Energy Materials: Advances made watching atoms move

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Developing the energy technologies of the future will rely heavily on advances in materials – whether it be safe reliable nuclear reactors, next-gen solar cells, or thermoelectric devices for waste heat recovery. Understanding how to control the flow of energy carried by the motion of atoms in materials (phonons, molecular modes, etc.) is often crucial. In this talk, I will highlight two examples, one on a photovoltaic (solar) material[1], and the other on a thermoelectric material[2]. Hot-carrier solar cells convert sunlight to electricity more efficiently than do conventional solar cells by harnessing charge carriers before they lose energy to heat. A key to keeping electric charges hot longer is blocking the phonons that transport heat away from the charge carriers. We use neutron scattering and other techniques to show that thermal transport can be reduced by swapping out a lighter isotope for a heavier one in the organic molecule of the high-performance photovoltaic material methylammonium lead iodide. The effect on phonons of the heavier isotope[1] delays the cooling of hot-carriers and extending their useful lifetime for energy conversion. For thermoelectric efficiency an ideal is the phonon glass–electron crystal, in which phonons are blocked but electrons are not. This drives research on strategies to scatter or localize phonons while minimally disrupting electrons. Anharmonicity has the potential to do both, even in perfect crystals, and *ab initio* simulations predict that thermoelectric lead selenide is anharmonic enough to support intrinsic localized modes (ILMs) that stop transport. We experimentally observe high-temperature localization using neutron scattering but find that localization is not isolated to ILMs – zero group velocity develops for a significant section of a phonon branch on heating above a transition in the anharmonic dynamics[2]. These examples highlight how observing the motions of atoms can bare new strategies for enhancing the performance of energy materials.

References:

1. M. E. Manley *et al.* Giant isotope effect on phonons and thermal conductivity in methylammonium lead iodide. *Science Adv.* **6**, aaz1842 (2020).
2. M. E. Manley *et al.* Intrinsic anharmonic localization in thermoelectric PbSe. *Nature Commun.* **10**, 1928 (2019).