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Supplementary Information for

The Centrosymmetric Li_2NaN: A Superior Topological Electronic Material with Critical-Type Triply Degenerate Nodal Points

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I. Computational details

We perform first-principles calculations in the framework of density functional theory, which is implemented in the Vienna ab initio Simulation Package [1-3]. For ionic potentials, The generalized gradient approximation with the Perdew-Burke-Ernzerhof realization is used [4]. The cutoff energy is chosen as 500 eV, and the Brillouin zone (BZ) is sampled with a Γ-centered *k* mesh of size 13×13×13 for geometry optimization and self-consistent calculations. The energy convergence criterion is set as 10^{-6} eV. To investigate the topological surface states, we construct the localized Wannier functions [5,6], and calculate surface spectra by using the WANNIERTOOLS package [7] combined with the iterative Green's function method [8].

II. Band structure under MBJ potential

Since the GGA potential sometimes underestimates potential band gaps, here we check the band structure of Li_2NaN by using a combination of modified Becke-Johnson exchange potential with local density approximation (MBJLDA) [9]. As shown in Figure S1, we can observe that the critical-type TDNPs in Li_2NaN retain under the MBJ calculation.

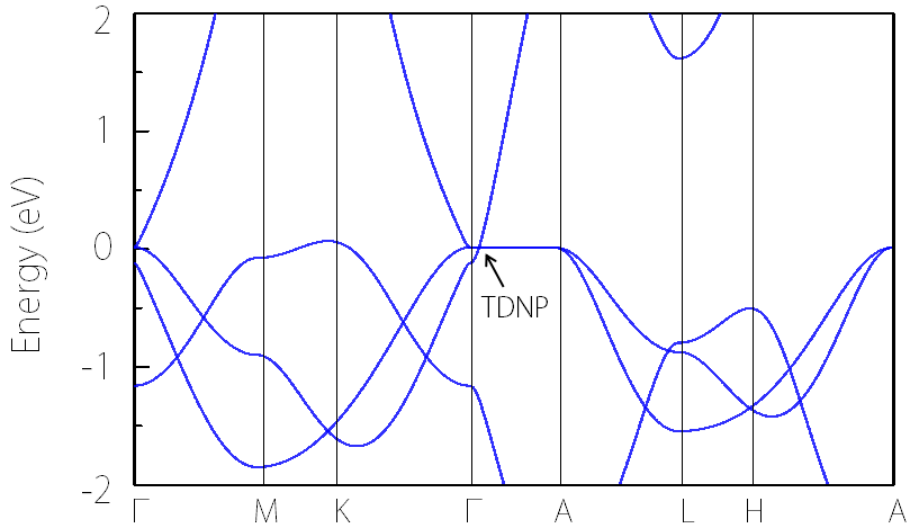

Figure S1. Band structure of Li_2NaN under MBJLDA calculation. The arrow points out the position of TDNP.

III. Band structure on some high-symmetry lines

In the maintext, Fig. 1(a) does not include the band structure on some high-symmetry lines such as L-M and K-H. Here in Figure. S2 (a) and (b) we provide the band structures for these missed paths. We can find the bands on these paths are far away from the Fermi level.

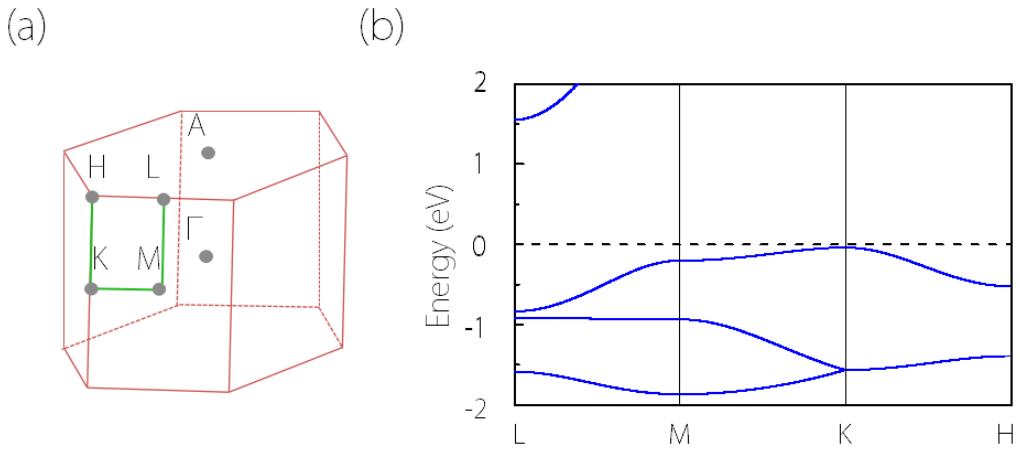

Figure S2. (a**)** The bulk Brillouin zone and selected k-path. **(**b**)** The band structure of Li_2NaN along the L−M−K−H path.

SUPPLEMENTARY REFERENCES

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