SUPPLEMENTARY INFORMATION

First-principles comparative study of perfect and defective CsPbX₃ (X=Br, I) crystals

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Heat capacity and discrepancy between samples

While performing several experimental runs for the heat capacities, we observed discrepancy between samples. Considering CsPbl₃, these discrepancies take the form of a different behavior at T< 2 K. As shown in Fig. S1, there is a remarkable hump at very low temperatures for sample Sl2, and the continuous decrease below indicates a significantly reduced Debye temperature Θ_D (T \rightarrow 0) and deviations from a T³ Debye-type power law.



Figure S1. Experimental heat capacity C_p of (a) CsPbI₃ and (b) CsPbBr₃ divided by T^3 .

Instead, sample SI1 shows a normal saturation behavior in the quantity C_p/T^3 indicating a Debye temperature of approximately 110 K (see main text, Fig. 3). The strong deviation from the Debye behavior observed for SI2 is likely due to impurities or to the presence of structural defects. Considering instead CsPbBr₃ (Fig. S1b), here 2 different samples present quite different magnitude of the heat capacity at T around 8 K. We believe that the reason for this discrepancy is the presence of 2 phases corresponding to CsPbBr₃, one tetragonal and one monoclinic. We therefore advise to perform such experiments on multiple samples and being aware of the potential pitfalls stemming from the samples themselves.