Direct Experimental Evidence for Defect Tolerance in Pb-Halide Perovskites, at last

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For progress in science, distinguishing between ideas or suggestions and solid experimental facts is critical, especially if it concerns a key issue. Such is the case for the widespread use of “defect tolerance” (DT) to explain the exceptionally good properties of halide perovskites (HaPs) for solar cells, LEDs and detectors. Even though DT lacked direct experimental evidence, it became a “fact” in the field. DT in semiconductors implies that structural defects do not translate to electrical and optical effects (e.g., due to charge trapping), associated with such defects. We present the first direct experimental evidence for DT in Pb-HaPs by comparing the structural quality of 2-dimensional (2D), 2D-3D, and 3D Pb-iodide HaP single crystals with their optoelectronic characteristics using high-sensitivity methods. Importantly, we get information from the materials’ bulk, because we sample at least a few hundred nanometers, up to several micrometers, from the sample’s surface, which allows for assessing intrinsic bulk (and not only surface-) properties of HaPs.

This combined approach yields experimental evidence for DT in the 3D, 2D-3D, and 2D HaPs crystals, i.e., the differences in density of structural defects does NOT translate into the corresponding differences in optoelectronically active defects.

In summary, DT in Pb-HaPs suggests that the dynamic Coulumbic screening in intrinsically “soft” and polarizable materials provides a design principle to achieve some co-existence of structural imperfections and close-to-optoelectronic perfection in materials. As such, DT can bridge any time lag between damage and self-healing to minimize effects of imperfections, to make materials more sustainable. In addition, our experimental design can guide the search for, and design of other materials with DT.