Pressure engineering of the Dirac fermions in quasi-one-dimensional Tl$_2$Mo$_6$Se$_6$

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Abstract

Topological band dispersions other than the standard Dirac or Weyl fermions have garnered the increasing interest in materials science. Among them, the cubic Dirac fermions were recently proposed in the family of quasi-one-dimensional (q-1D) conductors A$_2$Mo$_6$X$_6$ (A = Na, K, In, Tl; X = S, Se, Te), where the band crossing is characterized by a linear dispersion in one $k$-space direction but the cubic dispersion in the plane perpendicular to it. It is not yet clear, however, how the external perturbations can alter these nontrivial carriers and ultimately induce a new distinct quantum phase. Here we study the evolution of Dirac fermions, in particular the cubic Dirac crossing, under external pressure in the representative q-1D Tl$_2$Mo$_6$Se$_6$ via the first-principles calculations. Specifically, it is found that the topological properties, including the bulk Dirac crossings and the topological surface states, change progressively under pressure up to 50 GPa where it undergoes a structural transition from the hexagonal phase to body-centered tetragonal phase. Above 50 GPa, the system is more likely to be topologically trivial. Further, we also investigate its phonon spectra, which reveals a gradual depletion of the negative phonon modes with pressure, consistent with the more three-dimensional Fermi surface in the high-pressure phase. Our work may provide a useful guideline for further experimental search and the band engineering of the topologically nontrivial fermions in this intriguing state of matter.

Keywords: cubic Dirac fermions, topological superconductivity, quasi-one-dimensional superconductors

(Some figures may appear in colour only in the online journal)
1. Introduction

The search for new topological states has become the cynosure of condensed matter physics since the discovery of topological insulators [1, 2]. With the advent of Dirac and Weyl semimetals (DSMs and WSMs), the research interest in topological phenomena has largely shifted towards various breeds of topological metals or semimetals, including the topological nodal-line semimetals and those with fermionic excitations beyond 4-fold (Dirac) or 2-fold (Weyl) degeneracies [3], e.g. the threefold/sixfold/eightfold degenerate point nodes [4, 5].

More recently, a new type of topological fermion has been theoretically proposed, namely the cubically dispersed Dirac semimetal (CDSM) [6, 7]. The CDSMs possess linear band crossing along one principle axis but the cubic dispersions in the plane perpendicular to it. Interestingly, some members in this family, like Tl2Mo6Se6, Na2Mo6Se6 and In2Mo6Se6, are also superconducting at ambient pressure. Remarkably, a novel disorder-enhanced superconductivity was recently proposed in Tl2Mo6Se6 by theory, sparking renewed interest in these materials [20–22].

The questions may arise, however, as to how robust these Dirac fermions in Tl2Mo6Se6 are to the variations in the lattice parameters or in its one-dimensionality, and how fragile these topological properties are to other instabilities, such as charge-density waves that are often observed in q-1D materials. All these questions invoke more studies on this newly proposed topological material, both theoretically and experimentally. On the other hand, it is well established that pressure can effectively modify the atomic and electronic structure of a material, giving rise to the novel phases with unusual physical properties, such as a new superconducting phase. In this sense, it is highly desirable to study the topological evolution of the band structure of Tl2Mo6Se6 under pressure and search for new possible phases in it.

In this work, by means of the first-principles calculations, we study the pressure evolution of the band structure of Tl2Mo6Se6 up to 150 GPa, with special focus on its topological properties. We identify a possible topological phase transition within the P63/m structure below 50 GPa. Above 50 GPa, a structural phase transition takes place which drives the system into a topologically trivial phase. The bulk-boundary correspondence has also been studied which explicitly reveals a dramatic modification of the surface states under pressure. The calculated phonon spectra shed light on the possible Peierls distortion in this system. The prediction made in this work shall open up avenues for further study of novel physical properties associated with this newly proposed q-1D topological CDSM. This work may also stimulate the study of cubic Dirac dispersion in other areas of physics, including topological phases of excitations such as magnons and polaritons [23, 24].

