

Supplementary Information

**2D CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> hybrid halide perovskite structural  
and compositional properties a DFT study**

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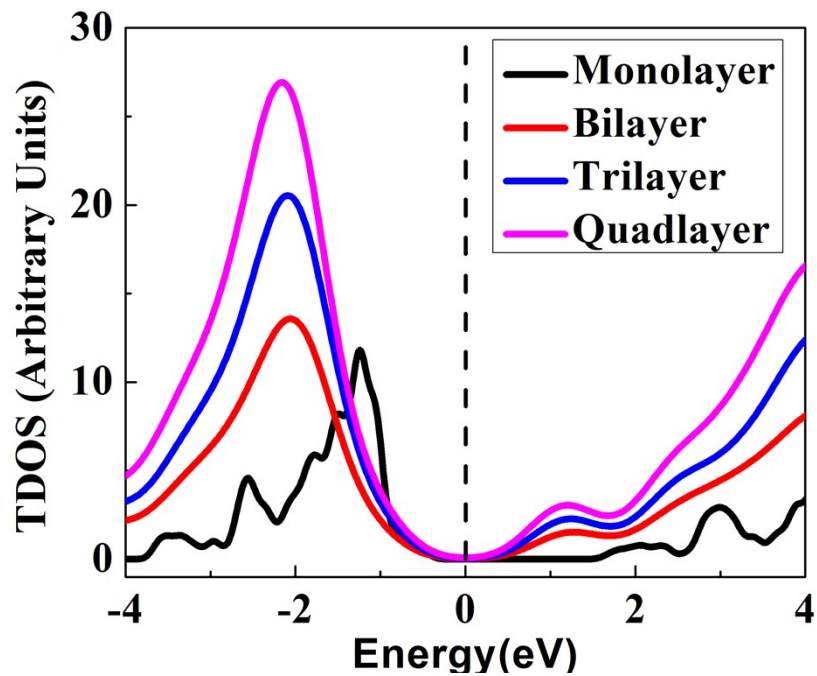


Figure S1: Calculated total density of states (TDOS) for mono, bi, tri, and quad layers of 2D  $\text{CH}_3\text{NH}_3\text{PbI}_3$ .

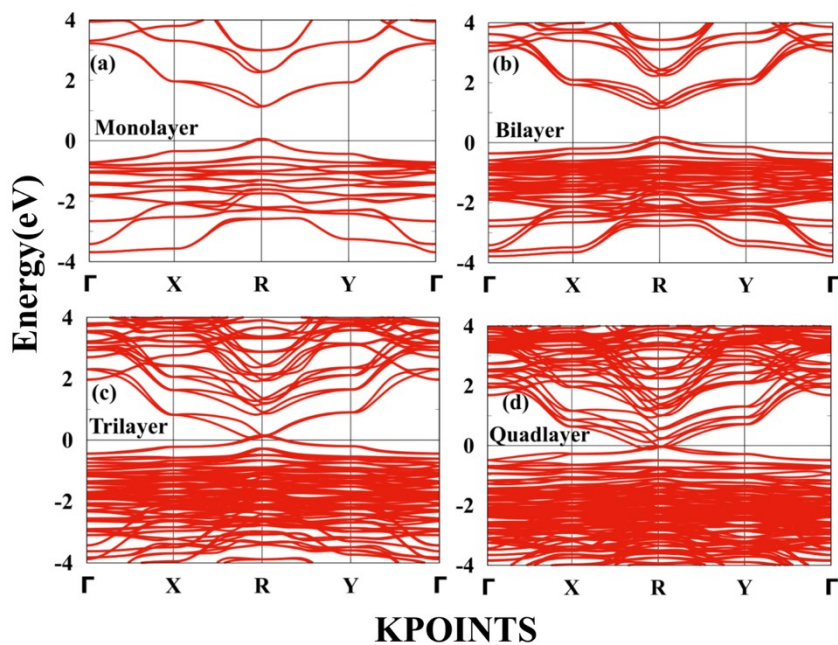


Figure S2. Calculated SOC band structure of (a) monolayer, (b) bilayer, (c) trilayer, and (d) quad-layer  $\text{CH}_3\text{NH}_3\text{PbI}_3$ .

