Structure, phase stability, half-metallicity, and fully spin-polarized Weyl states in compound NaV₂O₄: An example for topological spintronic material

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Here we systematically investigate the structure, phase stability, half-metallicity, and topological electronic structure for a topological spintronic material NaV₂O₄. The material has a tetragonal structure with excellent dynamical and thermal stabilities. It shows a half-metallic ground state, where only the spin-up bands are present near the Fermi level. These bands are demonstrated to form a nodal line with the double degeneracy on the $k_z = 0$ plane. The nodal line is robust against spin-orbit coupling, under the protection of the mirror symmetry. The nodal line band structure is very clean, thus the drumhead surface states can be clearly identified. Remarkably, the nodal line and drumhead surface states have the 100% spin polarization, which are highly desirable for spintronics applications. In addition, by shifting the magnetic field in-plane, we find that the nodal line can transform into a single pair of Weyl nodes. The nodal-line and Weyl-node fermions in the bulk, as well as the drumhead fermions on the surface are all fully spin-polarized, which may generate interesting physical properties and promising applications.

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I. INTRODUCTION

The discoveries of the Dirac and Weyl semimetal with nontrivial band topology sparked a revolution in condensed matter physics [1-10]. The unique linear band crossing in these topological semimetals cause a wide range of exotic transport and optical phenomena [11–16]. According to different band crossings in the electronic structure, topological semimetals can be classified into several groups such as nodal line semimetals [17–20], Weyl-Dirac semimetals [21–28], nodal-chain semimetals [29,30], and nodal surface semimetals [31–33]. Among them, the nodal line semimetal has attracted particular interest because it can be seen as the parent state of various quantum states, such as the topological insulator and Weyl semimetal states [34,35]. Previously, the studies on nodal line semimetals were mainly conducted in the absence of spin-orbit coupling (SOC) [36,37], under the protection of the mirror symmetry or the combing of the time reversal and the inversion symmetries.

In magnetic topological materials, the magnetic ordering breaks the time-reversal symmetry, so additional symmetry is required to protect the topological state. Historically, pyrochlore iridate [5] and half metal HgCr₂Se₄ [24], which host several pairs of time-reversal-breaking Weyl nodes, were the earliest proposal of magnetic topological semimetals. Later, more magnetic Weyl semimetals were proposed, including the stacking Kagome lattice Mn₃Sn/Ge [38] and Heusler compounds such as Co₂TiX (X = Si, Ge, or Sn) [39,40], and so on. Soon after, great progress was made in magnetic Dirac semimetals, and several candidates in CuMnAs [41], orthorhombic LaMnO₃ [42], MnF₃ [43], and EdCd₂As₂ [44] were proposed. Very recently, it a few reports emerged on the magnetic nodal line semimetals (NLSMs) in threedimensional materials Fe₃GeTe₂ [45], β -V₂OPO₄ [46], and Li₃(FeO₃)₂ [47] and two-dimensional ones LaCl [48,49], MnN [50], and CrAs₂ [51]. Unlike nodal lines in a nonmagnetic system, the spin-polarization in magnetic topological semimetals creates the topological electrons potential for spin manipulation and spintronics applications. Specifically, topological states in spintronics are believed to provide special advantages such as strong spin-momentum locking [52], high charge-current to spin-current conversion efficiency [53–55], high electron mobility and long spin diffusion length [56,57], and efficient spin filtering [58]. Materials combining nontrivial topological states and high spin polarization would stimulate the high speed and low energy consumption of the spintronics concept. For this consideration, topological half-metals are the most desirable because the fermions in them can show a 100% spin-polarization. However, candidate materials for topological half-metals, especially for nodal line half-metals, are quite limited currently.