2. Methods

We employed the WIEN2K code [25] with generalized gradient approximation (GGA) [26] to calculate the electronic band structures. The muffin tin radii were chosen to be 2.5 a.u. for Tl, and 2.33 a.u. for Mo and Se. A tight-binding model based on Wannier functions [27] was constructed to obtain the topological properties, using Tl s and p, Mo d, and Se p orbitals with spin–orbit coupling (SOC) included. The surface states spectrum were calculated with the surface Greens functions as implemented in the WannierTools code [28]. We used the Quantum-ESPRESSO program [29] to perform the calculations of phonon spectra and electron–phonon couplings. The cutoffs were chosen as 50 Ry for the wave functions and 400 Ry for the charge density. Furthermore, we employed the evolutionary crystal structure prediction method USPEX [30–32] to determine the high-pressure structures.

3. Results

In this section, we shall describe how the application of the external pressure affect the bulk electronic structure, phonon stability and topological surface states of Tl2Mo6Se6 in turn,
followed by a structure prediction at higher pressures. At ambient pressure, Tl$_2$Mo$_6$Se$_6$ crystallizes in the hexagonal $P6_3/m$ space group as reported previously [8]. The crystallographic structure of Tl$_2$Mo$_6$Se$_6$ and the corresponding Brillouin zone with high-symmetry $k$-points are illustrated in figure 1. The crystalline structure consists of a 1D condensation of an infinite number of Mo$_6$Te$_6$ units running along the $c$-axis, separated by the monovalent Tl$^+$ cations. The face-sharing Mo$_6$ octahedra can be viewed as Mo$_3$ triangles related to each other by a screw axis; as such, the crystal structure is nonsymmorphic. Each Mo$_3$ triangle has one extra electron donated by the Tl$^+$ ion.

We now focus on the pressure evolution of the band structure, with close attention to its Dirac crossing points. The calculated bulk band structure and Fermi surface with SOC under three representative pressures (0, 30, 50 GPa) are shown in figure 2. Our results for the ambient pressure (figure 2(a)) are in good agreement with previous reports [6, 7]. There are
two bands crossing the Fermi level. The bands along the $c$ axis ($\Gamma$–A and $\Gamma$–L) are highly dispersive. In contrast, the dispersions along the $\Gamma$–M–K–$\Gamma$ ($k_z = 0$ plane) and A–H–L ($k_z = \pi$ plane) are relatively flat, reflecting the q-1D feature of the structure. The SOC splitting is clearly visible between A and L points. Within the energy window of $\sim 1$ eV around the Fermi level, there are only two linear bands from conduction and valence bands crossing at A and L points from $\Gamma$. As extensively discussed in [7], the band crossing at A has a linear dispersion along $\Gamma$–A and becomes cubically dispersed in the perpendicular directions, e.g. along A–H, thus confirming the cubic Dirac fermions at A. By contrast, the Dirac point at L has linear dispersions along all directions in momentum space albeit with highly anisotropic velocities, consistent with an anisotropic Dirac cone. It should be remarked that there are possibly more Dirac-like crossings in the path of $\Gamma$–A at 300–500 meV above the Fermi level. However, these Dirac-like points are beyond the scope of our current interest in this study. Furthermore, the Fermi surface analysis has been performed to determine the band type using SKEAF (supercell K-space extremal area finder) [33]. It is shown that Mo-derived 4$d$ orbital dominates at the Fermi level and the blue dispersion in figure 2(a) is hole-like while the red one is electron-like. The bulk Fermi surface with color-coded Fermi velocity are visualized in the right panel (figure 2(d)), which is composed of two parts: the outer hole-like FSs and the inner electron-like FSs near the top and bottom boundaries of the first Brillouin zone. The flatness of the FSs also indicates the q-1D feature at ambient pressure. As the pressure increases, however, the band dispersion is dramatically reconstructed (see figures 2(b) and (c)). Distinctly different from the ambient case, there are totally five bands crossing the Fermi level for 30 and 50 GPa. At 30 GPa, the original Dirac bands shifts upward at L point and a new Dirac point arises at the Fermi level from the original valence bands, resulting in two Dirac crossings at the same $k$-point separated by $\sim 200$ meV in energy. At 50 GPa, this new Dirac point shifts further up in energy and touches with the original Dirac point, making a fourfold degenerate point at L. On the other hand, the cubic Dirac point at A is largely unchanged up to 50 GPa except that it moves up or down in energy. As for the Fermi surface, the original flat q-1D FSs become more three-dimensional under pressure, especially in the Brillouin zone center where a barrel-like electron pocket emerges at 30 GPa and 50 GPa. This is conceivably because the dissociated Tl atoms at zero pressure become bonded with their neighboring Se ions and form the Tl–Se$_6$ cuboid with pressure. Meanwhile, the face-sharing Mo$_6$ octahedra collapse at high pressure. As a consequence, the dramatic change in the bonding induced by pressure causes the reconstruction of charge distribution, band dispersion and Fermi surface morphology.

