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Defect physics in halide perovskites, double perovskites and perovskite alternatives¹

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Despite the rapid improvement in record power conversion efficiency (PCE) over the past six years, the commercialization of organic–inorganic Pb halide perovskite solar cells is still facing serious challenges such as cell instability against moisture and temperature and the inclusion of toxic Pb. Recently, non Pb containing halide perovskites, double perovskites and perovskite alternatives have attracted attention. To evaluate the potential of these non Pb-containing halide materials as photovoltaic absorbers, it is necessary to understand and compare the defect properties in both Pb halide and non Pb-containing halide materials. In this talk, we will first review our theoretical understanding of the superior defect tolerance properties, i.e., the dominant defects exhibit shallow levels and do not cause serious nonradiative recombination, in Pb halide perovskites through first-principles density-functional theory calculations. We will elucidate that the superior defect properties are attributed to the combination of strong antibonding coupling between Pb lone-pair *s* orbitals, perovskite symmetry, high ionicity and large lattice constant. We will further discuss the effects of the crystal structures and chemical compositions of double perovskites and perovskite alternatives on the defect properties. We will then show that the defect tolerance properties decrease in double perovskites and perovskite alternatives, suggesting less promising photovoltaic properties.

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