Seminar announcement

Thursday, March 20, 2025
2:00 pm
WSI, Seminar room S 101
Exclusively in person

"Self-healing in photovoltaic materials: Chemical insights from antimony chalcogenides and chalcohalides"

Contemporary photovoltaic materials research has devoted a significant effort to elucidate what makes halide perovskites unique. In this talk, I will consider possible origins of self-healing—a prominent property commonly ascribed to halide perovskites and considered by some as a part of the reason for their exceptional performance as PV materials. I will describe our efforts to push the boundaries of the current understanding of the self-healing process's chemistry and elucidate potential sources for propelling this property by looking at non-halide perovskites that show (a particular type of) self-healing.

In this talk, I will first describe the results of a study of a solid-state transformation reaction of antimony trichalcogenides to form chalcohalides (and the reverse reaction). This will be the setting for a subsequent description of a vibrational spectroscopy study of the self-healing reaction following intense light irradiation. Using Raman spectroscopy, we identified common intermediate species in the self-healing reaction in antimony trichalcogenides and chalcohalides. Comparing five different materials with a similar space group symmetry enabled us to uncover the common structural feature that leads to self-healing in these materials. We rationalize the chemical reaction and point at bonding states at the bottom of the conduction band as central origins in propelling a 'hidden phase,' which ensues (a particular type of) a self-healing reaction. Finally, we recently examined if this rationale overlaps with a novel chemical bonding concept by examining the homologue series of bismuth-antimony trichalcogenides. We found a reciprocal correlation between the three occurrences: metavalent bonding and bonding states at the bottom of the conduction band and photo-induced phase transition. The prevalence of self-healing semiconductors is restricted to a few selected cases, limiting understanding of the phenomenon. Expanding the variety and number of self-healing materials and uncovering the underlying solid-state reactions will facilitate developing self-healing electronic building blocks for making animate electronic devices.

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