Figure 3 depicts the phonon spectra of Tl$_2$Mo$_6$Se$_6$ under 0 GPa, 30 GPa and 50 GPa (all with P6$_3$/m space group). At 0 GPa, soft phonon modes are found in the $k_z = 0$ plane ($\Gamma$–M–K–$\Gamma$) as well as in the directions of $\Gamma$–A and $\Gamma$–L, indicating that such a high-symmetry semimetallic structure is dynamically unstable against density wave formation. In 1D systems, Peierls demonstrated that at low temperature an instability can be induced by the coupling between carriers and a periodic lattice. Such an instability induces a charge ordering phenomenon and a metal–insulator phase transition [34]. Such an electron–phonon-driven transition is expected to be second order. If one applies a distorted structure with a reduced symmetry of space group $P\bar{3}$, the negative phonon modes would naturally be depleted with an electronic band gap opened (semimetal–insulator transition) [7]. Alternatively, as we apply a pressure to the undistorted structure, the negative phonon modes would be progressively eliminated. As shown in figure 3(c) at 50 GPa, no soft phonon mode can be observed. This is consistent with the experimental finding that pressure can gradually tune this family of materials away from a metal–insulator transition, making them more metallic and in some extreme cases, becoming superconducting [10, 12, 13].

The bulk-boundary correspondence in topology prompts us to study its surface states under pressure. We calculate the surface band structure on the (001) plane using a tight-binding model based on maximally localized Wannier functions, as shown in figure 4. As the Dirac point in a DSM could be understood as two degenerate Weyl points with opposite chirality, one might expect that there are two copies of Fermi arcs on the DSM surface, forming a ring with two singularities at the surface projection of the Dirac points in the bulk [35–39]. Recently, however, Kargarian et al argued that the Fermi arcs on the DSM surface are not topologically protected [40] and can be continuously deformed into a closed Fermi

![Figure 3. Calculated phonon dispersions at (a) ambient pressure, (b) 30 GPa, and (c) 50 GPa.](image-url)
Figure 4. Calculated surface band structures at (a) 0 GPa, (b) 30 GPa, (c) 50 GPa; (d)–(f) the corresponding surface state spectra on the (001) plane. The red dots in (d) and (e) are the projection of the bulk Dirac points. Bright red lines denote the surface states.

countour without any symmetry breaking. From figure 4(d), one can clearly see the closed Fermi contour surrounding the $\Gamma$ point, instead of two Fermi arcs connecting the projection of the bulk Dirac nodes. Under 30 GPa, the Fermi contour on DSM surface is continuously deformed into the one shown in figure 4(e) without any symmetry breaking. At 50 GPa, only few surface states survived, which denotes weak topological character. The calculated $Z_2$ index suggests the possible topological phase transitions under pressure within this $P6_3/m$ phase: $Z_2$ index is 1 (0, 010) at zero pressure; at 30 GPa, the calculated $Z_2$ invariant numbers are 1 for $k_z = 0$, $k_y = 0$, and $k_x = \pi$ plane, and zeros for other planes, thus the topological index is 1 (0, 010), which indicates a strong topological material; at 50 GPa, only few surface states survive with topological index (0, 001), which denotes weak topological character. As a result, in the $P6_3/m$ phase, $\text{Tl}_2\text{Mo}_6\text{Se}_6$ may undergo a second order topological phase transition from a DSM to a strong topological metal and then to a weak topological metal.

