Ram Seshadri Group: Functional Materials for Energy Conversion and Storage [3/2018]

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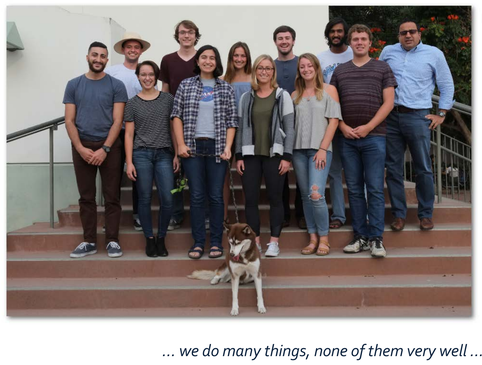
The group (photos from October 1017) + Dr. Joya Cooley

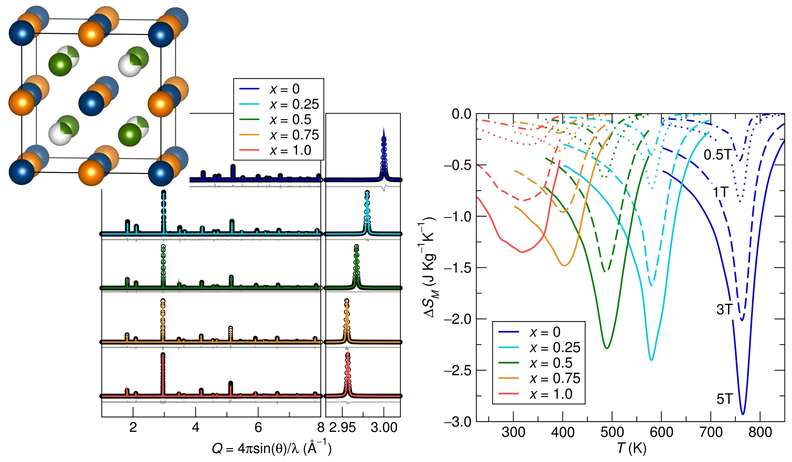
Human and canine graduate students + postdoctoral fellow Dr. Jason Grebenkemper



Undergraduate interns

... we do many things, none of them very well ...

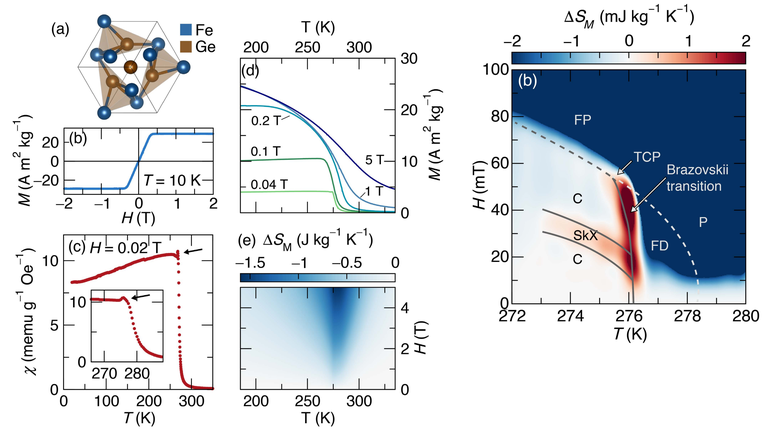
Magnetocaloric materials: Heusler/half-Heusler solid solutions



The half-Heusler magnet MnNiSb is able to form a complete solid solution with the half-Heusler $MnNi_2Sb$. The compounds are temperature-tunable magnetocalorics with applications ranging from refrigeration to waste-heat recovery.

Levin, Bocarsly, Wyckoff, *Pollock*, *Seshadri*, *Phys. Rev. Mater.* 1 (2017) 075003(1–8)

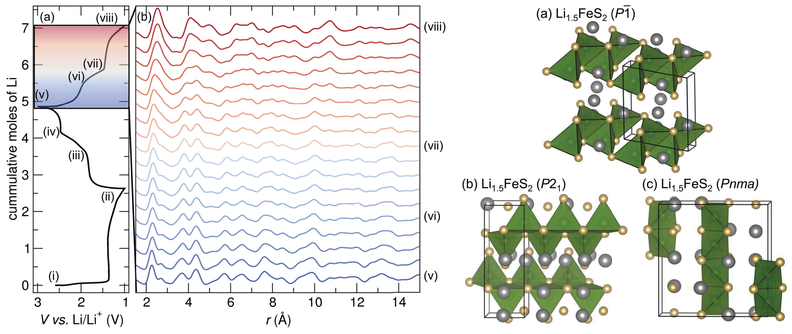
Mapping complex spin textures in topological magnets (skyrmions)



Careful magnetization measurements allow the magnetic phase diagram of the prototypical skyrmion host crystal FeGe to be mapped out, through the transformation to a magnetic entropy map, shown on the right.

