Hybrid Halide Compounds with Electroactive Organic Cations

This recent innovation in organic-inorganic hybrid materials 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.

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

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

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

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

Amorphous Metal Chalcogenide Strategies for Li–Battery Conversion Electrodes

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

Heuser Thermoelectric with Spontaneously Formed Coherent Precipitates

The discovery of an NISnO can be effective semiconductors and thermoelectric materials, but suffer from relatively large thermal conductivity. We find that adding excess Co to the formation of these materials, leads to spontaneously formed precipitates of the full Heuser phase, NbCoSn, that act as scattering centers for phonons. The results are reduced thermal conductivity, and enhanced thermoelectric properties.

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 latter significant capacitive and other contributions that these carbons can make to the estimated charge-storage capacity.


Developing a Simple Computational Proxy for Screening Magnetocaloric Materials

The development of the magnetic properties of the various samples 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.