Details in diffusion: Finding and controlling defects in halide perovskite semiconductors

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Semiconductors are a broad class of materials that exhibit a gap between occupied and unoccupied electronic states. This gap is tunable and gives rise to unique optical and electronic properties; as a result, semiconductors form the basis of established technologies including microprocessors, lasers, and solar cells. Crystalline semiconductors are a subset of this broad class of materials with characteristic long-range order, where the electronic structure is well-defined by molecular orbitals within the repeat unit. And while they are often conceptualized as perfect crystals, crystalline semiconductor devices are engineered with imperfections in mind owing to their outsized influence on the bulk material properties. For instance, silicon solar cells are manufactured to simultaneously exclude deleterious electron-scattering dopants (e.g., titanium) and include dopants that allow for a useful internal junction to form (e.g., boron, phosphorous). Here, I highlight the prevalence of defect-forming reactions occurring in the halide perovskites, an emergent class of semiconductors with applications in optoelectronic technologies including solar cells and light-emitting diodes. I present our complementary efforts to quantify, characterize, and mitigate point defect formation and diffusion in halide double perovskites, with a particular emphasis on the role of the halogen vacancy. We found that halogen vacancy defects are involved in a spontaneous external defect equilibrium that influences electronic properties, effectively self-doping the crystal. The connections between point defect structure and electronic doping, as well as bulk stability considerations, will be discussed for the class of technologically relevant halide perovskite semiconductors.