Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for

Emergence of Topological Nodal Loops in Alkaline-Earth Hexaborides XB_6 (X=Ca, Sr, Ba) under Pressure

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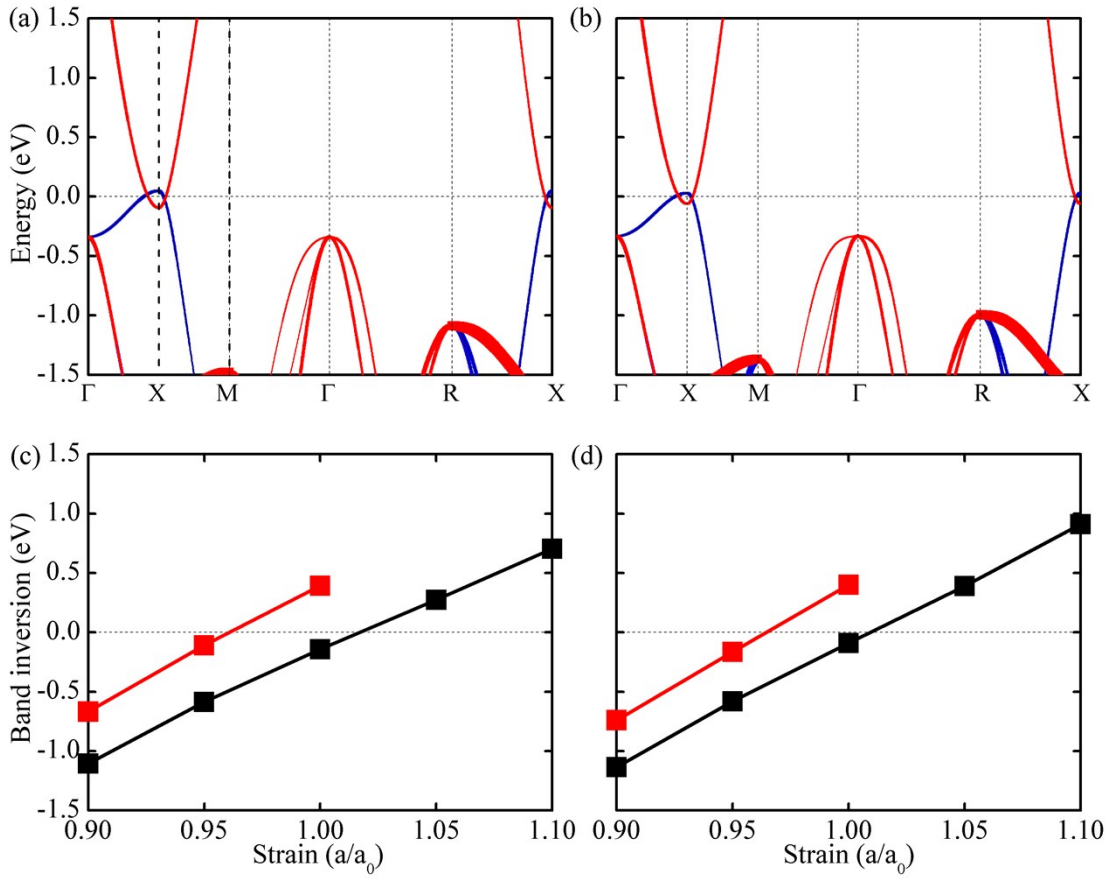

FIG. S1. (Color online) Projected band structures of (a) CaB_6 and (b) SrB_6 from GGA-PBE without SOC. The blue and red color show B p_x (p_z) and p_y orbitals, respectively. Evolution of the band inversion between the bonding and anti-bonding bands at X point of (c) CaB_6 and (d) SrB_6. Negative values indicate the existence of band inversion. Black: GGA-PBE. Red: HSE06.

