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Supplementary Information for

Topological nodal lines and nodal points in the antiferromagnetic material β-Fe_2PO_5

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I. Electronic band structure at other magnetic configurations

The electronic band structures of β-Fe_2PO_5 under the NM, AFM2 and AFM3 states are shown in Fig. S1 (a)-(c), and that for the FM state is shown in Fig. S2 (a)-(d). We find β-Fe_2PO_5 exhibits quite interesting topological band structure under the FM state. As shown in Fig. S2 (a)-(d), band crossings in R1, R2 and R3 form Weyl nodal line, type-II Weyl point, and Dirac nodal line, respectively.

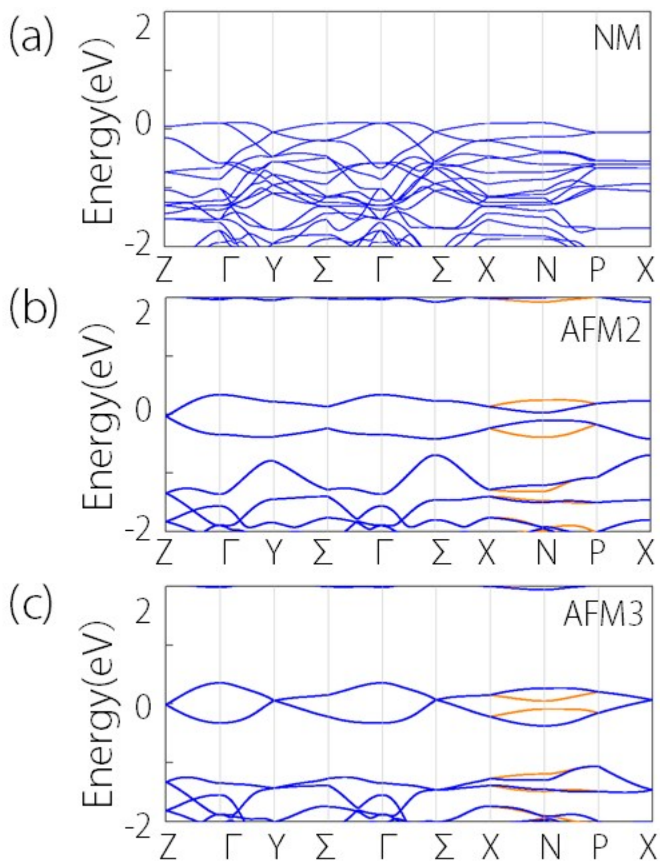

Fig. S1 Electronic band structure of β-Fe_2PO_5 in the (a) NM (b) AFM2 and (c) AFM3 states. In (b) and (c), bands in the spin-up and spin-down channels are shown by the blue and orange lines, respectively.

