Type-II Dirac cones and electron-phonon interaction in monolayer biphenylene from first-principles calculations

Peng-Fei Liu, Jingyu Li, Chi Zhang, Xin-Hai Tu, Junrong Zhang, Bao-Tian Wang, and David J. Singh

1Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, China
2Spallation Neutron Source Science Center, Dongguan 523803, China
3Key Laboratory of Materials Physics, Institute of Solid State Physics, HFIPS, Chinese Academy of Sciences, Hefei 230031, China
4Foshan (Southern China) Institute for New Materials, Foshan 528200, Guangdong, China
5College of Electrical Engineering, Henan University of Technology, Zhengzhou 450001, China
6School of Physics and Physical Engineering, Qufu Normal University, Qufu 273165, China
7LCP, Institute of Applied Physics and Computational Mathematics, Beijing 100088, China
8Collaborative Innovation Center of Extreme Optics, Shanxi University, Taiyuan, Shanxi 030006, China
9Department of Chemistry, University of Missouri, Columbia, Missouri 65211, USA
10Department of Physics and Astronomy, University of Missouri, Columbia, Missouri 65211, USA

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We report a first-principles investigation of electronic structure, topological bands, and electron-phonon interactions in metallic biphenylene sheets. Biphenylene is a recently synthesized sp2-bonded carbon allotrope. We find coupling of electrons at the Fermi surface to very high frequency carbon-derived phonons, analogous to superconducting MgB2. This leads to low-temperature weak coupling superconductivity due to an unusual combination of exceptionally large logarithmically averaged phonon frequency $\omega_{\text{ave}}=1369$ K and moderate electron-phonon coupling. The electronic structure shows a two-band Fermi surface dominated by C p orbitals and a pair of type-II tilted Dirac cones along the $\Gamma$–Y line at the Brillouin zone boundary. Berry curvature and edge-state calculations show that monolayer biphenylene is a two-dimensional $Z_2$ topological material. Thus, monolayer biphenylene is predicted to be a topological superconductor based on C p orbitals and high-frequency phonons.

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I. INTRODUCTION

Carbon is exceptional in the diversity of its allotropes arising from its combination of strong directional covalent bonding and competition between different hybridization schemes, particularly sp, sp2, and sp3 bonding [1]. The strong bonding leading to highly dispersive energy bands and generally high stability of the allotropes has provided exciting platforms for realizing novel physics. These include graphite [2], diamond [3], carbon nanotubes [4], fullerenes [5], graphene [6], and others [1]. Graphene, in particular, provides a platform for a wide variety of novel behaviors associated with its Dirac cones at the Fermi level [6,7]. These include ballistic charge transport [8], the quantum spin Hall effect [9], Klein tunneling [10], exceptional carrier mobilities [11], Majorana zero modes [12], and other phenomena [13]. This motivates searches for and investigation of other Dirac materials [14–18], especially materials based on carbon and analogs of them.

Carbon-based superconductivity provides the possibility of exceptionally high critical temperatures due to the possibility of coupling to high-frequency phonons with strong electron-phonon matrix elements arising from the strong bonding and light mass of carbon, as well as the possibility of novel features associated with topological aspects of the electronic structure of some carbon allotropes, especially graphene. This was anticipated in the discovery of electron-phonon superconductivity MgB2, which is closely related to graphene. MgB2 has an exceptionally high ambient pressure critical temperature of $T_c=39$ K [19], based on coupling to high frequency modes as well as two-gap superconductivity [20,21]. In fact, the unique carbonlike characteristics of MgB2, specifically high-energy scales, has enabled elucidation of two-gap superconducting physics [22]. Additionally, similar and higher critical temperatures have been discovered in doped fullerenes, which, in addition, provide a platform for investigating superconductivity in proximity to metal insulator transitions and magnetism [23]. Finally, graphene itself has been shown to be an exciting superconductor when modified through doping or twisting [24–32]. Superconductivity with $T_s \sim 5.9$ K is found Li-decorated monolayer graphene [33]. Superconductivity has also been observed in Ca-decorated graphene [34,35]. First-principles theory shows that these are well explained as electron-phonon superconductors [28,36,37].

