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Supplementary information for "Pressure effects on the structures and electronic properties of halide perovskite $CsPbX_3$ (X=I, Br, Cl)"

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As indicated in the manuscripte, we carried out the phonon calculation for predicting the stability of pressure-induced structures. Here, we use a supercell approach as implemented in the PHONOPY code.[1] Figs. S1-S3 show the phonon-dispersion curves for different pressure-induced phases of $CsPbX_3$(X=I, Br, Cl).

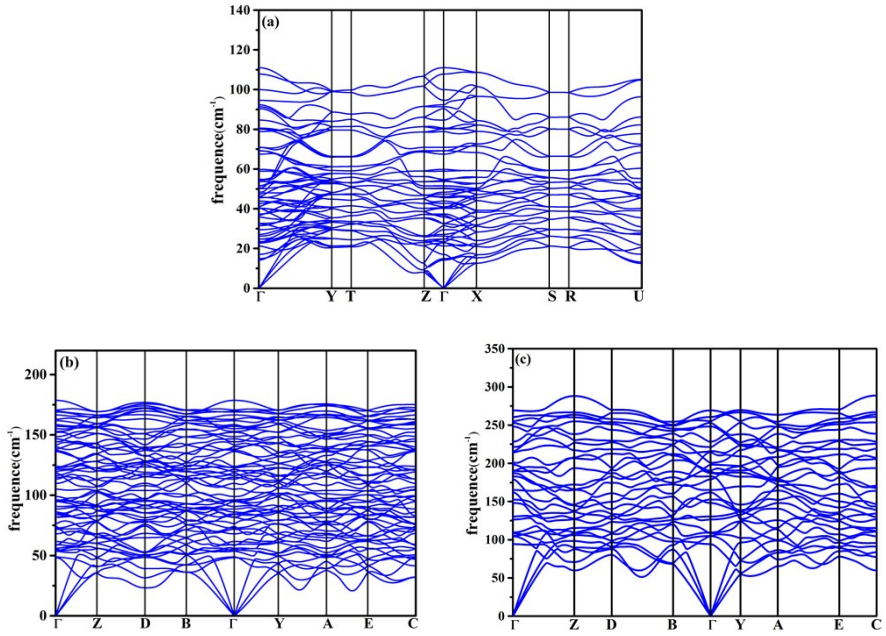

Fig. S1. Calculated phonon-dispersion curves for (a) non-Pv-*Pnma* (0 GPa), (b) *C2/m* I (20 GPa), (c) *C2/m* II (70GPa) phases of $CsPbI_3$