We further use crystal structural prediction techniques to find energetically stable structures of $\text{Tl}_2\text{Mo}_6\text{Se}_6$ under extremely high pressures. The calculated enthalpy-pressure ($\Delta H - P$) curves are plotted in figures 5(a) for the structures of interest. Several crystallographic structures shown in figure 5 are found to be the stable/metastable phases with lower energies at high pressures. In our calculations, we find three candidate structures under high pressures: orthorhombic $Cmcm$ phase, tetragonal $P4mm$ phase and body-centered tetragonal $I4mm$ phase. Among these candidates, body-centered tetragonal phase has the lowest enthalpy when the pressure is larger than 50 GPa. Thus, with increasing pressure, $\text{Tl}_2\text{Mo}_6\text{Se}_6$ may undergo a structural phase transition, from the hexagonal $P6_3/m$ to $I4mm$ structure at about 50 GPa. The unit cell of $I4mm$ structure consists of one formula unit, containing edge-sharing Mo–Se$_8$ cubes. Mo ions are located at the center of the cube and TI ions stay in the space between the cubes. The calculated band structure, Fermi surfaces and Brillouin zone with high-symmetry $k$ points are shown in figures 5(e)–(g) for the $I4mm$ structure at 80 GPa. As noted, there are six bands crossing the Fermi level, constructing the complicated three dimensional Fermi surfaces. The further topological band analysis shows that the $I4mm$ structure is a topological trivial phase.

In order to estimate the superconducting $T_c$ of $\text{Tl}_2\text{Mo}_6\text{Se}_6$ under pressure, we performed the linear response calculations of its electron–phonon properties, and estimated the critical temperature through the Mc-Millan Allen–Dynes formula [41, 42]

$$k_B T_c = \frac{\hbar \omega_{\text{th}}}{1.2} \ln \left[ \frac{1.04(1 + \lambda)}{\lambda - \mu^* (1 + 0.62 \lambda)} \right],$$

where $\omega_{\text{th}}$ is the logarithmically averaged phonon frequency, $\lambda$ is the electron–phonon coupling constant, and $\mu^*$ is the Coulomb pseudopotential which is set to be 0.1 in the calculations. We evaluate the pressure-dependent electron–phonon coupling constant $\lambda$ and the superconducting transition temperature $T_c$ shown in figure 6. It is found that both $\lambda$ and $T_c$ decrease, while $\omega_{\text{th}}$ increases with increasing pressure. Several other compounds have similar behaviors, especially at high pressures [43–45]). The electron–phonon coupling constant given by phonon calculations ranges from 0.44 to 0.57, with corresponding $T_c$ from 2.5 K to 5.0 K. This result can be verified by further experimental studies at high pressure.

4. Discussion and conclusion

When interacting electrons are spatially confined in the reduced dimensions, they show an enhanced tendency toward exotic electronic ground states, which makes them a fascinating topic of research, both theoretically and experimentally [46]. Q-1D systems provide an excellent playground in which to explore electronic correlations in low dimensions as they exhibit a rich variety of physical phenomena, including non-Fermi-liquid behaviors, superconductivity, charge density wave distortion and so on [46, 47]. It is well established theoretically that the conventional picture of Fermi liquid theory does not apply when interacting electrons are confined to a single dimension, i.e. the Fermi liquid approach breaks down spectacularly in 1D metals [18]. Instead, it can be described by
the Tomonaga–Luttinger liquid paradigm, where the elementary excitations are collective spin and charge modes, propagating with different velocities and leading to spin-charge separation [18]. Surprisingly, for the q-1D molybdenum chalcogenides $A_2\text{Mo}_6X_6$, no experimental investigation has as yet been done in this respect, primarily due to the unfavorable sample dimensions of the single crystals available for the spectroscopic measurements, such as ARPES and STM.

