Supplementary Information for

Topological nodal line state in superconducting NaAlSi compound

Lei Jin,[a,b] Xiaoming Zhang,[*, a,b] Tingli He,[a,b] Weizhen Meng,[a,b] Xuefang Dai,[a,b] and Guodong Liu[*, a,b]

[a] State Key Laboratory of Reliability and Intelligence of Electrical Equipment, Hebei University of Technology, Tianjin 300130, China.

[b] School of Materials Science and Engineering, Hebei University of Technology, Tianjin 300130, China.

E-mail: zhangxiaoming87@hebut.edu.cn; gdliu1978@126.com

I. Band structure of NaAlSi by HSE06

Since PBE computations may underestimate the band gap, we have checked the band structure by HSE06 calculations. As shown in Fig. S1, the band crossings in region-A and region-B retain under HSE06 calculations.

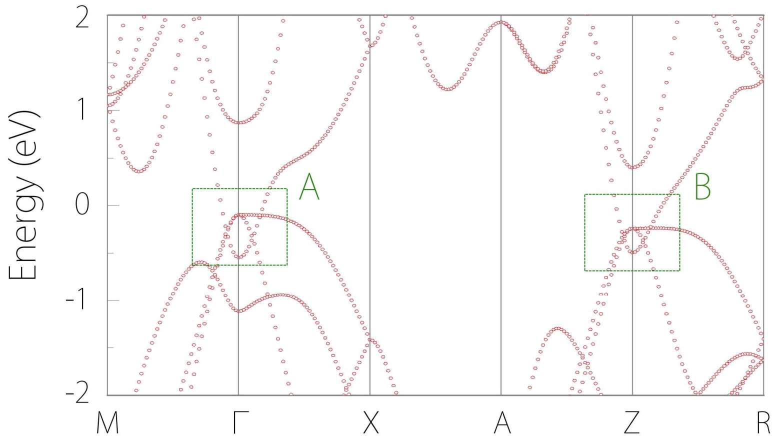

Fig. S1 Electronic band structure of NaAlSi by HSE06 computation

II. The phonon dispersion spectrum for NaAlSi

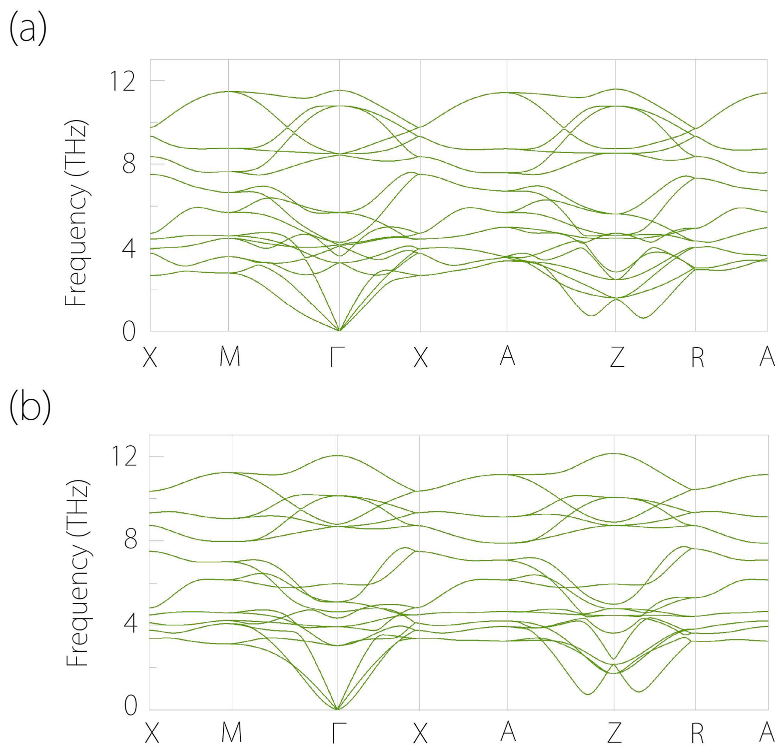

Fig. S2 Phonon dispersion spectrums of NaAlSi under (a) 5% and (b) 2% compressive strains

III. Classification of topological materials

Topological materials can be distinguished by several indicators. For example, depending on the conductivity of bulk band structure, topological materials can be classified into topological insulators (which have insulating bulk state) and topological semimetals/metals (which show semimetallic/metallic bulk state with linear band crossing near the Fermi level). Topological semimetals/metals (TMs) can also be classified into different categories, for example: based on the dimensionality of the band-crossing, TMs can be classified as nodal point, nodal line, and nodal surface TMs, which possess zero-dimensional nodal points, one-dimensional nodal lines, and two-dimensional nodal surfaces in the low-energy band structures (see Fig. S3); depending on the degeneracy of the crossing bands, TMs can be classified as Dirac, Weyl, triply, sixfold, and eightfold-degenerate nodal point ones; depending on the slope of crossing bands, TMs can be classified into type-I and type-II ones (see Fig. S4). These different topological states can be easily identified by checking the electronic band structures.

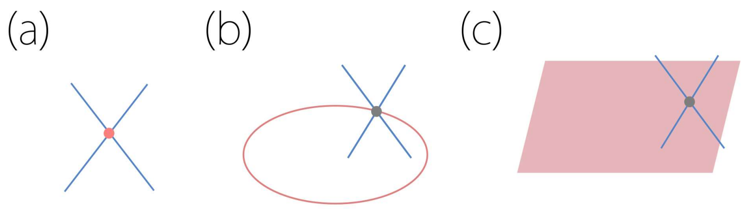

Fig. S3 Schematic illustrations of (a) the nodal point, (b) the nodal line and (c) the nodal surface.

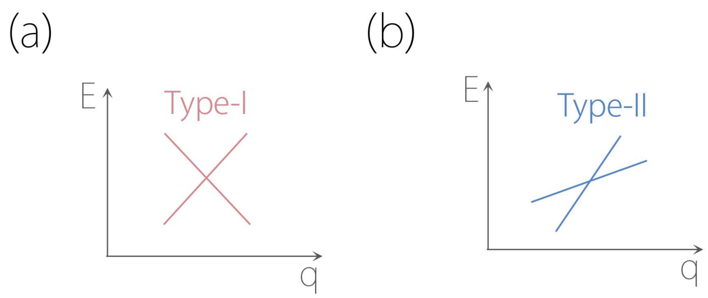

Fig. S4 Schematic illustrations of (a) type-I and (b) type-II band dispersions in the momentum-energy space.