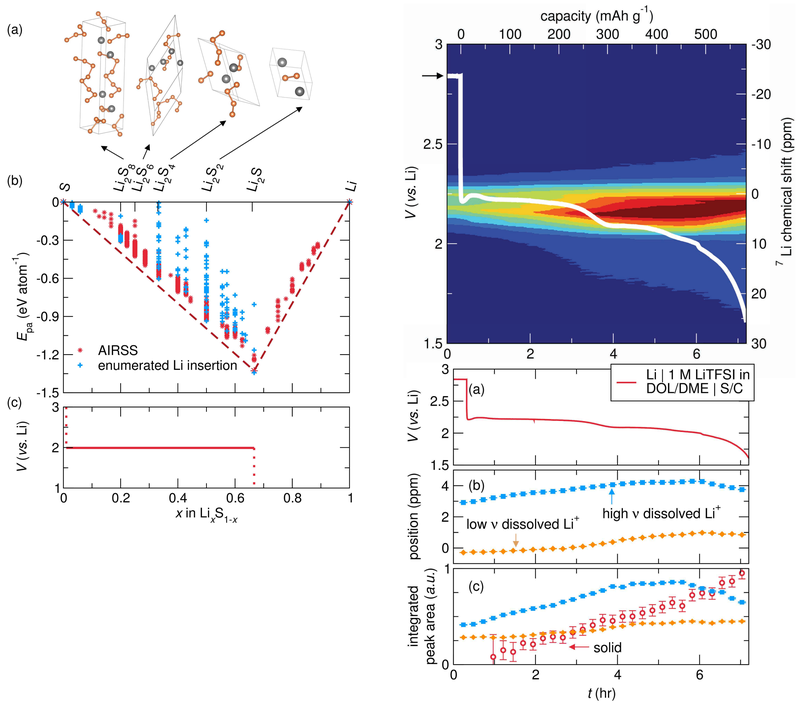
Fundamental science of halide perovskites and related materials



In collaboration with the Chabinyc and Wudl groups, we are examining new materials, fundamental science, device performance, and theory of main group halide compounds related to perovskites. In the example above, DFT calculations on some lead-based compounds point to the level of theory required to describe the electronic energy levels, including absolute energetics such as ionization energies, with reasonable accuracy. Also seen is the evolution of electronic structure with dimensionality.

Brgoch, Lehner, Chabinyc, 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 (2015) 27721–27727.

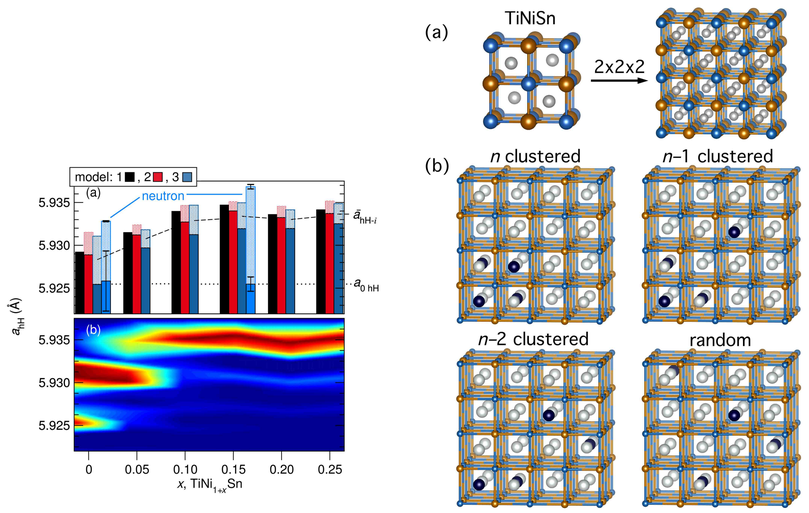
Li–S batteries



A combined experimental and DFT study (collaboration with the Van der Ven group) of the Li–S cell, including through the use of in-situ ^{7}Li NMR (collaboration with the Grey group at Cambridge) has suggested that there are no intermediate compositions between Li and Li$_2$S.

See, Leskes, Griffin, Britto, Matthews, Emly, Van der Ven, Wright, Morris, Grey, Seshadri, Ab initio structure search and in situ ^{7}Li NMR studies of discharge products in the Li–S battery system, *J. Am. Chem. Soc.* 136 (2014) 16368–16377.

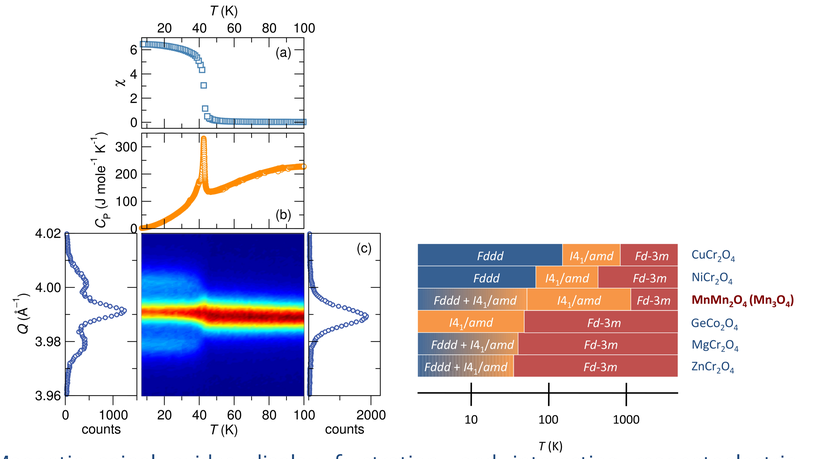
Intermetallic thermoelectrics



In collaboration with the Pollock group, we have been studying robust, high-performing, and inexpensive thermoelectric materials based on the Ti–Ni–Sn system. Here synchrotron X-ray and neutron scattering are employed in conjunction with DFT calculations on supercells to determine the possible structure of solid-solution intermediates between TiNiSn and TiNi$_2$Sn.

Douglas, Chater, Brown, Pollock, Seshadri, Nanoscale structural heterogeneity in Ni-rich half-Heusler TiNiSn, *J. Appl. Phys.* 116 (2014) 163514(1–7).

Magnetostructural phase transitions in spinels



Magnetic spinel oxides display frustration, and interesting magnetoelectric behavior. We have employed high-resolution synchrotron X-ray data, acquired at the 11BM beam-line at APS to study symmetry-lowering transitions that accompany magnetic ordering. The panel on the left displays such studies on Mn_3O_4. On the right are the complete list of compounds studied by us.

Kemei, Harada, Seshadri, Suchomel, Structural change and phase coexistence upon magnetic ordering in the magnetodielectric spinel Mn_3O_4, *Phys. Rev. B* 90 (2014) 064418(1–8).

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