These results raise the question of whether an intrinsic 2D sp2-bonded carbon allotrope with topological Dirac cones and
superconductivity without requiring doping, twisting, or strain can be found. This would offer the potential for a highly stable, readily realizable platform for investigating topological superconductivity. Here we investigate biphenylene as a candidate and find that it is, in fact, a topological superconductor, with features related to those of MgB$_2$, particularly the coupling to high-frequency phonons, but in a weak coupling regime.

Biphenylene is a planar $sp^2$-hybridized carbon allotrope with intrinsic Dirac cones. Similar to graphene, it is atomically thin. However, the structure is more complex and is comprised of approximately square four-membered, six-membered, and eight-membered carbon rings [38]. The possibility of synthesizing biphenylene has been recognized for some time. This motivated several attempts and synthesis and the discovery of interesting related phases with potential practical applications [39–41]. Finally, biphenylene was recently experimentally synthesized [42] and shown to be a stable metal [43–45]. Here we show that besides being a metal, biphenylene is both a topological metal and superconducting. We find that there is a pair of type-II Dirac cones derived from C $p_z$ orbitals approximately 0.63 eV above the Fermi energy in monolayer biphenylene and that the material is an electron-phonon superconductor. It exhibits a nontrivial $Z_2$ topological invariant exhibiting protected edge states at the boundaries with one-way propagation.

II. COMPUTATIONAL METHODS

Our first-principles calculations were performed in density-functional theory with the local density approximation and norm-conserving pseudopotentials [46,47]. We used a plane-wave basis as implemented in the QUANTUM ESPRESSO (QE) package [48,49], with plane-wave basis set cutoffs of 80 Ry for the wave functions and 320 Ry for the charge density. The zone sampling in the self-consistent calculations was done with a Methfessel-Paxton smearing of 0.02 Ry on a $20 \times 16$ Monkhorst-Pack grid k-mesh [50]. The internal atomic positions are fully relaxed with a threshold of 10 meV/Å for the forces. We used periodic supercells with a length of 20 Å along the $z$ direction, perpendicular to the biphenylene sheets.

The phonon dispersions were calculated within density-functional perturbation theory [51] on a $10 \times 8$ q-mesh using the Phonon code in the QE package. The mode-resolved magnitudes of the electron phonon coupling (EPC) $\lambda_{q\nu}$ were calculated as [52,53]

$$\lambda_{q\nu} = \frac{\gamma_{q\nu}}{\pi N(E_F)\omega_{q\nu}^2},$$

where $\gamma_{q\nu}$ is the phonon linewidth, $\omega_{q\nu}$ is the phonon frequency, and $N(E_F)$ is the electronic density of states at the Fermi level. The $\gamma_{q\nu}$ are calculated as

$$\gamma_{q\nu} = \frac{2\pi \omega_{0\nu}}{\Omega_{BZ}} \sum_{k,n,m} |\xi_{kn,k+q\nu}^\nu|^2 \delta(\epsilon_{kn} - \epsilon_F) \delta(\epsilon_{k+q\nu} - \epsilon_F),$$

where $\Omega_{BZ}$ is the volume of the Brillouin zone, the $\epsilon_{kn}$ ($\epsilon_{k+q\nu}$) are the Kohn-Sham eigenvalues, and $\xi_{kn,k+q\nu}^\nu$ are the EPC matrix elements [55]. The Eliashberg electron-phonon spectral function $\alpha^2 F(\omega)$ is then calculated by

$$\alpha^2 F(\omega) = \frac{1}{2\pi N(E_F)} \sum_{q\nu} \frac{\gamma_{q\nu}}{\omega_{q\nu}} \delta(\omega - \omega_{q\nu}).$$