In this work, we report an ideal nodal-line half-metal state in the NaV₂O₄ compound. Its topological band structure shows the following features: (i) the band crossing forms one nodal line with double degeneracy near the Fermi level; (ii) the nodal line has a 100% spin-polarization because it arises from the states in a single spin channel; (iii) the nodal line can survive under SOC, protected by symmetry; (iv) the nodal line is robust against lattice strain and effective onsite U values; (v) the nodal line has a large linear energy region

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(a)



FIG. 1. (a) Side and (b) top views of the conventional cell of NaV_2O_4 compound. (c) The primitive cell and (d) the bulk Brillouin zone with the corresponding (001) surface Brillouin zone of NaV_2O_4 compound.

and shows definite spin-polarized drumhead surface states. In addition, we show that the nodal line can transform into a single pair of Weyl nodes by shifting the magnetization into in-plane. The work provides excellent material to investigate the novel properties of fully spin-polarized fermionic states with time-reversal breaking.

II. METHODS

In this work, first-principles calculations were performed by using the Vienna *ab initio* simulation package [59]. The exchange-correlation potential was adopted by the generalized gradient approximation (GGA) of the Perdew-Burke-Ernzerhof (PBE) function [60]. The cutoff energy was set as 500 eV. The Brillouin zone was sampled by a Monkhorst-Pack [61] k-mesh with a size of $15 \times 15 \times 15$. During our calculations, we applied the GGA + U method to account for the three-dimensional (3D) orbitals of the V atom [62,63]. The U value for V was chosen as 4 eV, and the Hund's exchange parameter J is taken as 0. To be noted, slightly shifting the U values and J values will not change the conclusion of our work. For lattice optimization, the selfconsistent field convergence for the total energy and the force variation were set as 10^{-7} eV and 0.001 eV/Å, respectively. The phonon spectrum are calculated by using the NANODCAL package [64]. The topological surface states are calculated based on the maximum-localized Wannier functions, by using the WANNIERTOOLS package [65,66]. Detailed computational tests are shown in the Supplemental Material Ref. [67].

III. CRYSTAL AND MAGNETIC STRUCTURES

The compound NaV₂O₄ has a tetragonal structure with the space group $I4_1/amd$ (No. 141) and the point group of D_{4h} . The crystal structure is shown in Figs. 1(a) and 1(b). We can find that the fundamental blocks of the Na-V-O system consist of the stacks between the NaO₄ tetrahedra and VO₆ octahedra.



FIG. 2. (a) The calculated phonon spectrum and (b) the total potential energy fluctuation of NaV_2O_4 during the AIMD simulation at 300 K.

In the structure, the Na and V atoms are located at the 4b(0.000, 0.250, 0.375) and the 8c (0.000, 0.000, 0.000) Wyckoff sites, respectively. The O atoms occupy the 16h Wyckoff sites (0.000, μ , ν). Figure 1(c) shows the primitive cell form of the NaV_2O_4 compound. One conventional unit cell contains two units of such a primitive cell. The structure of NaV₂O₄ was initially proposed by the Materials Project [68], which was demonstrated to be energetically and dynamically stable. Here, we want to point out that in the database, four typical structures for NaV₂O₄ are proposed. We compared the energy among them, and find the structure focused in this work is among the lowest energy. In addition, among different phases of NaV₂O₄, only the current one shows the novel topological half-metal band structure. Thus, in the following we focus on the structure for detailed discussions. In this work, the structure of the NaV₂O₄ compound has been fully relaxed. The optimized lattice values are a = b = 6.053 Å, c = 9.008 Å, $\mu = 0.036$, and $\nu = 0.772$.

Here, we check the stability of the obtained structure. In Fig. 2(a), we show the phonon spectrum of the NaV₂O₄ compound. We can find that the material has a nice dynamical stability with no imaginary modes in the entire Brillouin zone. We also performed the *ab initio* molecular dynamics (AIMD) simulations to estimate the thermal stability of the obtained structure. The evolution of free energy for NaV₂O₄ compound at 300 K during the AIMD simulation is shown in Fig. 2(b). After running 2000 steps (3 ps) at 300 K, we find no bonds broken or geometric reconstructions in the final state. These results show the NaV₂O₄ compound is also thermodynamically stable.

