Supplementary Information for

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

L.-Y. Gan,$^{1,2}$ R. Wang,$^{1,3}$ Y. J. Jin,$^1$ D. B. Ling,$^4$ J. Z. Zhao,$^1$ W. P. Xu,$^1$ J. F. Liu,$^{1,*}$ and H. Xu$^{1,*}$

$^1$Department of Physics, South University of Science and Technology of China, Shenzhen 518055, China

$^2$Key Laboratory of Advanced Technology of Materials (Ministry of Education), Superconductivity and New Energy R&D Center, Southwest Jiaotong University, Chengdu, 610031 Sichuan, China

$^3$Institute for Structure and Function & Department of Physics, Chongqing University, 400030 Chongqing, China

$^4$Department of Physics, Anhui University, Hefei 230601, China
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) BaB₆, (b) CaB₆, and (c) SrB₆ at the strain of 0.95.