The total EPC $\lambda$ can be calculated in two ways. These are integrations of the EPC constant $\lambda_{q\nu}$ in the full Brillouin zone for all phonon modes or by integrating the Eliashberg spectral function $\alpha^2 F(\omega)$ [54]:

$$\lambda(\omega) = \sum_{q\nu} \lambda_{q\nu} = 2 \int_0^{\omega_0} \frac{\alpha^2 F(\omega)}{\omega} d\omega.$$\phantom{.}(4)

The superconducting transition temperature, $T_c$, is determined from the calculated EPC constant $\lambda$ by the McMillan-Allen-Dynes formula,

$$T_c = f_1 f_2 \frac{\omega_{log}}{1.2} \exp \left[ -\frac{1.04(1 + \lambda)}{\lambda - \mu^*(1 + 0.62\lambda)} \right],$$

where $\mu^*$ is the effective screened Coulomb repulsion constant, $\omega_{log}$ is the logarithmic average frequency,

$$\omega_{log} = \exp \left[ \frac{2}{\lambda} \int_0^{\infty} \frac{d\omega}{\omega} \alpha^2 F(\omega) \log \omega \right],$$

and $f_1$ is the correction factor when $\lambda > 1.3$ [55]. As discussed below, we find lower values of $\lambda$ characteristic of weak coupling, and used values of $\mu^* = 0.1$ and $f_1 f_2 = 1$.

We analyzed the electronic structure in terms of Wannier orbitals to examine the electronic structure of nanoribbons for edge states. The Wannier tight-binding (TB) Hamiltonian was constructed from the first-principles Bloch functions by projecting the states onto maximally localized Wannier functions (MLWFs) [56] using the WANNIER90 package [57,58]. In the model, the MLWFs are derived from six C $p_z$ orbitals. The nontrivial boundary-edged states are calculated from the imaginary part of the surface Green’s function [59] as obtained with the WANNIERTOOLS package [60]. Fermi surfaces colored as a function of an arbitrary scalar quantities in this paper are drawn by using the FERMI-SURFER program [61].

III. RESULTS AND DISCUSSION

A. Atomic structure and electronic properties

Layered biphenylene forms in the centrosymmetric orthorhombic space group $Pmmn$ (No. 47). The monolayer is illustrated in Fig. 1. There are two crystallographically distinct C positions: C1, site symmetry 4c; and C2, site symmetry 2p. The optimized lattice constants are $a=3.75$ Å and $b=4.51$ Å. These compare well with a prior calculation ($a=3.76$ Å and $b=4.52$ Å) [38]. Importantly, the structure is clearly anisotropic between the $a$ and $b$ directions. This leads to the expectation of anisotropic physical properties. The structure is based on three types of C rings: tetragons hexagons and octagons, with C–C bond lengths ranging from 1.40 Å to 1.45 Å. These compare well with a prior calculation [38].

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FIG. 1. Structure of monolayer biphenylene in a top view. The unit cell, bond lengths, and angles are as indicated by the solid black lines. This shows that monolayer biphenylene has a truly planar structure.

The calculated band structure and corresponding electronic density of states are shown in Fig. 2. The band structure is metallic with two bands crossing the Fermi level. This is in accord with prior calculations [38,62] and experimental $dV/dI$ spectra [42]. As shown in the orbital-resolved band structure of Fig. 2(a), the $p_{x,y}$ orbitals hybridize with the $s$ orbitals to form 18 strong covalent in-plane $\sigma$ bonds. The unhybridized $p_z$ orbitals form six relatively weak out-of-plane $\pi$ bonds. The third and fourth $\pi$ bands contribute to the Fermi surface. Thus the Fermi surface is derived from $\pi$ orbitals. As seen, the valence and the conduction bands touch along the $\Gamma$-Y line with linear dispersion to form intrinsic type-II Dirac cones approximately 0.63 eV above the Fermi level [Figs. 2(b) and 3(b)]. Also, as seen in Fig. 3(a), the valence band contributes elliptical hole pockets around Y, while the conduction band forms elliptical electron pockets around the S points. Thus, the Fermi surface has two Fermi pockets. These Fermi surfaces are compensating with equal areas corresponding to the even electron count, but have different average velocities.