From the transport point of view, a Tomonaga–Luttinger liquid manifests a gross violation of an empirical law, i.e. the Wiedemann–Franz (WF) law which states that the ratio of the electronic thermal conductivity $\kappa_e$ to the electrical conductivity $\sigma$ at a given temperature $T$ is equal to a constant called the Lorenz number, $L_0 = \kappa_e / \sigma T = 2.44 \times 10^{-8} \text{ W} \cdot \Omega \cdot \text{K}^{-2}$ and reflects that the same quasiparticles are responsible for both the thermal and electrical transport. This law was found to be

Figure 5. (a) Calculated enthalpy curves for $P4mm$ (circles), $P6_3/m$ (down-triangles) and $I4mm$ (up-triangles) phases with respect to the $Cmcm$ structure (squares), as a function of pressure from 0 to 150 GPa. Crystal structure of (b) $I4mm$, (c) $Cmcm$, and (d) $P4mm$. (e)–(g) The band structure, top view of Fermi surfaces and the Brillouin zone of the $I4mm$ structure at 80 GPa, respectively. The bands crossing the Fermi level in (e) are marked by different colors.

Figure 6. (a) The logarithmically averaged phonon frequency $\omega_n$, (b) electron–phonon coupling constant $\lambda$, and (c) superconducting $T_c$ as a function of pressure in the $I4mm$ structure.
strongly violated in the q-1D purple bronze Li_{0.9}Mo_{0.17}O due to its spin-charge separation \[48–50\]. In the future, a similar test can be done for the q-1D A_{2}Mo_{6}X_{6} to search for the possible non-Fermi liquid behavior therein.

Q-1D conductors are prone to the Peierls distortion, forming the charge density modulation in real space. Indeed, some members in A_{2}Mo_{6}X_{6} family, such as Na_{2}Mo_{6}Se_{6}, Rb_{2}Mo_{6}Se_{6}, Rb_{2}Mo_{6}Te_{6}, etc. undergo a metal–insulator transition at low temperatures, suggesting the CDW formation \[12, 13\]. For Tl_{2}Mo_{6}Se_{6}, there are two types of samples, one with metallic ground state while the other having resistivity upturn at low temperatures \[9\]. This fact suggests that Tl_{2}Mo_{6}Se_{6} is actually on the border of the Peierls transition, consistent with its q-1D Fermi surface and the soft phonon revealed in our calculations. Under a uniform pressure, our calculations suggest more three dimensionality of the electronic structure, in line with the experimental finding of the better metallicity at a small hydrostatic pressure \[10\]. Interestingly, a uniaxial strain induces a metal-to-insulator transition in Tl_{2}Mo_{6}Se_{6} \[15\]. The mechanism for this opposite trend under uniaxial and hydrostatic pressure merits a further study.

Tl_{2}Mo_{6}Se_{6} also becomes superconducting below 3–5 K, depending on the sample quality. Very recently, Huang et al. proposed that Tl_{2}Mo_{6}Se_{6} is a time-reversal invariant topological superconductor induced by intersublattice pairing, favoring a spin-triplet order parameter with \(E_{2u}\) symmetry \[22\]. Like topological superconductor Cu_{1.5}Bi_{2}Se_{3}, this odd-parity pairing would spontaneously break the rotational symmetry in its gap function and produce a nematic order \[51–56\]. Certainly, it would be very interesting to probe the possible nematic superconductivity in Tl_{2}Mo_{6}Se_{6} by, e.g., the high-resolution angle dependent calorimetric study \[55\].

To summarize, via first-principles calculations, it is predicted that the topological properties of the q-1D conductor Tl_{2}Mo_{6}Se_{6} change dramatically with pressure up to 50 GPa, above which a structural phase transition takes place to drive the system into a topologically trivial phase. Our calculations also reveal the pressure dependence of the topological surface and the phonon modes. Recently, it was predicted that, in the presence of strong interactions, DSM or WSM can easily undergo a continuous quantum phase transition into either an axion insulator or a rotational symmetry-breaking nematic state \[57\]. Our results establish Tl_{2}Mo_{6}Se_{6} as an ideal arena for further exploring various topological phenomena associated with different types of topological fermions and may potentially be useful for engineering these nontrivial carriers in future applications.

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