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First-Principles Calculation of the Topological Nodal-Line Semimetal $FeGe_2$

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Abstract: The electronic and topological properties of $FeGe_2$ with a tetragonal crystal structure were investigated via first-principles calculations. The results demonstrate that $FeGe_2$ in this structure exhibits anti-ferromagnetism, with two bands crossing the Fermi level nesting each other at high-symmetry points in the Brillouin zone, forming a nodal ring where the nodes intersect in momentum space. Additionally, it possesses nontrivial topological surface states. Upon inclusion of SOC (spin-orbit coupling), there are no significant changes observed in the band structure, nodal features, or surface states, indicating the persistence of its topological nodal-line characteristics.

Key words: Topological semimetal, first-principles calculations, electronic property, topological property.

1. Introduction

The topological semimetal is a class of materials with nontrivial band structures in momentum space, where their conduction and valence bands intersect to form degenerate points or lines [1]. Near these degenerate points or lines, the dispersion relation of quasi-particles can be described by Dirac type or Weyl type Hami-ltonians, which are fundamentally different from the usual Schrödinger-type Hamiltonians. The surface states of topological semimetals also exhibit topo-logically protected characteristics, such as surface states and Fermi arcs. Different types of topological semimetals have distinct features; for instance, the surface states of Weyl semimetals can form Fermi arcs connecting different Weyl points, while nodal-line semimetals can exhibit two-dimensional drumhead states with dispersion relations that approximate zero, leading to divergent surface state densities [2, 3]. The surface states of topological semimetals can induce novel physical phenomena such as high-temperature super-conductivity, magnetism, and anomalous Hall effects [4-7], which can be applied to practical electronic or spin devices with low dissipation. Currently, most known topological semimetals are non-magnetic, while research on magnetic topological semimetals is still in its early stages.

On the other hand, Fe-Ge compounds have attracted interest due to their intriguing magnetic and thermoelectric properties [8-10]. Among them, $FeGe_2$ has been a focal point of numerous experimental and theoretical studies [11-14]. $FeGe_2$ exhibits two characteristic temperatures: $T_{N1} \sim 289$ K, which is the second-order Neel transition temperature from paramagnetic to asymmetric spin density wave, and $T_{N2} \sim 264$ K, which is the first-order transition temperature from asym-metric spin density wave to collinear antiferromagnetic low-temperature phase. Similarly, FeGe, which poss-esses a Kagome lattice structure, represents the first member in the Fe-Ge family to exhibit topological properties associated with charge density [15, 16]. It is particularly important to investigate whether similar properties exist in other compounds within the Fe-Ge system. However, there is currently scarce literature regarding the topological properties of $FeGe_2$.

We employ first-principles calculations and discover the existence of topological nodal-line semimetallic

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characteristics in $FeGe_2$. These topological nodal-line features are highly stable, persisting even when considering SOC (spin-orbit coupling), thus avoiding topological phase transitions. Our theoretical model and computational findings unveil the topological nodal-line properties in $FeGe_2$ and their experimental observability, providing an ideal platform for the study of topological nodal-line semimetals.

2. Experimental Setup

The present study employs the first-principles calculation software package VASP [17, 18] to compute the band structure and DOS (density of states) of the $FeGe_2$ system within the framework of condensed matter physics. Here, the exchange-correlation function is addressed through the GGA (generalized gradient approximation), and the pseudopotentials are treated using the PAW (projector augmented wave) method. Throughout the computational process, initially, a *k*-point grid of 11×11×11 is set. The energy cutoff is set to 520 eV, with convergence criteria for energy and force being 10^{-6} eV and -0.02 eV/Å, respectively. Subsequently, the Wannier90 software package is utilized to fit the band structure and construct a tight-binding model. Finally, WannierTools is employed to compute three-dimensional band structures, surface states, Fermi arcs, and other topological properties on a 101×101 grid.