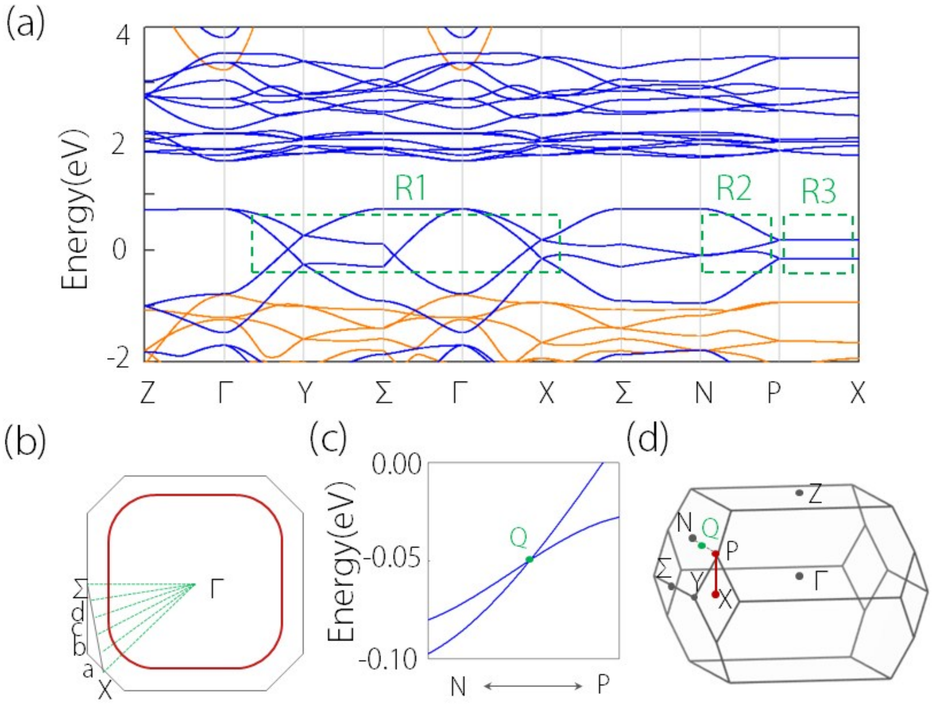

Fig. S2 (a) Electronic band structure of β-Fe_2PO_5 in the FM state. Bands in the spin-up and spin-down channels are shown by the blue and orange lines. R1, R2 and R3 highlight the band crossings along the *k*-paths *Γ*-*Y*, *X*-*Γ*-*Σ*, *N*-*P*, and *P*-*X* respectively. (b) The profile of the Weyl nodal line in R1. (c) Enlarged band structure for R2. Q is a type-II Weyl point. (d) The bulk Brillouin zone and the positions for the type-II Weyl point and Dirac nodal line along *P*-*X*.

II. Electronic band structures at different U values

Our calculations show the band crossings near the Fermi level in β-Fe_2PO_5 will not change when U shifts in the range from 0 eV to 10 eV.

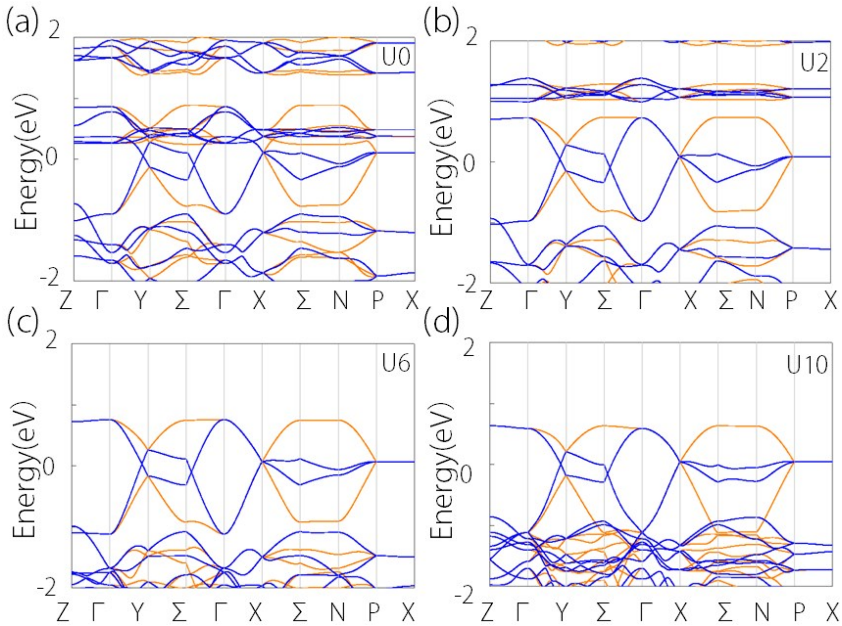

Fig. S3 Band structure of β-Fe_2PO_5 calculated by the GGA+U method with different U values: (a) U = 0 eV, (b) U = 2 eV, (c) U = 6 eV, (d) U = 10 eV. Bands in the spin-up and spin-down channels are shown by the blue and orange lines.

III. Electronic band structures under MBJLDA functional

The MBJLDA calculation shows a similar band structure with GGA that all the linear band crossings near the Fermi level retain in β-Fe_2PO_5.

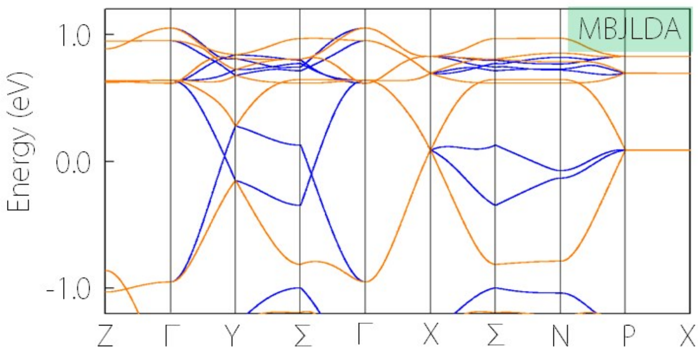

Fig. S4 The electronic band structure of β-Fe_2PO_5 under the MBJLDA functional.

IV. Electronic band structures under different lattice distortions

We find the Weyl nodal line in β-Fe_2PO_5 is very robust upon lattice distortion (which usually happens during the preparation of materials). Our calculations show the band crossings at the Γ-Y and Γ-Σ paths can retain under 10% tensile and compressive lattice distortions.