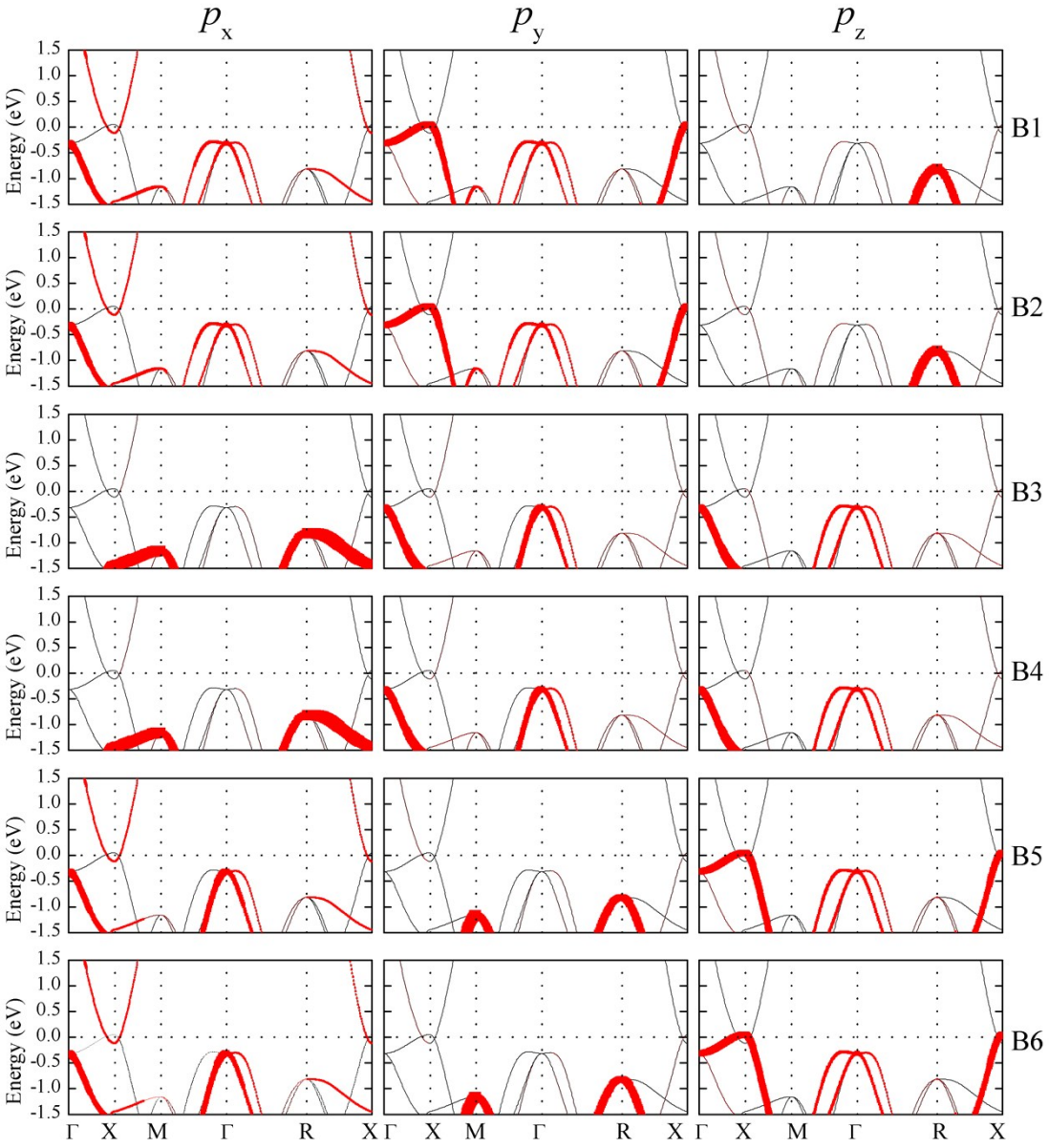

FIG. S2. (Color online) Projected band structures of B *p* orbitals.