3. Experimental Results

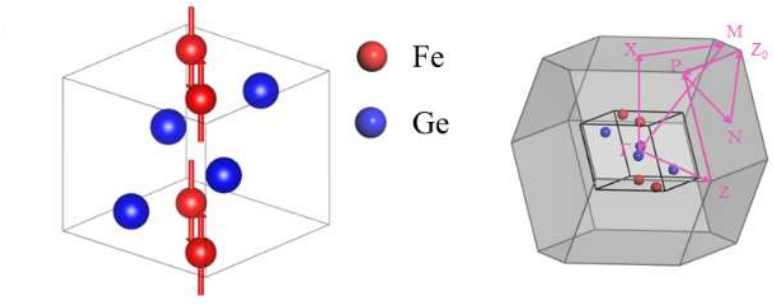
3.1 Crystal Structure

$FeGe_2$ belongs to the tetragonal crystal system, with its space group being I4/mcm, and lattice parameters of $a = b = 5.908$ Å and $c = 4.957$ Å. The structure of the $FeGe_2$ unit cell is illustrated in Fig. 1. Fig. 1a depicts the unit cell structure of $FeGe_2$, where red represents Fe atoms, blue represents Ge atoms, and the red arrows indicate the magnetization direction of Fe atoms, which is anti-ferromagnetic [9] Fig. 1b depicts the corresponding first Brillouin zone and high-symmetry paths.

3.2 Electronic Structure

In this paper, we investigate the influence of orbital coupling on the band structure and DOS of $FeGe_2$, both with and without SOC. Figs. 2a and 2b respectively depict the band structure (left) and DOS (right) without SOC and with SOC. Firstly, in the band structure shown in Fig. 2a, it is evident that three bands intersect the Fermi level (marked in red, blue, and green), indicating semimetallic behavior. Simultaneously, the TDOS (total density of states) corresponding to Fig. 2a is non-zero at the Fermi level, supporting the conclusion of the system's semimetallic nature. Further inspection reveals the appearance of band crossings near the high symmetry point Γ, indicative of topological properties in the absence of SOC. Upon closer examination of the DOS in Fig. 2a, it is noticeable that the Fe 3d orbitals play a decisive role in the electron behavior within the energy range (-2, 2) eV.

SOC plays a crucial role in the electronic structure and physical properties of materials. Fig. 2b displays the band structure and DOS under the influence of SOC. Comparing with Fig. 2a, it is observed that SOC



(a) (b)

Fig. 1 (a) Side view of unit cell; (b) The first Brillouin zone and high-symmetry paths.