Furthermore, we can estimate the mechanical properties of the NaV_2O_4 compound by using the stress-strain method. Tetragonal crystal structure totally possesses five independent



FIG. 3. The calculated directional-dependent mechanical properties for NaV_2O_4 . For the shear modulus and Poisson's ratio, the blue shaded surface indicates the maximum values and the green surface for the minimum ones.

elastic constants, which include C_{11} , C_{12} , C_{13} , C_{33} , C_{44} , and C_{66} . Other mechanical parameters such as the bulk modulus *B*, the Young's modulus *E*, the shear modulus *G*, and the Poisson's ratio ν can be derived from these elastic constants. As shown in Fig. 3, we can observe strong mechanical anisotropy for all the mechanical parameters. The mechanical stability of the NaV₂O₄ compound can be estimated based on the generalized elastic stability criteria. For a stable tetragonal crystal structure, the following conditions are required:

$$C_{11} > 0,$$

$$C_{33} > 0,$$

$$C_{44} > 0,$$

$$C_{66} > 0,$$

$$C_{11} - C_{12} > 0,$$

$$C_{11} + C_{33} - 2C_{13} > 0,$$

$$2(C_{11} + C_{12}) + C_{33} + 4C_{13} > 0.$$
(1)

By checking our results, we find all conditions in (1) are satisfied in the current NaV_2O_4 compound. This indicates that the material could be mechanically stable. Specifically, we focus on the Young's modulus, which can reflect the rigidity of the material. For materials with similar structure, the larger of the Young's modulus, the less likely the material is to deform. For current NaV_2O_4 , the Young's modulus is calculated to be 178 Gpa, which is larger or comparable with several synthesized materials in a similar structure, such as tetragonal BiFeO₃ (142 Gpa) [69], ZnO (110 Gpa) [70], and tetragonal ZrO₂ [71] (192 GPa).

Before studing the electronic band structure, we need to determine the ground magnetic state in the NaV_2O_4 compound first. In NaV₂O₄, the magnetic moment is almost carried by the transition metal element V. To determine the ground magnetic state, we compared the total energies by assigning the V moments in different magnetic configurations, including nonmagnetic (NM), ferromagnetic (FM), and antiferromagnetic (AFM). Our results confirm that the energy of the FM state is far lower (5.55 eV) than the NM state. We performed careful calculation to compare the energy between FM and AFM states. We first performed the calculation in the unit cell of NaV₂O₄, where two AFM states including AFM1 and AFM2, were considered [see Fig. S1(a) in the Supplemental Material Ref. [67]]. Then we compared their energies at different U values of V (0, 1, 2, 3, 4, 5), shown as Fig. S1(b) in the Supplemental Material [67]. We find the FM state always possesses the lowest energy at different U values. In addition, we also considered different magnetic configurations in the $1 \times 1 \times 2$ and $2 \times 2 \times 1$ supercells (see Figs. S2 and S3 in the Supplemental Material [67]). We find that the FM state is most energetically stable in all considered magnetic configurations. These results show the NaV₂O₄ compound tends to show FM magnetic ground state. In the following, we adopt the FM state as the ground state to study electronic band structure of NaV₂O₄. We also display the band structure for the AFM states in the Supplemental Material [67]. We find NaV_2O_4 can also show Weyl points and nodal lines under AFM states. In the ground state, the magnetic moment is estimated to be 6 μ_B per unit cell. Moreover, the easy magnetization direction is determined to along the out-of-plane [001] direction, which is about 0.67-meV lower than typical in-plane directions.

IV. ELECTRONIC BAND STRUCTURE

A. Nodal line and Weyl nodes without SOC

Based on the FM ground state, here we investigate the topological band structure of NaV₂O₄ compound. At first, the SOC is not included in the calculations. The spin-resolved band structure and the density of states (DOSs) are shown in Figs. 4(a) and 4(b). We can observe that the material shows a metallic band structure in the spin-up channel. From the given total and partial DOSs, we find these states are mostly contributed by the V-d orbitals. Whereas, the material shows an insulating feature in the spin-down channel, with the band gap as large as 3.75 eV. These results suggest that NaV₂O₄ is an excellent half metal with a 100% spin polarization of conducting electrons. Remarkably, we can observe three linear band crossing points (P1, P2, and Q) in the spin-up bands [see Fig. 4(a)], which occur in the k-paths Γ -Y, Γ -X, and N-P, respectively. All these band crossings locate quite close to the Fermi level. Here, we want to point out that both the band crossings and the half-metal band structure in NaV2O4 can also be obtained in other calculation methods (see Figs. S5 and S6 in the Supplemental Material [67]).