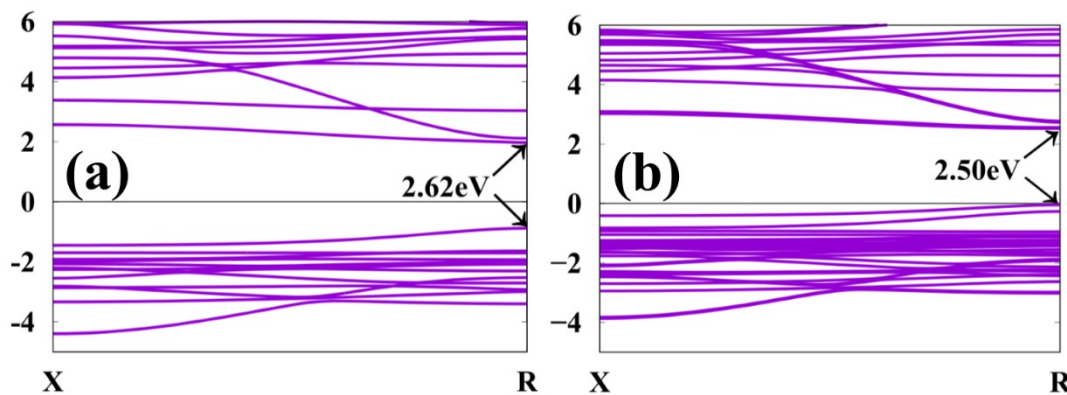


Figure S3. Calculated HSE band structure of (a) monolayer, (b) bilayer  $\text{CH}_3\text{NH}_3\text{PbI}_3$ .

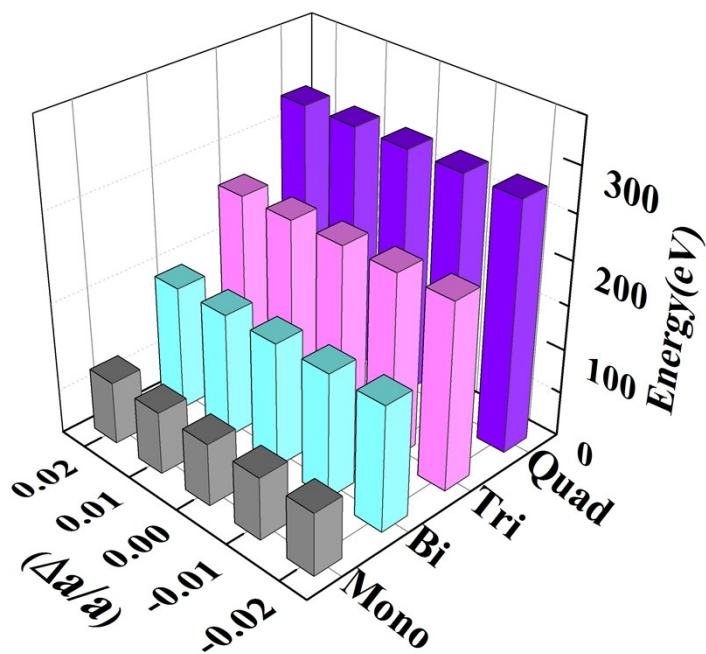


Figure S4. The variation of formation energy with applied tensile and compressive strain.