The Fermi surfaces colored to indicate relative Fermi velocity are shown in Fig. 3(a). The ratio between the maximum and minimum velocity is approximately 4.2. This reflects the very different slopes of the bands comprising the Fermi surface as seen in the band structure, for example, the high velocity of the lower band coming from $\Gamma$ and crossing the Fermi level along $\Gamma$-Y, as compared to the relatively weak dispersion of the band crossing the Fermi level along X-S. Thus, the hole pocket around Y has higher Fermi velocity than the electron pocket around S, leading to the expectation that the electrical transport will be dominated by hole carriers, while the density of states will be dominated by the electron carriers. This is opposite to iron-based superconductors and many other superconductors where hole Fermi surfaces are heavier than the electron Fermi surfaces in terms of Fermi velocities [63]. We note that, similar to graphene, spin orbit is expected to have an extremely small effect as a consequence of the small atomic number of carbon [64,65].

B. Topological numbers and edge states

As may be noted, graphene, which is a Dirac material, has an intrinsic nontrivial topological band feature [9]. Especially in light of this, it is important to determine whether 2D biphenylene with its Dirac cones is also topological. Biphenylene has a structure with inversion symmetry. Therefore, we can verify the nontrivial topological nature of a biphenylene sheet via the $\mathbb{Z}_2$ topological invariant. This number comes directly from the parities of the occupied bands at time reversal invariant momentum (TRIM) points [66,67]. The

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<td>$\Gamma$</td>
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TABLE I. The calculated parity eigenvalues of the 12 occupied spin-degenerate bands at four TRIM points for monolayer biphenylene.
FIG. 4. Berry curvature $\Omega \xi$ distributions (a) in the Brillouin zone and (b) along the high-symmetry lines for single-layer biphenylene.

The parities $\xi(i)$ of 12 occupied valence bands for the biphenylene monolayer are given in Table I. The parity products for the occupied states at the TRIM points are calculated, by $\delta(k_i) = \prod_{\nu=1}^{12} \xi(i)$, to be $+1$, $+1$, $-1$ and $+1$ for $\Gamma$, $X$, $Y$, and $S$, respectively. This yields a nontrivial topological invariant $\nu = \prod_{i=1}^{4} \delta(k_i)$. This result clearly indicates the presence of nontrivial topological states in biphenylene.

To further confirm the topological nature of the Dirac points, we calculate the Berry curvature via

$$\Omega^\xi_n(k) = i \langle u_n(k) | \nabla_k | u_n(k) \rangle,$$  

(7)

where $u_n(k)$ represents the Bloch wave function of the $n$th band. In Fig. 4, a pair of Dirac points at the boundary of the Brillouin zone could show the positive and negative Berry curvature distributions. These then would serve as the source and sink of the Berry curvature in the momentum space, respectively. We calculate the Berry phases [68,69] by

$$\gamma_n = \oint_C \Omega^\xi_n(k) \cdot dk.$$  

(8)

For this purpose, we define a circle on the $k_z = 0$ plane centered at the Dirac point to calculate the Berry phase [70]. The needed radius of the circle is arbitrary as long as it does not cover another Dirac point. We find that the Berry phase for the Dirac point is either $\pi$ or $-\pi$, indicating that the crossing points are indeed pairs of topologically nontrivial points with opposite Berry phases [68].

Nontrivial topology in a 2D crystal can be also characterized via the topologically protected edge states due to the bulk-edge correspondence [71,72]. We used a TB model as mentioned above to construct a supercell of a one-dimensional nanoribbons. As discussed in the case of graphene [72], two representative nanoribbons, one with a zigzag configuration shown in Fig. 5(a) and one with an armchair configuration shown in Fig. 5(b) were constructed by cutting the biphenylene sheet. For the armchair-edged boundary, as shown in Fig. 5(c), the topologically protected edge states originate from the Dirac points and disappear into the bulk states. This confirms the nontrivial topological phase in monolayer biphenylene. In the case of the zigzag-edged ribbon, as indicated in Fig. 5(d), we find an absence of $d-1$-dimensional edge states. This is consistent with the above topological chirality analysis where only the $Y$ point hosts odd parity and gives rise to the topological band.

