

Defects, defect tolerance, and self-healing in lead halide perovskites: a first principles perspective

Leeor Kronik
Department of Molecular Chemistry and Materials Science,
Weizmann Institute of Science,
Rehovoth 76100, Israel

Abstract

Among many riddles posed by halide perovskites, the surprising apparent near-absence of harmful defects stands out. This is usually ascribed to defect tolerance or to self-healing. Here, I will present first-principles studies that attempt to explain selected experimental results from various spectroscopies, in terms of specific chemical and physical scenarios of the underlying chemical behavior.