First, we focus on the two band crossing points P1 and P2 in the spin-up channel. The enlarged band structure near P1 and P2 is shown in Fig. 5(a). It is worth noticing that both the k-paths Γ -X and Γ -Y situate in the mirror-invariant plane $k_z = 0$, which can protect a nodal line. To examine whether P1 and P2 are isolate nodal points or belong to a nodal line, we calculated the band structure in several other k-paths, namely



FIG. 4. Electronic band structure and the projected density of states of NaV₂O₄ in (a) spin-up channel and (b) spin-down channel. In (a) the band crossing points in the *k*-paths Γ -*Y*, *X*- Γ , and *N*-*P* are denoted as *P*1, *P*2, and *Q*, respectively. In (b) the size of the band gap is labeled.

 Γ -*a*, Γ -*b*, Γ -*c*, Γ -*d*, and Γ - Σ [see Fig. 5(b)]. Together with Γ -*X* and Γ -*Y*, these *k*-paths can reflect the band signature of the entire Brillouin zone. The band structure on these *k*-paths is shown in Fig. 5(c). It is clearly found that all the *k*-paths Γ -*a*, Γ -*b*, Γ -*c*, Γ -*d*, and Γ - Σ show a linear band crossing point, suggesting the presence of a nodal line in



FIG. 5. (a) The enlarged view of band structure near *P*1 and *P*2 points. (b) Illustration of the nodal line in the $k_z = 0$ plane and selected *k*-paths through the nodal line. (c) Band structure along the selected *k*-paths in (b). (d) The shape of nodal line in the Brillouin zone. (d) The Berry phase along the *k*-paths *X*- Γ -*Y* in the $k_z = 0$ plane.

the $k_z = 0$ plane. As shown in Fig. 5(c), the linear energy range near the nodal line is large with the size of about 0.5 eV. In Fig. 5(d), we map the profile of the nodal line in the $k_z = 0$ plane, it centers the Γ point, and has a square symmetry. The nodal line is protected by the mirror symmetry M_{τ} because the two crossing bands have opposite mirror eigenvalues (+1 and -1), as verified by our DFT calculations. As discussed above, the nodal line in NaV₂O₄ is located in the $k_7 = 0$ plane and is protected by the mirror symmetry M_z . The topological invariant of such a nodal line could be treated as a variation of the quantized Berry phase with respect to the mirror plane [72,73], which is related to the change at the end of the one-dimensional system along a path across the nodal line in the $k_z = 0$ plane. Here we choose the k-path $X-\Gamma-Y$ to show this point. As shown in Fig. 5(e), the Berry phase indeed shows a jump when the path crosses the nodal line. These results further confirm the topological feature of the nodal line in NaV2O4.

We checked that the little group at Γ point belongs to D_{4h} , which is generated by S_{4z} , C_{2x} , M_z . Since the nodal ring lying on $k_z = 0$ plane is protected by the mirror symmetry, consequently, the two bands are characterized by the different eigenvalues (g_z) of mirror symmetry M_z , corresponding to $g_z = 1$ and $g_z = -1$. Thereby, in the invariant space of mirror symmetry, M_z is given by

$$M_z = \sigma_z. \tag{2}$$

Generally, the two band Hamiltonian takes the form of $\mathcal{H}(k) = \sum_i d_i(\mathbf{k})\sigma_i$, (i = x, y, z). Here, we consider up to the second order of *k*. Then the commutation between the mirror symmetry and effective Hamiltonian satisfies that

$$M_z \mathcal{H}(\mathbf{k}) M_z^{-1} = \mathcal{H}(k_x, k_y, -k_z).$$
(3)

Such a relationship requires that $d_x(\mathbf{k})$ and $d_y(\mathbf{k})$ cannot have the second order of \mathbf{k} due to $\{\sigma_{(x/y)}, \sigma_z\} = 0$. Given that the time-reversal symmetry (\mathcal{T}) acts on one spin-channel in the half-metal system just like acts on a spinless system, it only has a complex conjugation satisfying $\mathcal{TH}(\mathbf{k})\mathcal{T}^{-1} = \mathcal{H}(-\mathbf{k})$. Such that the terms linear to σ_x and σ_z cannot appear.

