MS18-P15 | THERMOCHROMIC LEAD-FREE HALIDE DOUBLE PEROVSKITES

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Lead-free halide double perovskites with diverse electronic structures andoptical responses, as well as superior material stability show great promise for a range of optoelectronic applications. However, their large bandgaps limit their applications in the visible light range such as solar cells. In this work, an efficient temperature-derived bandgap modulation, that is, an exotic fully reversible thermochromism in both single crystals and thin films of Cs2Ag-BiBr6 double perovskites is demonstrated. Along with the thermochromism, temperature-dependent changes in the bond lengths of Ag–Br ($R_{Ag–Br}$) and Bi–$Br_{(RBi–Br)}$ are observed. The first-principle molecular dynamics simulations reveal substantial anharmonic fluctuations of the $R_{Ag–Br}$ and $R_{Bi–Br}$ at high temperatures. The synergy of anharmonic fluctuations and associated electron–phonon coupling, and the peculiar spin–orbit coupling effect, is responsible for the thermochromism. In addition, the intrinsic bandgap of $Cs_2AgBiBr_6$ shows negligible changes after repeated heating/cooling cycles under ambient conditions, indicating excellent thermal and environmental stability. This work demonstrates a stable thermochromic lead-free double perovskite that has great potential in the applications of smart windows and temperature sensors. Moreover, the findings on the structure modulationinduced bandgap narrowing of $Cs_2AgBiBr_6$ provide new insights for the further development of optoelectronic devices based on the lead-free halide double perovskites.