FIG. 5. Structural models for ribbons of single-layer biphenylene with (a) armchair-edged and (b) zigzag-edged boundaries. To clearly display the nanoribbons, we replace some of the repeated periodic cells by dotted lines. Momentum-resolved local density of states projected on the edges of semi-infinite nanoribbons for (c) armchair and (d) zigzag boundaries. The black lines in (c) and (d) indicate the band structure of monolayer biphenylene.
C. Phonons and electron-phonon interactions

Figure 6 shows the phonon dispersions and the projected phonon density of state over the whole frequency range. The results are in accord with prior calculations [38,62,73,74]. The absence of unstable modes in the Brillouin zone confirms the dynamic stability of monolayer biphenylene with a planar structure. The highest phonon frequency is approximately 209 meV, which is slightly larger than in the case of graphene [70]. There are six atoms per unit cell in biphenylene, leading to 18 phonon branches in the dispersion: three acoustic and 15 optical branches. The acoustic branches are an out-of-plane (ZA), an in-plane transverse (TA), and an in-plane longitudinal (LA) branch. These cross several low-frequency optical branches. The ZA mode around the Γ point has a parabolic dispersion characteristic of a planar material, while the LA and TA modes show linear dispersions near the Γ point.

We used in-house postprocessing programs to determine atomic characters and directions [75,76] based on \(|e_{\nu j}(\vec{q}, \vec{q})|^2\), where \(e\) is the polarization vector of the \(j\)th atom and the \(\nu\)th band at \(\vec{q}\) along the \(\alpha\) direction. The phonon dispersions colored according to the contributions of different C sites and vibrational directions are shown in Figs. 6(a)–6(c). The out-of-plane C vibrations mainly contribute to the lower energy phonons. The high-energy phonons, above 100 meV, are almost entirely from the in-plane vibrations. This is similar to graphene.

We now turn to superconductivity, which we discuss based on the calculated electron-phonon Eliashberg spectral function \(\alpha^2 F(\omega)\). As seen in Fig. 6(d), phonons from 119 to 130 meV, dominated by the in-plane vibrations that modulate C–C bond lengths, make the main contributions to the EPC based on the calculated \(\alpha^2 F(\omega)\). There are also significant contributions from even higher frequency modes as seen in the peak in the spectral function around 150 meV. This is different from the behavior of most other 2D superconductors, such as Cu2Si [77], borophene [78], B2O [79], and Cu-BHT [80]. In those materials, out-of-plane vibrations dominate the EPC.

The integrated EPC \(\lambda_{\text{tot}}(\vec{q})\), given by \(\lambda_{\text{tot}}(\vec{q}) = \sum_\nu \lambda_{\nu}(\vec{q})\), is plotted in Fig. 7. According to Eq. (1), when \(\omega_{q\nu}\) is zero, \(\lambda_{\text{tot}}\) goes to infinity. For it to make sense, we set the \(\lambda_{\nu}\) of the three acoustic branches at the Γ point to the nearest neighbor. As seen, optical phonons around the Γ point contribute strongly to the EPC. This is seen particularly along the Γ–S line. The overall EPC constant \(\lambda\) is approximately 0.3. This is a very small value for a superconductor. Nonetheless, superconductivity with a \(T_c\) of 0.59 K is predicted with \(\mu^* = 0.1\). The relatively high \(T_c\) for low \(\lambda\) is a consequence of the very high frequencies of the phonons that are coupled. The logarithmic averaged frequency \(\omega_{\text{log}}\) for biphenylene sheet is 1369 K. The critical temperature is larger than that predicted in hole-doped graphene [30], where \(\omega_{\text{log}} = 0.27\) and \(T_c\) in the order of \(\sim 10^{-4}\) K were reported. It is also much smaller than the values \(\lambda = 0.55\) and \(T_c = 5.1–7.6\) K in Li-decorated graphene [28] \((\omega_{\text{log}} = 0.71\) and \(T_c = 6.8–8.1\) K), in Ca-intercalated graphene [36], and \(\lambda = 0.42\) and \(T_c = 13\) K in heavily n-doped graphene [30]. The logarithmic averaged frequency \(\omega_{\text{log}}\) for biphenylene sheet is comparable to the value of \(\omega_{\text{log}} = 1316\) K in hole-doped graphene [30]. This implies an analogy between the superconductivity of hole-doped graphene and intrinsic undoped biphenylene. Finally, it should be noted that due to the weak coupling implied by the low \(\lambda\), the predicted value of \(T_c\) is highly sensitive to the choice of \(\mu^*\) although the prediction that the material is superconducting is robust in the usual range of \(\mu^*\) from 0.10 to 0.15.

