Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information – Computational Prediction of Structural, Electronic, Optical Properties and Phase Stability of Double Perovskites K_2SnX_6 (X = I, Br, Cl)

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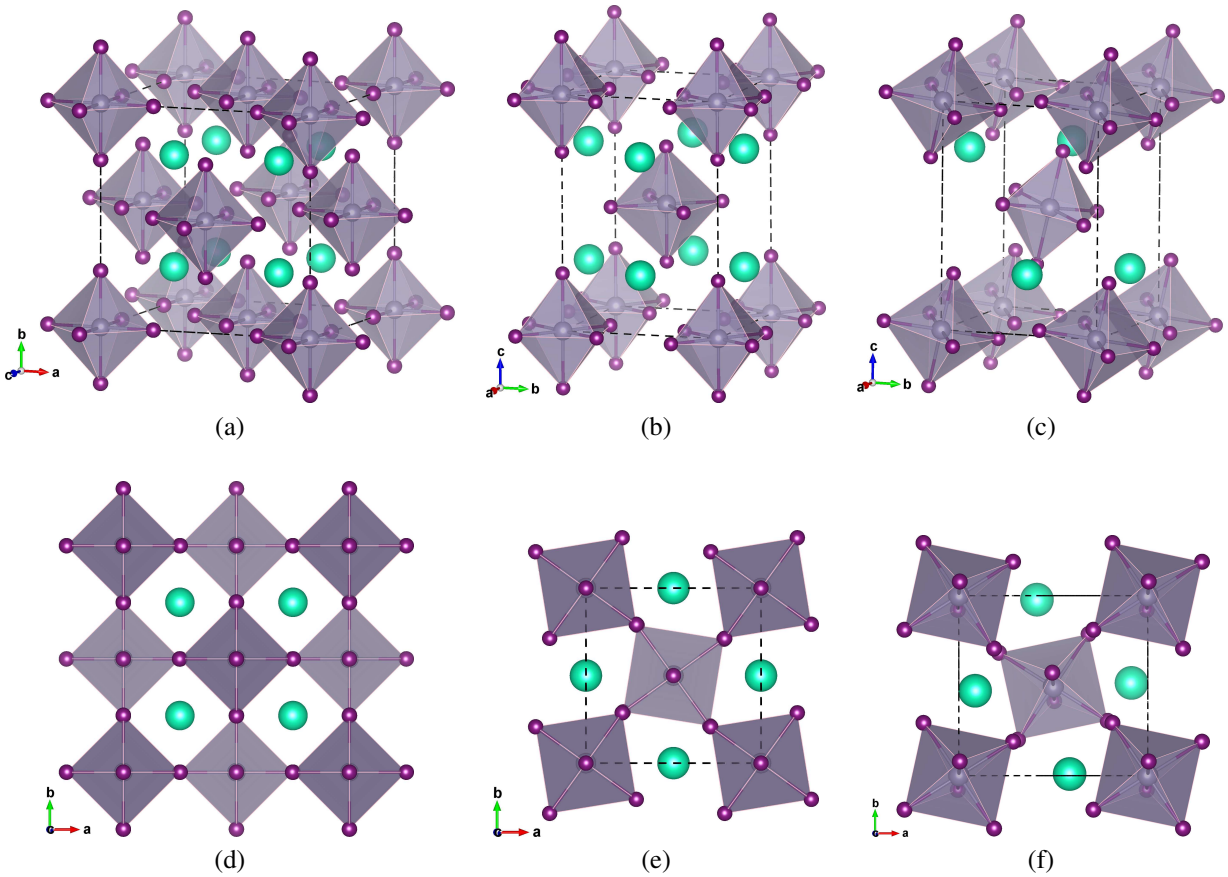

Figure S1. Polyhedral view of optimized crystal structures of (a), (d) cubic, (b), (e) tetragonal, and (c), (f) monoclinic K_2SnX_6 in perspective (top panel) and $x-y$ plane (lower panel) . Grey, purple and green balls represent Sn, X and K atoms, respectively.