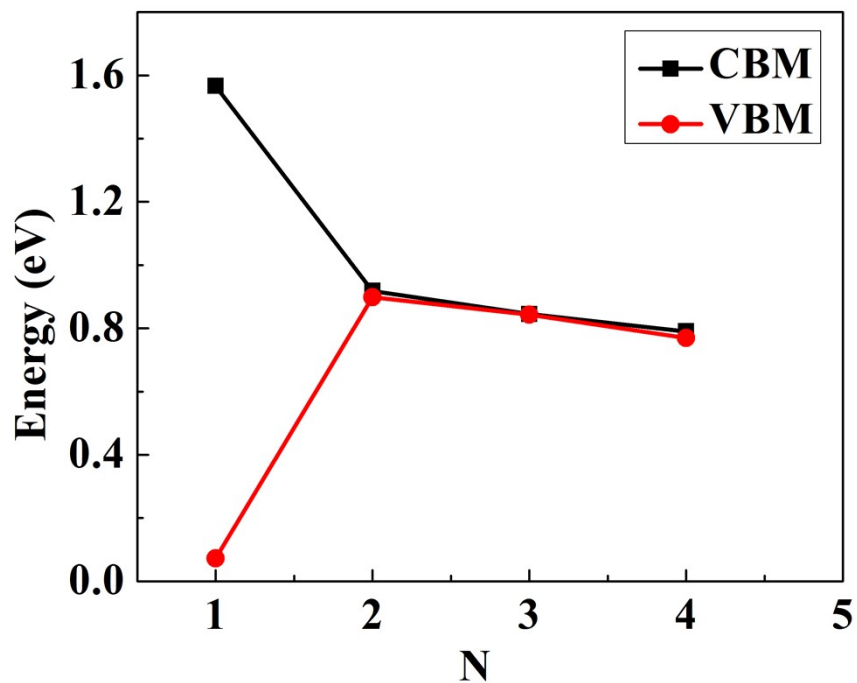


Figure S5. The variation in conduction band minimum (CBM) valence band maximum (VBM) Vs number of layers (N) of  $\text{CH}_3\text{NH}_3\text{PbI}_3$ .