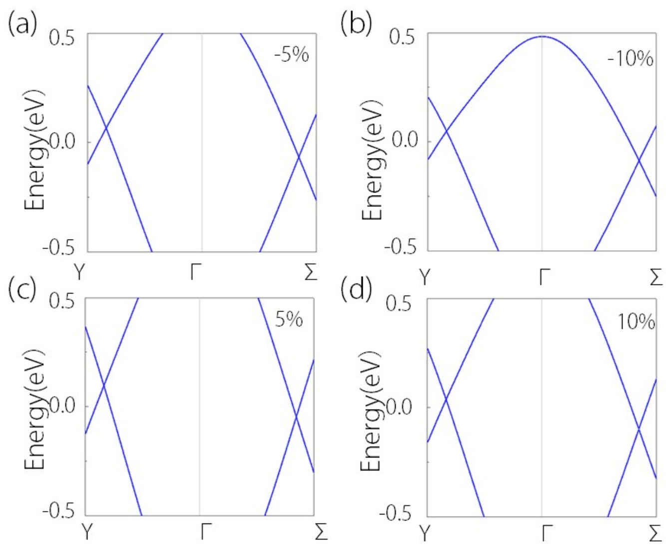

Fig. S5 Enlarged band structure of β-Fe2PO5 along the Y-Γ-Σ path under (a) 5% compressive, (b) 10% compressive, (c) 5% tensile, and (d) 10% tensile distortions.

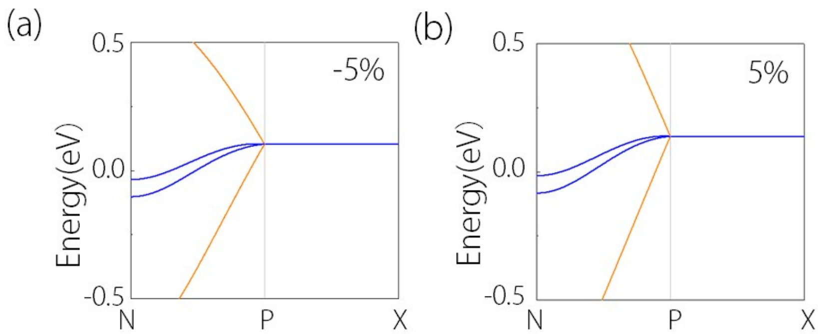

Fig. S6 Enlarged band structure of β-Fe2PO5 along the N-P-X path under (a) 5% compressive, and (b)5% tensile distortions.

V. Surface states of β-Fe_2PO_5

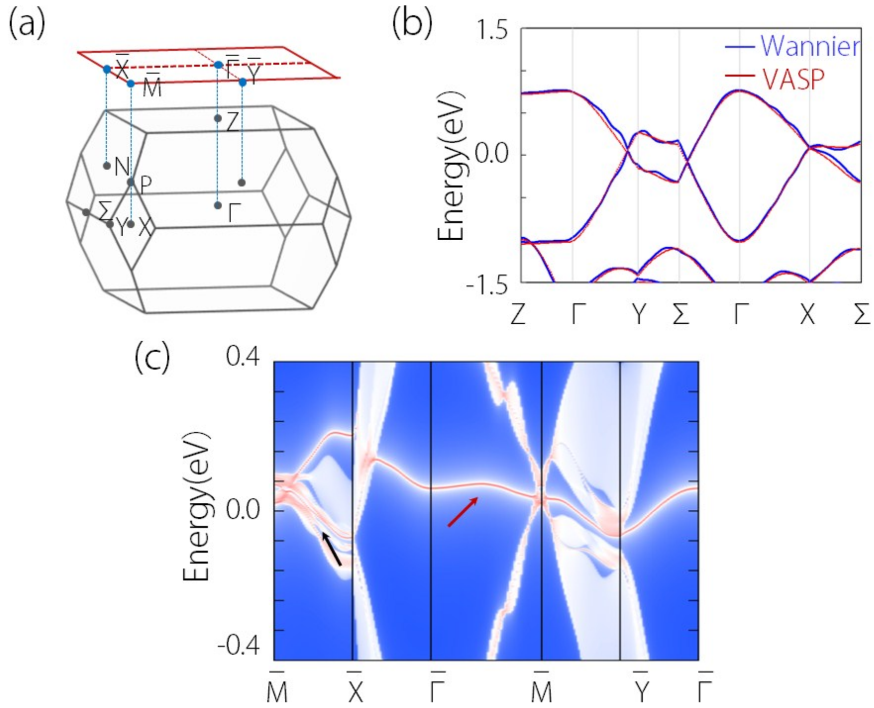

Fig. S7 (a) The bulk Brillouin zone and its projection onto the (001) surface projection of β-Fe_2PO_5. (b) Comparison of band structure from DFT and the Wannier. (c) The (001) surface band structure of β-Fe_2PO_5. In (c), the surface bands for the Weyl nodal line and Dirac point are pointed by the red and black arrows, respectively.