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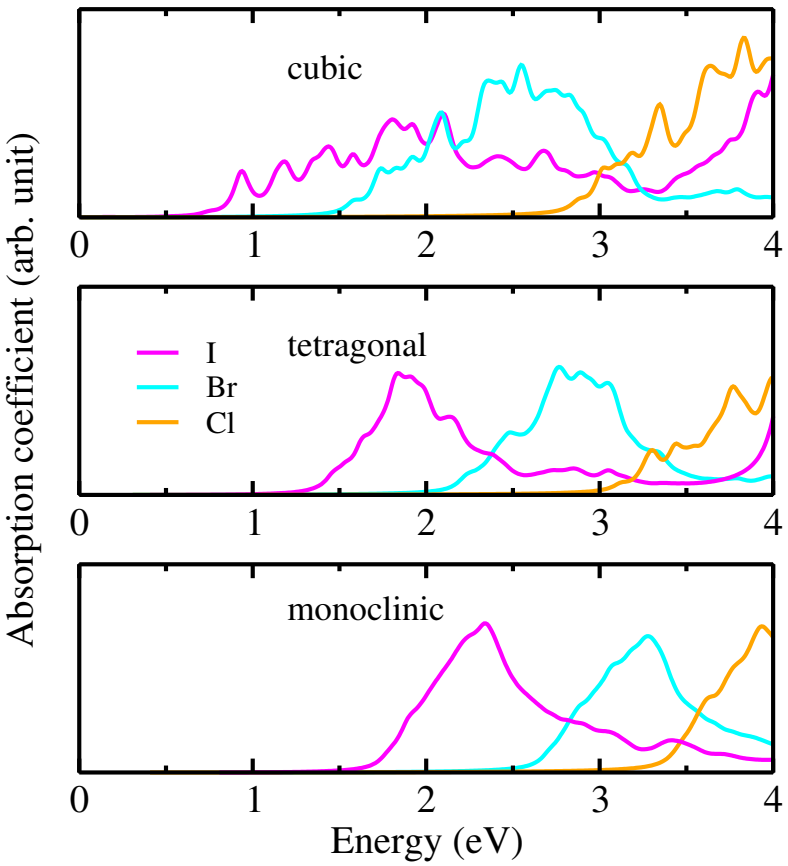

Figure S2. Light-absorption coefficients calculated within the density functional perturbation theory for the cubic, tetragonal, and monoclinic phases of K_2SnX_6 (X = I, Br, Cl).

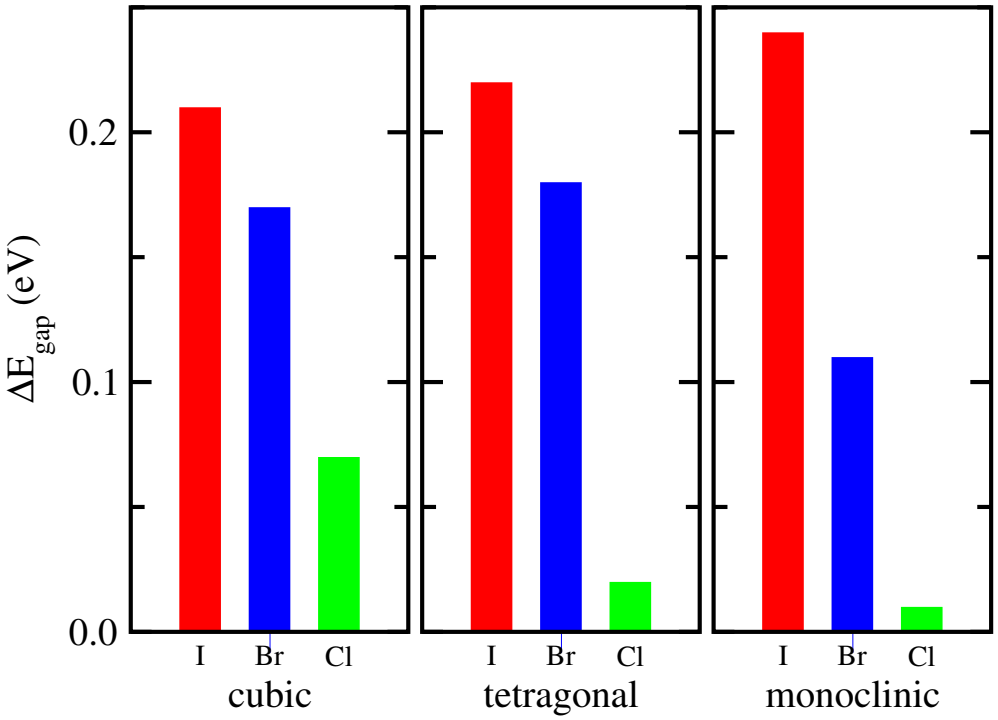

Figure S3. Band gap differences between HSE and HSE+SOC calculations for the cubic, tetragonal, and monoclinic phases of K_2SnX_6 (X = I, Br, Cl).