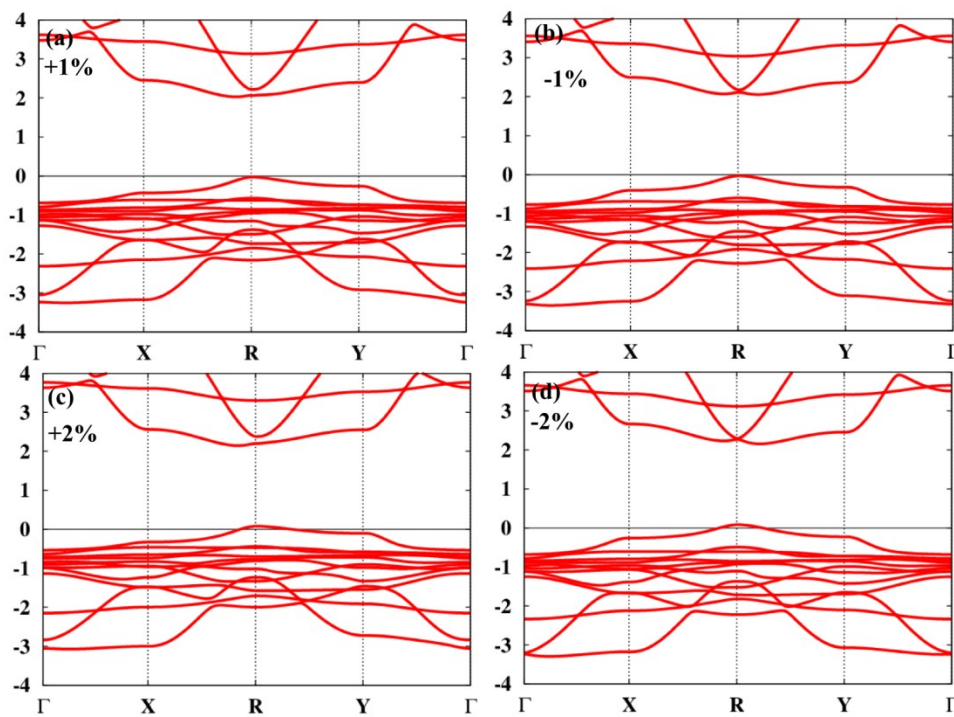
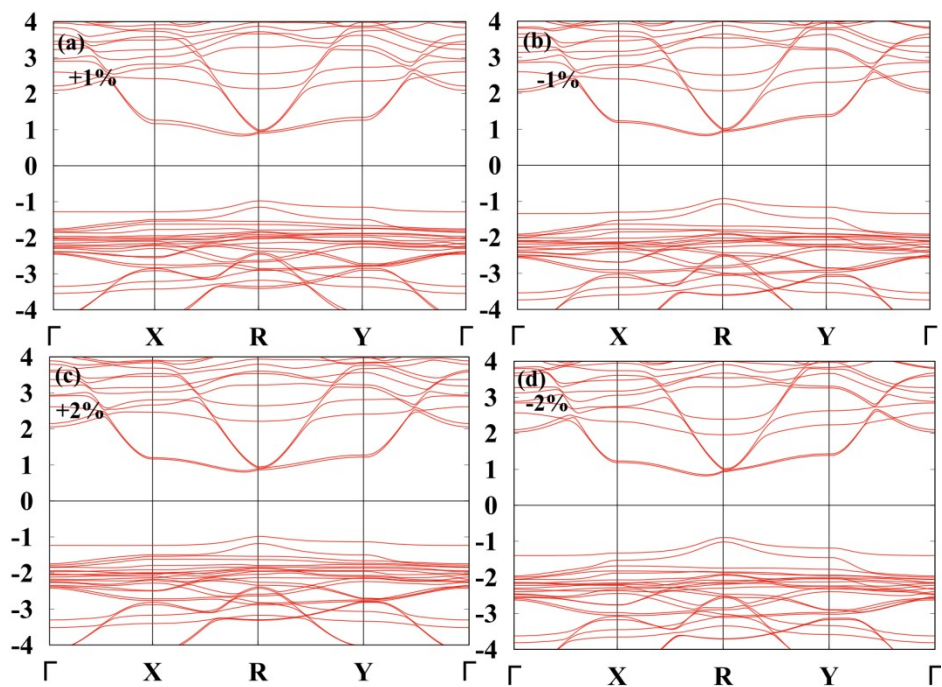
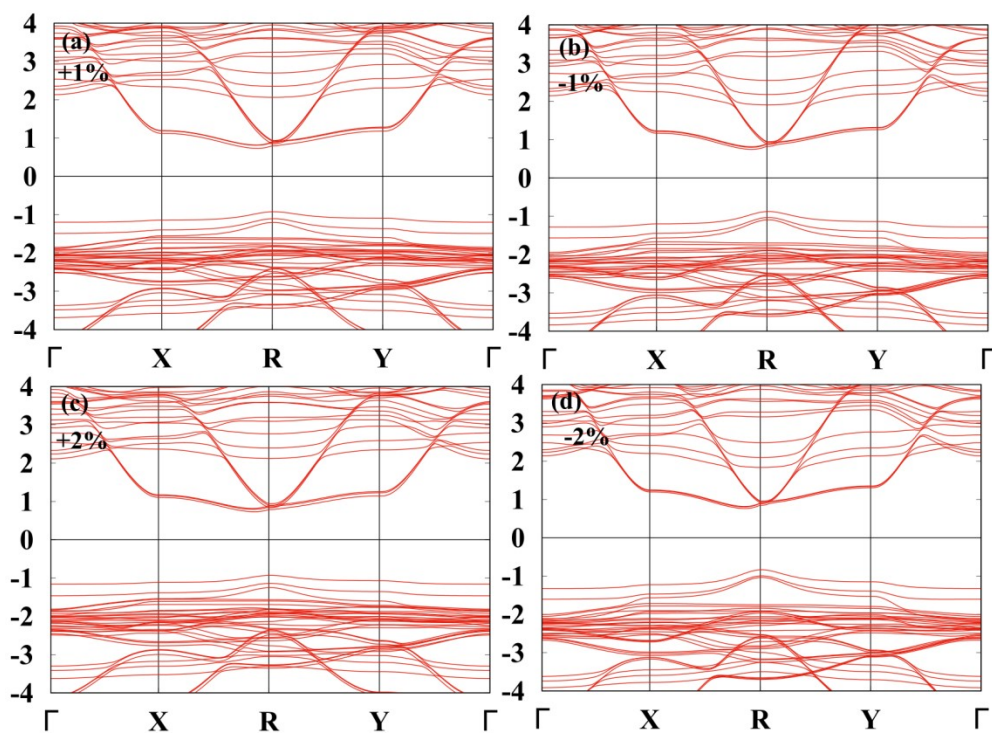


Figure S6. The variation in band gap under the tensile and compressive strain of monolayer of  $\text{CH}_3\text{NH}_3\text{PbI}_3$ .