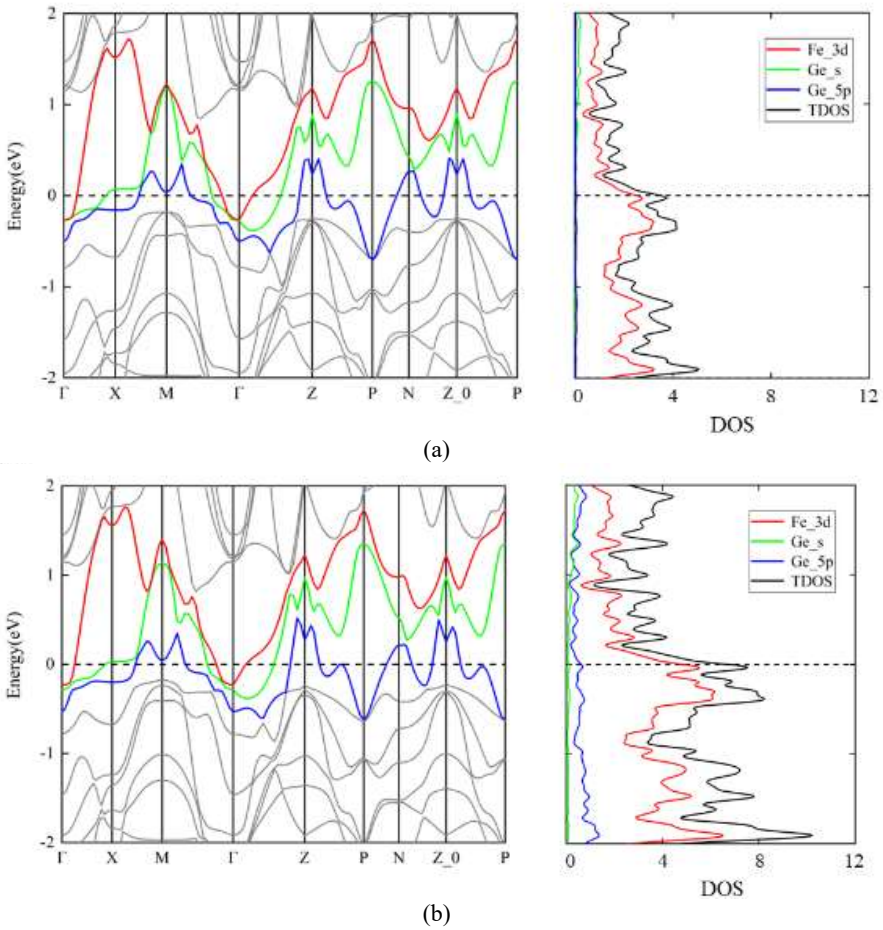
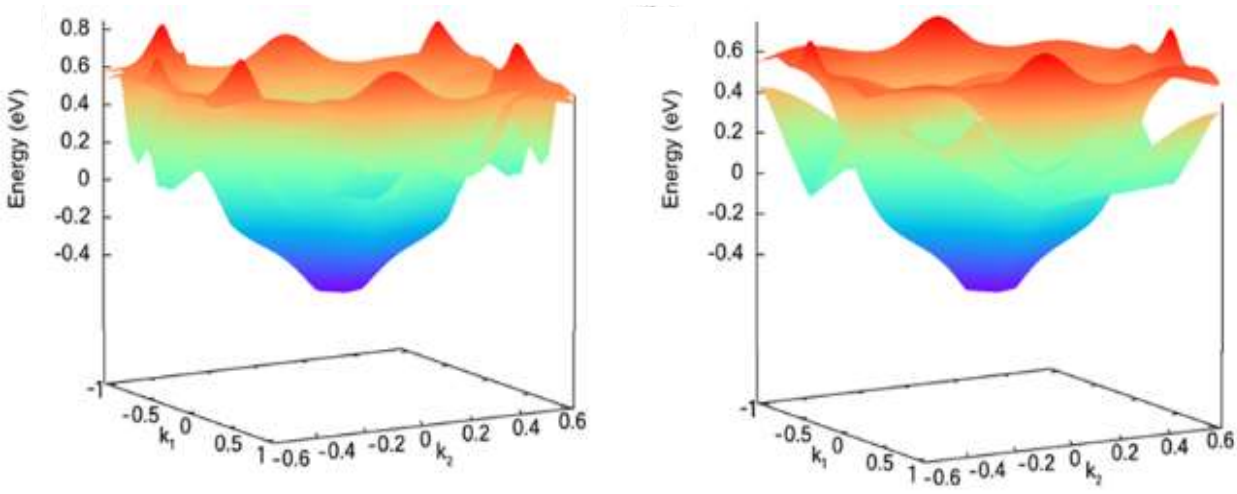


Fig. 2 (a) The band structure (left) and DOS (right) without SOC; (b) The band structure (left) and DOS (right) with SOC.

introduces a band gap of approximately 0.05 eV, indicating a slight alteration in the system's behavior. Although SOC causes the band crossings at the high-symmetry point Γ to open a gap, the overall effect remains minimal due to the small magnitude of the gap. Additionally, under SOC, three bands still intersect the Fermi level (marked in red, green, and blue), and the TDOS at the Fermi level remains non-zero, indicating metallic behavior persists in the system. Further analysis of the DOS in Fig. 2b reveals a similar scenario to that without SOC, with Fe 3d orbitals contributing predominantly to the electronic states. In summary, the impact of SOC on this system is relatively minor.

3.3 Topological Properties

To achieve precise construction of tight binding models and thorough fitting, we utilize Fe's 3d and Ge's s, p orbitals as initial guess orbitals, employing the maximally localized Wannier function method for band fitting. As mentioned earlier, regardless of the presence of SOC, band crossings still occur near the high-symmetry point Γ. To illustrate the band crossing more vividly, we plot the three-dimensional band structure near the Γ point with and without SOC, as shown in Fig. 3. Fig. 3a depicts the case without SOC, showing a conical band nested with another conical band, indicating the presence of clean nodal rings at the high-symmetry point Γ in the absence of SOC. These nodal rings belong to type-II, characteristic of topological nodal semimetals [18]. Fig. 3b illustrates the situation with SOC. In this case, we observe that the crossing point where the gap opens still exhibits a conical band intersecting with another conical band in the three-dimensional band structure. It is evident that



(a) (b)

Fig. 3 (a) Three-dimensional energy band diagram at the high-symmetry point Γ without SOC; (b) Three-dimensional energy band diagram at the high-symmetry point Γ with SOC.

the presence of SOC results in band gap opening compared to the case without SOC, indicating a minimal impact of SOC on the system. Furthermore, the absence of changes in nodal rings under SOC suggests the preservation of topological nodal phases without undergoing a topological phase transition.

