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Tunable photostriction of halide perovskites through energy dependent photoexcitation

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Halide perovskites exhibit giant photostriction, that is, volume or shape changes upon illumination. However, the microscopic origin of this phenomenon remains unclear and there are experimental reports of both light-induced lattice expansion and contraction. Using a combination of molecular orbital theory and first principles methods, we find that different valence states have different bonding characters, leading to opposing strengthening or weakening of bonds depending on the photoexcitation energy. The overall trend is that light induces lattice contraction at low excitation energies, while giant lattice expansion occurs at high excitation energies, rationalizing experimental reports. More generally, the proposed microscopic mechanism is universal for all halide perovskites because their electronic band structures share the same orbital characters.

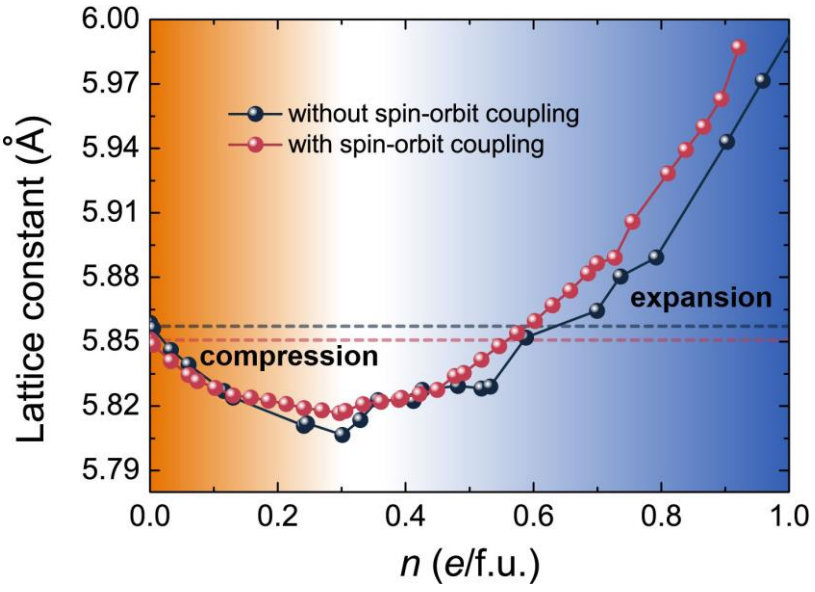

Figure 1 : Photostriction of $CsPbBr_3$ with and without spin-orbit coupling as a function of photoexcited carrier density.