**Figure S7.** The variation in band gap under the tensile and compressive strain of bilayer of  $\text{CH}_3\text{NH}_3\text{PbI}_3$ .



**Figure S8.** The variation in band gap under the tensile and compressive strain of trilayer of  $\text{CH}_3\text{NH}_3\text{PbI}_3$ .

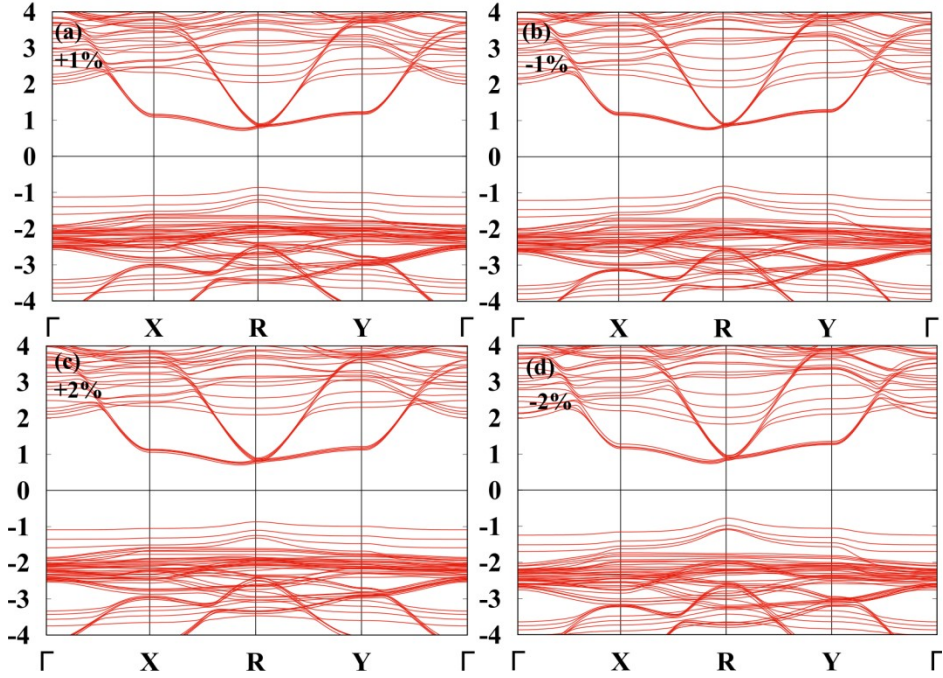


Figure S9. The variation in band gap under the tensile and compressive strain of quad-layer of  $\text{CH}_3\text{NH}_3\text{PbI}_3$ .

