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The group, April 2015

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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.

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.

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 TLMR (collaboration with the Grey group at Cambridge) has suggested that there are no intermediate compositions between Li and LiS

Intermetallic thermoelectrics

In collaboration with the Pollock group, we have been studying robust, high-performing, and inexpensive thermoelectric materials based on the Tl–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 TlNiSn and TlNiSn.

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 12BM beam-line at APS to study symmetry-lowering transitions that accompany magnetic ordering. The panel on the left displays such studies on MnO. On the right are the complete list of compounds studied by us.

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