Optical, Electronic, and Magnetic Engineering of «111» Layered Halide

Perovskites

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© 2018 American Chemical Society. Antimony and bismuth «111» layered perovskites have recently attracted significant attention as possible, nontoxic alternatives to lead halide perovskites. Unlike lead halide perovskites, however, «111» halide perovskites have shown limited ability to tune their optical and electronic properties. Herein, we report on the metal alloying of manganese and copper into the family of materials with formula Cs4Mn1-xCuxSb2Cl12 (x = 0-1). By changing the concentration of manganese and copper, we show the ability to modulate the bandgap of this family of compounds over the span of 2 electron volts, from 3.0 to 1.0 eV. Furthermore, we show that in doing so, we can also adjust other relevant properties such as their magnetic behavior and their electronic structure.