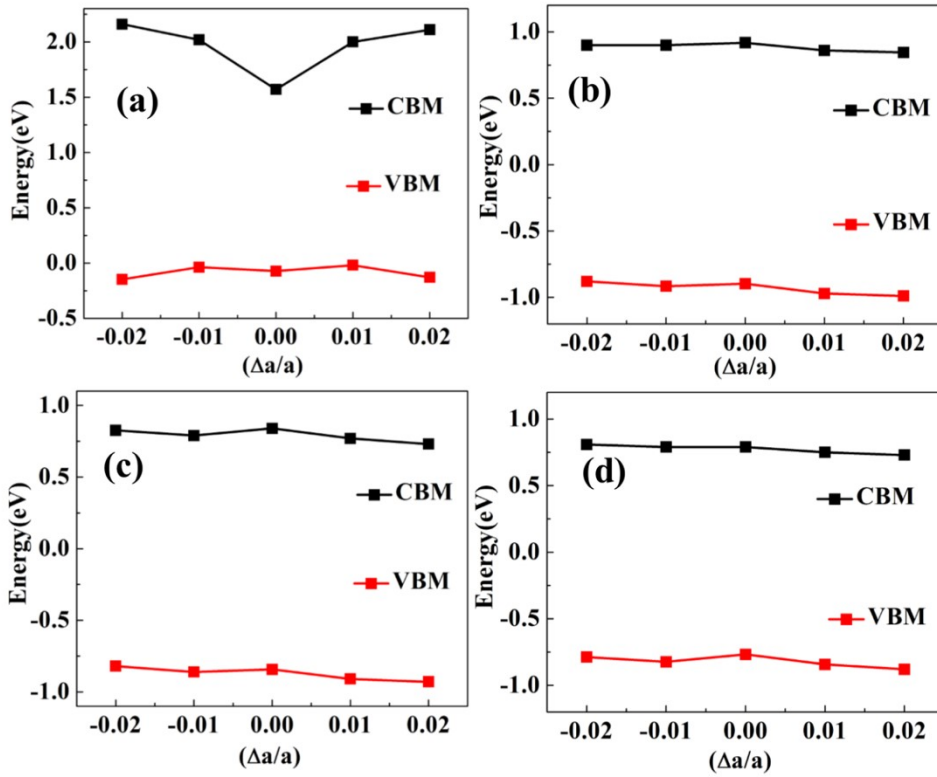


Figure S10. The variation in band gap under the tensile and compressive strain of (a) monolayer (b) bilayer (c) trilayer and (d) quad-layer of  $\text{CH}_3\text{NH}_3\text{PbI}_3$ .

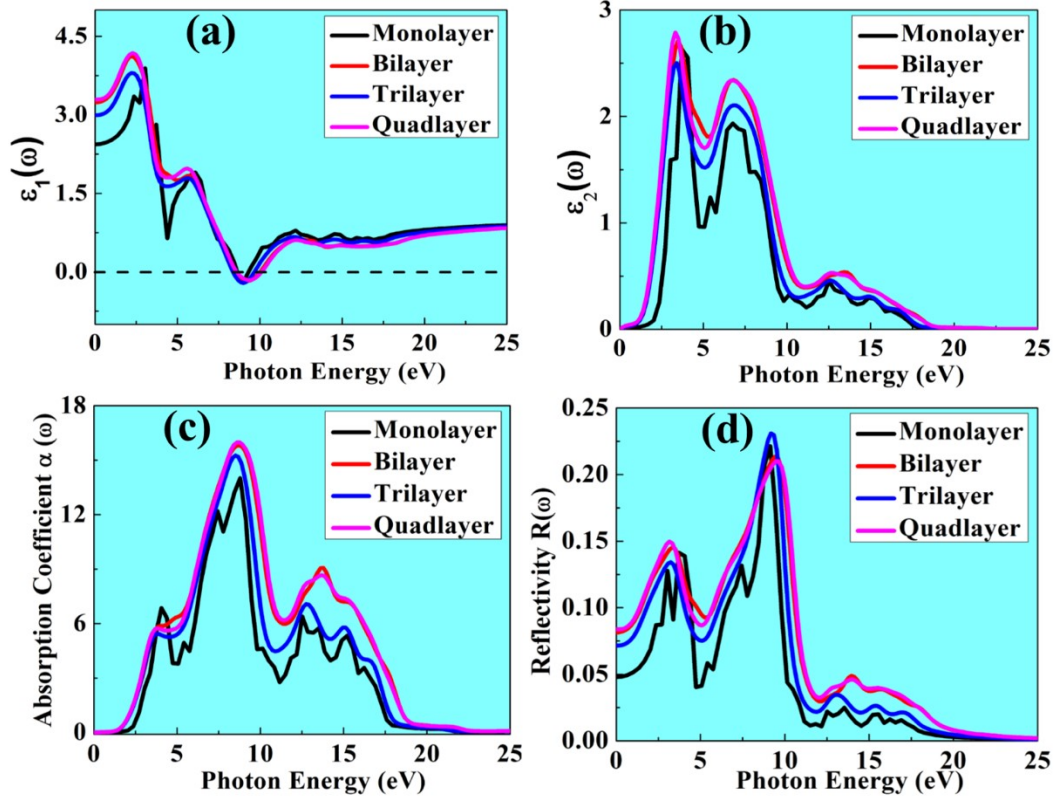


Figure S11. Optical properties of 2D multilayer  $\text{CH}_3\text{NH}_3\text{PbI}_3$  perovskites with (a) real, (b) imaginary dielectric functions, (c) absorption coefficient and (d) reflectivity.