Consequently, $d_z(\mathbf{k})$ only has the term which is even order of \mathbf{k} , including the constant term, whereas $d_x(\mathbf{k})$ vanishes. Together, with the remaining generators, one has

$$S_{4x}\mathcal{H}(\mathbf{k})S_{4x}^{-1}=\mathcal{H}(-k_y,k_x,-k_z),$$

$$C_{2x}\mathcal{H}(\mathbf{k})C_{2x}^{-1}=\mathcal{H}(k_x,-k_y,-k_z).$$

Finally, the effective Hamiltonian takes the form of

$$\mathcal{H}(\mathbf{k}) = [M_0 + Mk^2]\sigma_0$$

+[C + Ak_z^2 + B(k_x^2 + k_y^2)]\sigma_z + \gamma k_z \sigma_y. (4)

Here, parameters, M_0 , M, A, B, C, and γ are real parameters, and $k^2 = k_x^2 + k_y^2 + k_z^2$. We should point out that, to indicate a nodal ring on plane $k_z = 0$, BC < 0.

Drumhead surface state is a distinguishing feature of nodal line materials [36,74–78]. To study the surface states of the



FIG. 6. (a) The comparison of the band structure from the Wannier model and DFT. (b) Calculated (001) surface band structure with the drumhead surface states pointed by the black arrows. (c) The constant energy slice of the surface states at -3 meV. The energy level for -3 meV is indicated in the dashed line in (b). The numbers of the color bars in (b) and (c) are the log of the spectral weight.

nodal line in the NaV₂O₄ compound, we first construct a tight-binding model by projecting onto the Wannier orbitals. By examining the PDOSs in Fig. 4, we find the valence and conduction bands are contributed by the hybridization among Na-3s, V-3d, and O-2p orbitals. By projecting these orbitals, the Wannier band structure is constructed. As shown in Fig. 6(a), we find the Wannier band structure is in good agreement with the band structure from the DFT. Correspondingly, the surface spectrum can be obtained. We show the (001) surface band structure in Fig. 6(b). We can clearly observe the drumhead-type surface states around the $\overline{\Gamma}$ point originating from the projected nodal line, as pointed to by the arrows in the \bar{Y} - $\bar{\Gamma}$, \bar{M} - $\bar{\Gamma}$ and \bar{X} - $\bar{\Gamma}$ paths. In addition, in Fig. 6(c), we also displayed the slice of the surface states at -3 meV. The energy level for -3 meV is indicated in the dashed line in Fig. 6(b), which can exactly cut the drumhead surface states. In Fig. 6(c), the profile for the drumhead surface is pointed by the arrows. Such clear surface states greatly favor the experimental detection in the future. To be noted, the drumhead surface states in NaV₂O₄ are also fully spin-polarized, being different from those in nonmagnetic nodal line materials.

Next, we focus on the linear band crossing labeled as Q in the *N-P* path. The enlarged view of the band structure is shown in the left panel of Fig. 7(a). The three-dimensional plotting of band dispersion near Q is depicted in the right panel of Fig. 7(a). We can clearly find that point Q is, in fact, a Weyl node. The Weyl node locates quite close to the Fermi level (0.02 eV). Considering the crystal symmetry, there totally exist four pairs of such Weyl nodes in the system. The positions for a pair of Weyl nodes in the Brillouin zone are shown in Fig. 7(b). The projected spectrum on the (001) surface and the corresponding constant energy slice at 0.02 eV are shown in the Figs. 7(c) and 7(d), respectively. We can clearly observe the Fermi arc surface states connecting the Weyl nodes.



FIG. 7. (a) The enlarged view of band structure in the *N*-*P* path and the 3D plotting of band dispersion near the *Q* point. (b) The position of the *Q* point in the BZ. (c) Calculated (001) surface band structure and (d) the corresponding constant energy slices at E = 0.02 eV. The energy level for 0.02 meV is indicated in the dashed line in (b). The numbers of the color bars in (c) and (d) are the log of the spectral weight.