We further investigated the superconductivity by calculations using the density-functional theory for superconductors...
by solving the gap equation with the SUPERCONDUCTING-TOOLKIT package [81,82]:

\[ \Delta_{nk} = -\frac{1}{2} \sum_{n'k'} K_{nk'/k}^{el} + K_{nk'/k}^{el-\text{ph}} \frac{\Delta_{nk'}}{Z_{nk}} \times \tanh \left( \frac{\beta E_{nk'}}{2} \right), \]  

(9)

where \( K_{nk'/k}^{el} \), \( K_{nk'/k}^{el-\text{ph}} \), and \( Z_{nk} \) are the electron-electron kernel, electron-phonon kernel, and renormalization, respectively. As shown in Fig. 8, the calculated \( \lambda_k \) has a significant anisotropy on the Fermi surface with values varying from 0.15 to 0.23. However, only one peak is in the distribution \( \rho(\lambda_k) \), which implies that, although there are two sheets of Fermi surface, the material should be classified as a single-gap superconductor [28]. The momentum-resolved EPC parameter \( \lambda_{nk} \) on the Fermi surface is shown in the inset of Fig. 8. Comparing with the band structure in Fig. 2(b) and the Fermi surface plot in Fig. 3(a), one observes that the larger values of \( \lambda_k \) are on the Y-centered Fermi pockets dominated by the valence band. Overall, our calculated EPC \( \lambda = 0.19 \) and \( T_c = 0.46 \) K from the superconducting density functional calculation are in accord with the values (\( \mu^* = 0.1, \lambda = 0.3, T_c = 0.59 \) K) from the averaging and McMillan-Allen-Dynes formula.

IV. CONCLUSIONS

In summary, we investigated the electronic structure and EPC of the recently synthesized \( sp^2 \) carbon allotrope, single-layer biphenylene. We find that the Dirac cones in biphenylene sheet are of type-II and in pairs with opposite valued Berry curvature. The topological nature is confirmed by the presence of edge states and the nonzero topological \( Z_2 \) invariant. We also find low-temperature weak coupling single-gap superconductivity. This arises from the combination of a very high logarithmically averaged phonon frequency, dominated by the in-plane vibrations, with a relatively low EPC constant \( \lambda \). Thus monolayer biphenylene is predicted to be a topological superconductor and may therefore be a useful platform for studying the interplay of topological bands and superconductivity in an intrinsic material. It will therefore be of considerable interest to perform low-temperature experimental studies searching for superconductivity in biphenylene and its monolayers.

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APPENDIX

As shown in Fig. 9, the valence band (blue line) and the conduction band (red line) touch at the Dirac point with a tilted-over cone in energy-momentum space. In addition, the two bands along the \( \Gamma-Y \) line have slopes with the same sign, which is an intuitive criterion for type-II points [83].


D. Ferguson, D. J. Searles, and M. Hankel, Biphenylene and phagraphene as lithium ion battery anode materials, ACS Appl. Mater. Interfaces 9, 20577 (2017).