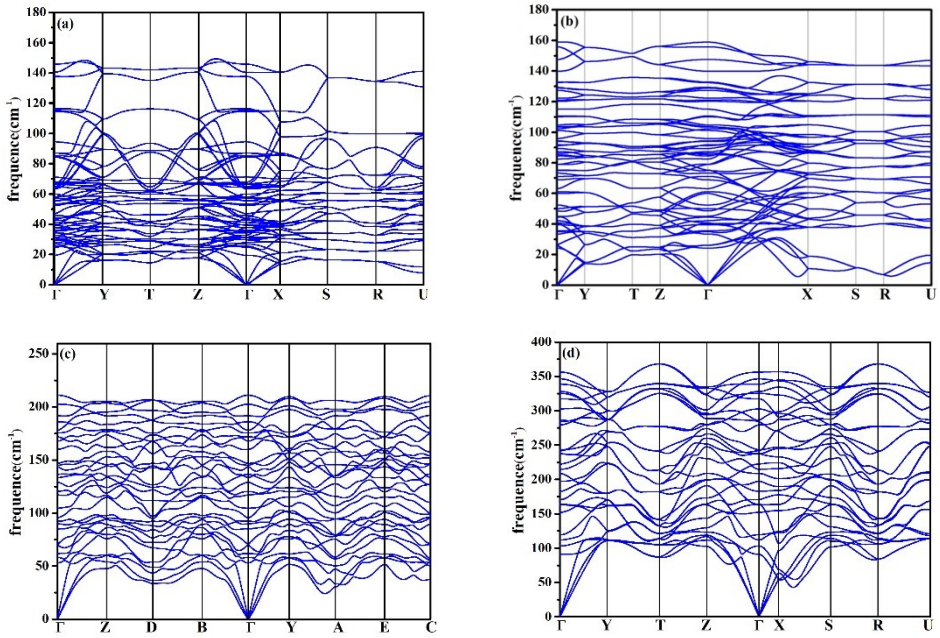

Fig. S2. Calculated phonon-dispersion curves for (a) Pv-*Pnma* (0 GPa), (b) non-Pv-*Pnma* (5 GPa), (c) *C2/m* I (20 GPa) , (d) *Cmcm* (70 GPa) phases of $CsPbBr_3$

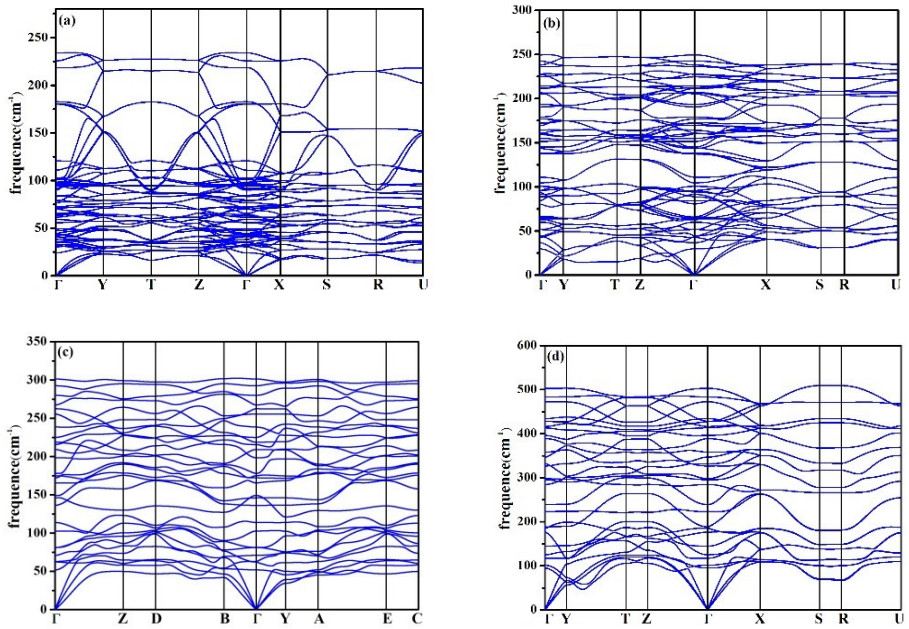

Fig. S3. Calculated phonon-dispersion curves for (a) Pv-*Pnma* (0 GPa), (b) non-Pv-*Pnma* (5 GPa), (c) *C2/m* I (20 GPa) , (d) *Cmcm* (70 GPa) phases of $CsPbCl_3$

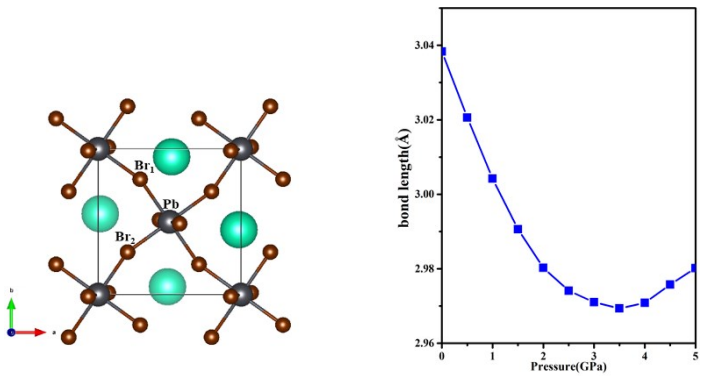

Fig. S4. The structure of $CsPbI_3$ Pv-*Pnma* phase (Right panel) and average of in-plane Br-Pb (Br_1-Pb and Br_2-Pb) bonds length (left panel).

1. A. Togo, F. Oba and I. Tanaka, *Phys. Rev. B*, 2008, **78**, 134106.