In order to present the intersecting situations more accurately and clearly, this study conducted a node search throughout the entire momentum space. The results are shown in Fig. 4, where Fig. 4a represents the results without SOC, and Fig. 4b represents the results with SOC. From Fig. 4a, we can observe a multi-nodal ring structure in momentum space, with a central circular ring surrounded by an elliptical ring nested within the central ring. Additionally, there are multiple band nodes around the nodal ring, indicating that such complex band structures will inevitably lead to exotic topological properties [20]. Meanwhile, after the introduction of SOC, more nodes emerge due to band splitting. However, as shown in Fig. 4b, the ring formed by nodes still persists, providing strong evidence for the topological nodal-line phase in $FeGe_2$.

In order to further investigate its topological properties, we calculate the surface states and Fermi arcs of $FeGe_2$ along the (001) direction, as shown in Fig. 5. Here, $\bar{\Gamma}$ and $\bar{P}$ represent the projections of the high-symmetry points Γ and P onto the (001) direction, while $\bar{N}$ and $\bar{N}$' represent the projections of N at different positions along the (001) direction. In Fig. 5a, the left panel depicts the surface states without SOC. Unlike typical topological nodal-line semimetals, $FeGe_2$ exhibits multiple non-dispersive surface states with spin-up polarization, which give rise to non-dispersive band crossings. Simultaneously, a drumhead like surface state crossing the Fermi level is observed at $\bar{P}$, providing additional evidence of the topological nodal-line nature of $FeGe_2$ [21]. On the other hand, Fermi arcs serve as an effective means to probe the system's topological properties. The Fermi arcs shown in Fig. 5b reveal elliptical Fermi arcs centered at the nodes caused by the system's topology. Figs. 5c and 5d depict the surface states and Fermi arcs of $FeGe_2$ under SOC. Upon observing Fig. 5c, it is evident that SOC breaks the surface states of $FeGe_2$, resulting in the splitting of surface bands. Despite this, some band crossings can still be observed above the Fermi level along the high-symmetry paths $\bar{\Gamma}$-$\bar{N}$ and $\bar{N}'$-$\bar{\Gamma}$, and the drumhead-like surface band at $\bar{P}$ remains, albeit shifted upwards. Turning to Fig. 5d, we observe a significant dissipation of Fermi arcs under SOC, leaving behind circular Fermi arcs on both sides, which remain distinctly visible.

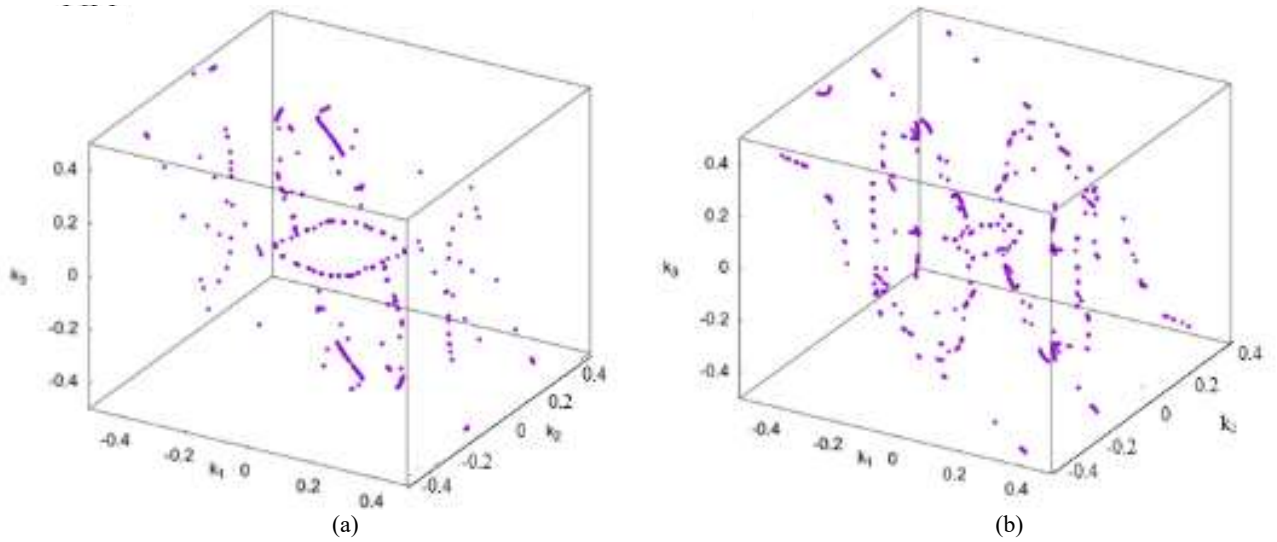


Fig. 4 (a) Momentum space nodes without SOC; (b) Momentum space nodes with SOC.