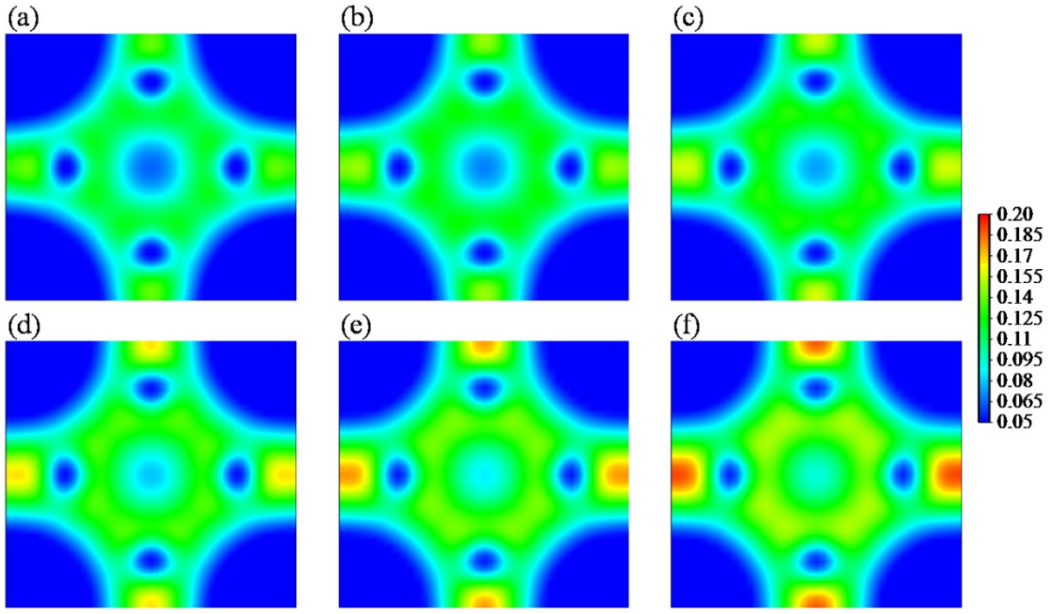

FIG. S3. (Color online) Charge density contours of the (001) plane formed by B3-B6 atoms as shown in Fig. 1a: (a) unstrained; (b)-(f) strained systems at a strain of 0.98, 0.96, 0.94, 0.92, and 0.90, respectively.

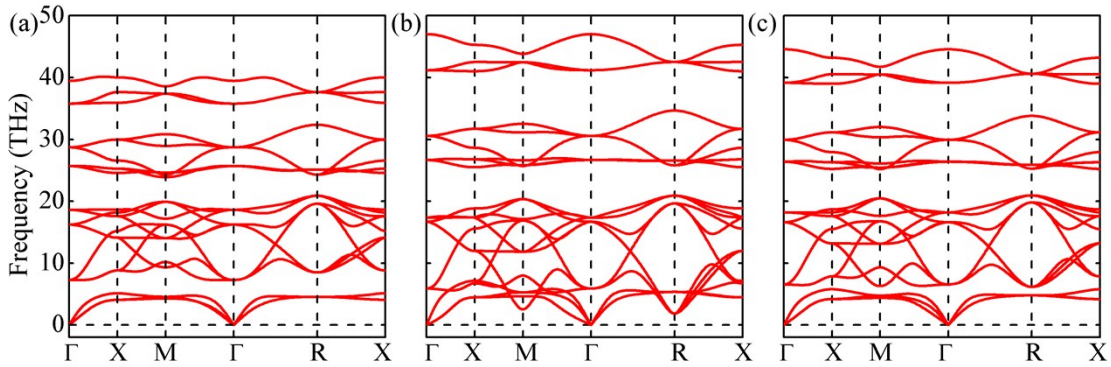

FIG. S4. (Color online) Phonon band dispersions of (a) BaB_6, (b) CaB_6, and (c) SrB_6 at the strain of 0.95.