B. Effects of SOC, lattice strain, and electron correlation

The above discussions are based on the electronic band structure without SOC. In the NaV_2O_4 compound, the SOC effect cannot be simply ignored because the material has considerable atomic weight. Figure 8(a) shows the band structure of NaV_2O_4 with SOC. We find the bands in both spin channels



FIG. 8. (a) Electronic band structure of NaV₂O₄ under SOC with magnetization along the [001] direction. The inset of (a) shows the band gap in the *N-P* path. (b) Schematic diagram of the fully spin-polarization nodal line in $k_z = 0$ plane under the [001] magnetization.

conjunct together, but the band details do not change much. A careful examination on the band structure at crossing points P1, P2, and Q finds that the crossing points P1 and P2 are retained under SOC while Q is gapped. As shown by the inset of Fig. 8(a), the gap size around Q is only 3.4 meV. We calculated the surface states (see Fig. S7 in the Supplemental Material Ref. [67]). We find the gap situates at 25 meV above the Fermi level. More importantly, the states around Q and their corresponding surface states still cross the Fermi level, which can contribute to the transport properties. Since the gap size is extremely small, the slightly gapped states may still show the features of the Weyl fermions. As the result, these states are promising to show similar transport phenomena with Weyl fermions such as the negative magnetoresistivity. We fully scanned the bands in the $k_z = 0$ plane, and find the crossing along the whole nodal line is retained. These results suggest the nodal line in the NaV₂O₄ compound is robust against SOC. This can be derived from the symmetry point of view. The material shows the easy magnetization along the out-of-plane [001] direction, and the mirror symmetry M_{z} is preserved under SOC. Our calculations show that the two crossing bands for the nodal line still have opposite mirror eigenvalues (+i and -i), which protect the nodal line from opening gaps under SOC. As the results, the NaV₂O₄ compound only shows a single nodal line in the $k_z = 0$ plane when SOC is included, as shown in Fig. 8(b).

The magnetic symmetry will change by shifting the magnetization direction, and the topological state may change accordingly. If in-plane magnetizations are applied in the NaV₂O₄ compound, the mirror symmetry M_z will be broken. In this occasion, the nodal line in the $k_z = 0$ plane should vanish. In Figs. 8(c) and 8(e), we show enlarged band structures with the magnetization along the in-plane [100] and [110] directions, respectively. For the [100] magnetization, we find the crossing points in the Γ -Y and Γ -X paths are gapped, but that in the Γ - Σ path is retained [see Fig. 8(c)]. We also checked the bands for other parts on the nodal line, and no other crossing point is found. Therefore, the NaV2O4 compound has transformed into a Weyl semimetal with a single pair of Weyl nodes in the Γ - Σ path [see Fig. 8(d)]. If the magnetization along the [110] direction, only the band crossing point in the Γ -X path is preserved [see Fig. 8(e)]. As the results, the system exhibits a single pair of Weyl nodes in the Γ -X path [see Fig. 8(f)]. In fact, the system always retains a pair of Weyl nodes under arbitrary in-plane magnetization, which is ensured by symmetry. Here, we use the [110] magnetization as an example, while the symmetry analyses for other cases are fundamentally the same. Under the [110] magnetization, the mirror symmetry M_{z} is broken, which gaps the nodal line. However, the system preserves the magnetic double point group C_{2h} . Along the Γ - Σ path, the little group is C_2 , which can allow the presence of Weyl nodes in this path.

The above discussions showed that the NaV₂O₄ compound takes the fully spin-polarized nodal line state in the easy magnetization direction and the state is robust against SOC. Here we further investigate the robustness of the fully spinpolarized line against lattice strain and the electron correlation effects. To ensure the fully spin-polarized nodal line state, two crucial conditions need to be satisfied: (i) an insulating band gap in the spin-up channel; (ii) band crossings in the spin-up channel. These conditions ensure the half-metal signature and the presences of nodal line.