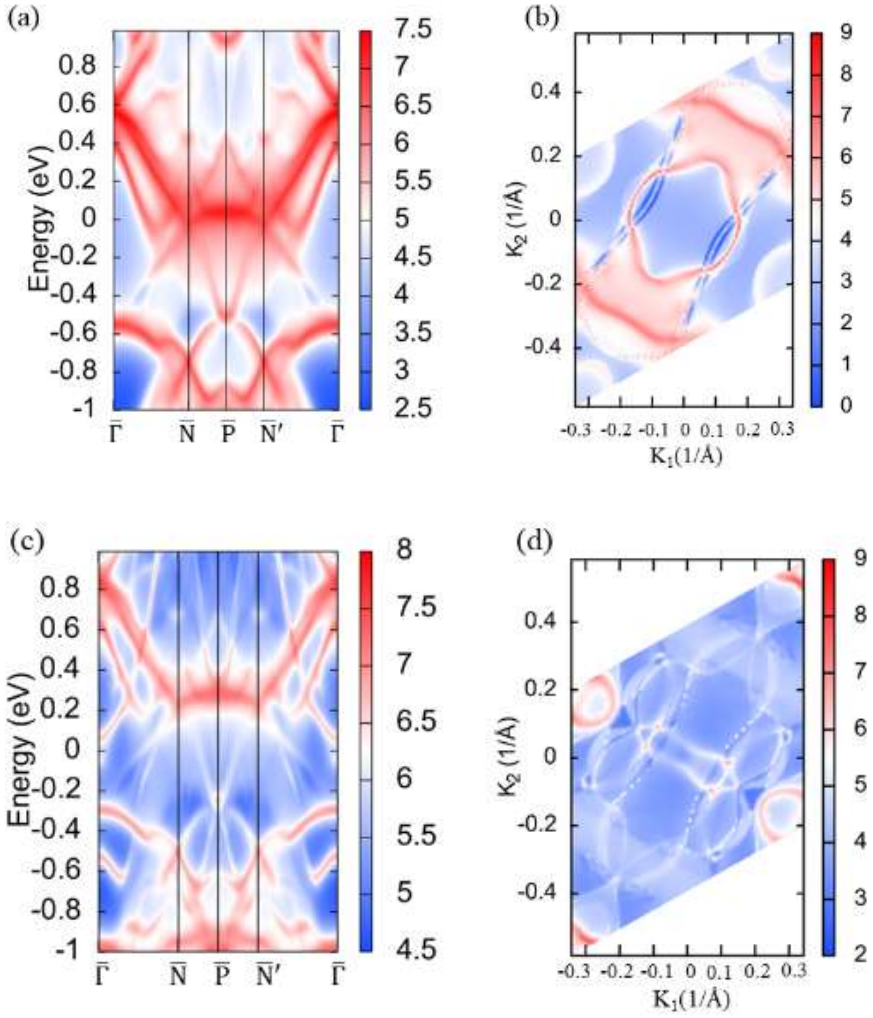


Fig. 5 Direction (001). (a) Surface state without SOC; (b) Fermi arc without SOC; (c) Surface state with SOC; (d) Fermi arc with SOC.

4. Conclusions

This paper investigates the electronic and topological properties of the $FeGe_2$ system using condensed matter physics language. The following conclusions are drawn: The band structure of the $FeGe_2$ system forms nested Fermi surfaces in momentum space, leading to the emergence of nontrivial drumhead surface states on its surfaces. Under the influence of SOC, the band structure of $FeGe_2$ undergoes partial gap opening, altering the original surface states while retaining the topological nodal features. Based on these findings, $FeGe_2$ is identified as a magnetic material exhibiting stable topological nodal properties, along with nontrivial topological surface states. This provides a theoretical foundation for subsequent experimental validations. These characteristics position $FeGe_2$ favorably for research on topological nodal semimetals and hold promise for applications in spintronics devices.

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