Bocarsly, Need, *Seshadri*, *Wilson*, arXiv:1802.09115

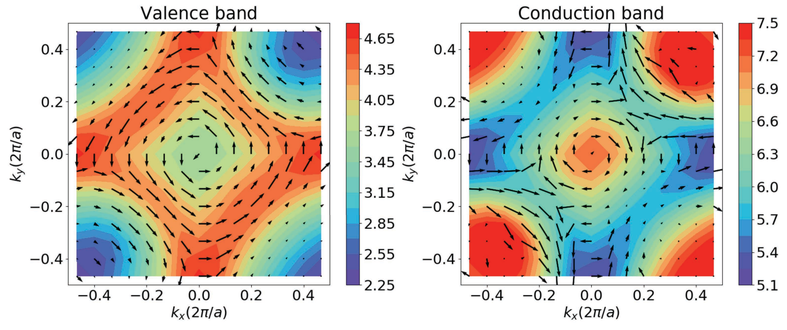
Conversion battery electrodes: The case of FeS_2



In a conversion (as opposed to intercalation) battery electrode, the crystalline structure of the electrode material is completely transformed in the process of charging and discharging. I*n operando* synchrotron X-ray pair distribution studies of electrode cycling, judiciously coupled with density functional theory calculations of intermediate structure stability helps unravel the details of what happens when pyrite FeS_2 is cycled.

Butala, Mayo, Doan-Nguyen, Lumley, Göbel, Wiaderek, Borkiewicz, Chapman, Chupas, Balasubramanian, Laurita, Britto, *Morris*, *Grey*, *Seshadri*, *Chem. Mater.* 29 (2017) 3070–3082.

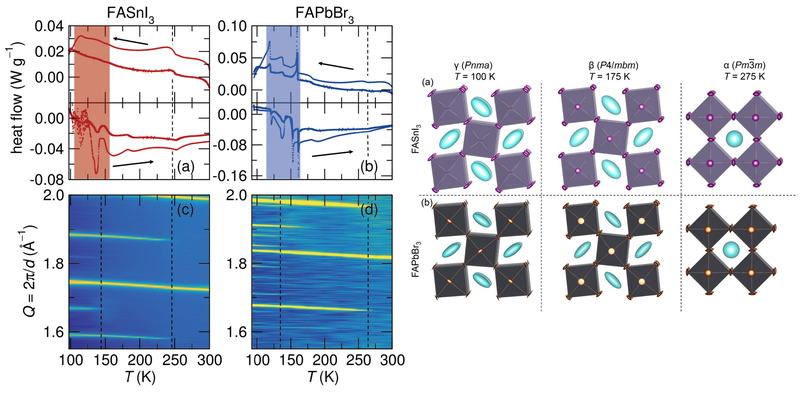
Topological materials: The nexus with energy materials



Valence band and conduction bands of a slightly distorted (111 off-centered Sn) rock-salt SnTe, showing the distinct spin texture in this topologically non-trivial material. We are interested in the question of whether such spin texturing can impact the use of these materials in energy conversion, *ie*. as thermoelectrics and photovoltaics.

Teicher, *Mukherjee*, *Seshadri* (unpublished)

Fundamentals of structure-property relations in halide perovskites



Hybrid halide perovskites display complex structural changes as a function of temperature as a consequence of octahedral titling, in conjunction with the dynamics of the organic cation on the *A*–site. We employ a combination of calorimetry, capacitance measurements, and high-resolution synchrotron X-ray scattering studies to unravel the details of these structural changes.

Schueller, Laurita, Fabini, Stoumpos, *Kanatzidis*, *Seshadri*, *Inorg. Chem.* 57 (2018) 695–701.

Support:

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