Computational studies of the structural and optical properties of organic-inorganic lead halide perovskites

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Due to their high power conversion efficiency, organic-inorganic lead halide perovskites have emerged as promising materials for next-generation solar cell devices. As the efficiency race continues for this revolutionary class of light-harvesting materials, many questions about the structural, electronic and optical properties of perovskite solar cells have still to be addressed. More particularly, the long-term stability of this kind of devices is an open question because various different crystalline phases exist in a narrow temperature range.[1] Mixed cation lead halide perovskites have attracted wide attention due to the possibility of tackling the problem of limited phase stability. Through a theoretical analysis of the phase stability of binary formamidinium (FA)-rich, cesium-rich FA/Cs and guanidinium (GUA)/FA mixtures as well as ternary Cs/GUA/FA mixtures, we propose a series of design principles for the synthesis of stable mixed cation lead halide perovskites that could be potential candidates for solar cell applications.[2]

In addition to this, an understanding of the correlations between different photo-physical properties and the atomistic characteristics of these materials is paving the way for the design of lead halide perovskites with enhanced optical properties.[3] For this reason, the anomalous low-temperature behavior of the photoluminescence spectra of cesium lead bromide is rationalized in terms of the structural characteristics of the material at low temperatures.

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