Next, we apply lattice strain to NaV₂O₄. To be noted, hydrostatic strain is applied here. Thus, all the crystalline symmetries are preserved. In Fig. 9(a), we show the positions of the valence band maximum (VBM) and the conduction band minimum (CBM) under 5% hydrostatic strains. Here "+" represents the tensile strain while "-" denotes the compressive strain. We can find that both the energies for VBM and CBM rise to higher energy levels with strain turning from the compressive to tensile one. However, the insulating gap corresponding to the Fermi level always remains during the period. We also checked the band structure in the spin-up channel, and found the crossing points P1 and P2 are always preserved. In Fig. 9(b), we show the position of P1 in the momentum space under different strains. We can find that P1 moves away from the Γ point with strain turning from a compressive to tensile one. However, the energy of P1 does not change much. A similar phenomenon is also observed for P2, as shown in Fig. 9(c). These results indicate that the size of the nodal loop in the NaV2O4 compound would become larger under tensile strain, but become smaller under compressive strain. In addition, we also investigate the robustness of the fully spin-polarized line state against the effective U values. For typical transition-metal elements such as Ti, V, Cr, Mn, and Fe, the U value is generally chosen among 2 to 5 eV. For example, the effective U for V is set to 3.0 eV in β -V₂OPO₄ [46], and that for Fe is set to 4.0 eV in $Li_3(FeO_3)_2$ [47]. Here we shift the U values of the V element from 0 to 8 eV. The results are shown in Figs. 9(d) to 9(f). As shown in Fig. 9(d), the size of the insulating gap in the spin-down channel can be different at different U values. U = 0 eV gives a decreased gap size, and moves the Fermi level closer to the bottom of the conduction band. U = 8 eV gives an increased gap size, and moves the Fermi level closer to the top of the valence band. In these extreme cases, the thermal broadening effects and correlation effects might reduce the spin-polarization from 100%. However, when U is chosen in the range of 2 to 6 eV, the material shows very nice half-metal band structures. In addition, as shown in Figs. 7(e) and 7(f), we find the crossing points P1 and P2 always preserve with U values from 0 to 8 eV. These results show the nodal line state in the NaV_2O_4 compound is quite robust.

V. DISCUSSIONS AND CONCLUSION

Before ending, we have two remarks. First, the nodal line in the NaV₂O₄ compound is almost ideal for further experimental detections in that (i) it locates slightly below the Fermi level, in the energy range of -8.7 meV to -1.5 meV; (ii) the nodal line band structure is fairly clean without other bands nearby; (iii) its linear energy range is as large as 0.5 eV; (iv) the nodal line is robust against SOC and lattice strain; (v) the drumhead surface states are very clear.

In addition, the nodal line state in the NaV_2O_4 compound also shows the following features: (i) it belongs to the type-I nodal line because all the crossings around the line have the type-I band dispersion; (ii) considering the system lacks the time-reversal symmetry, the nodal line has a double degeneracy; (iii) the nodal-line fermion and its corresponding



FIG. 9. (a) Illustration of the positions of valence band maximum (VBM) and conduction band minimum (CBM) in the spin-down channel under hydrostatic strain. The positive and negative values correspond to hydrostatic expansion and hydrostatic compression, respectively. During the period, the change of the position and the energy for crossing points P1 and P2 are shown in (b) and (c). (d), (e), and (f) are similar with (a), (b), and (c), but for the case under different U values of the V atom.

drumhead surface states are fully spin-polarized, which are drastically different with those in nonmagnetic system.

In conclusion, we revealed that the NaV_2O_4 compound is a half metal with fully spin-polarized nodal line and tunable Weyl states. We find the material has excellent dynamical, thermal, and mechanical stability. It shows a ferromagnetic ground state with the easy magnetization along the [001] direction. The spin-resolved band structure exhibits a metallic character in the spin-up channel, but an insulating one in the spin-down channel. Two spin-up bands cross with each other and form one nodal line and four pairs of Weyl nodes near the Fermi level. The nodal line and Weyl nodes have a 100% spin-polarization. Their nontrivial surface states are also spinpolarized, which were clearly identified. We find the nodal line is robust against SOC, protected by mirror symmetry. We further find that the nodal line can shift into a single pair of Weyl nodes by applying the magnetization in-plane. Moreover, the presence of fully spin-polarized nodal line in

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 NaV_2O_4 is robust against lattice strain and the effective onsite U values. The fully spin-polarized nodal line state proposed here is very promising for spintronics applications.

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