Chemical and structural stability of superconducting In$_5$Bi$_3$ driven by spin–orbit coupling

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Abstract

Relativistic effects play a prominent role in many electronic material properties such as the Rashba and Dresselhaus spin splitting in inversion asymmetric crystals, or the bulk band gap in topological insulators. By contrast, macroscopic material properties are typically not connected to relativistic phenomena. As an exception to this rule, we show that the macroscopic chemical and structural properties of superconducting In$_5$Bi$_3$ are driven by relativistic physics. In the non-relativistic limit In$_5$Bi$_3$ decomposes into elemental indium and bismuth, but the inclusion of relativistic spin–orbit coupling chemically stabilizes the In$_5$Bi$_3$ stoichiometry. Similarly, the structural stability of tetragonal In$_5$Bi$_3$ is driven by the spin–orbit interaction, which eliminates a phonon instability present in the non-relativistic limit. Low-temperature resistivity and heat capacity measurements show that In$_5$Bi$_3$ is a strong coupling superconductor, with a superconducting critical temperature of 4.2 K and a superconducting critical field of 0.3 T. The unconventional interplay between relativity with chemistry and structure, together with the presence of superconductivity, make In$_5$Bi$_3$ a versatile material that provides, for example, a simple model for the study of strong coupling superconductivity in quasiperiodic crystals.

1. Introduction

Relativistic effects play a prominent role in material properties, most prominently through the spin–orbit interaction which couples the spin and orbital electronic degrees of freedom [1]. In noncentrosymmetric crystals, the spin–orbit interaction leads to a splitting of the electronic states of opposite spin, associated with phenomena such as the Rashba [2, 3] and Dresselhaus [4] effects, recently extended to centrosymmetric crystals with asymmetric sites [5]. The manipulation of the spin textures arising in these materials, for example using electric fields in ferroelectric Rashba semiconductors [6], could be exploited in spintronics applications [7]. Combining noncentrosymmetric spin–orbit materials with superconductivity could lead to unconventional mixed singlet and triplet pairing states [8, 9]. In parallel, spin–orbit coupling also drives the bulk band gap in many topological materials [10–13], and also plays a prominent role in topological superconductors [14–16]. The latter can host Majorana quasiparticles that could find applications in quantum computers [17, 18]. The optoelectronic properties of materials can also be affected by spin–orbit coupling, for example it has been proposed that Rashba–like spin splitting could enhance carrier lifetimes in noncentrosymmetric semiconductors [19]. Interestingly, the spin–orbit interaction has occasionally been identified as even determining material properties that are not typically associated with relativistic effects, such as the voltage of the widely used lead-acid batteries [20].
In this work we explore the physical properties of superconducting In$_5$Bi$_3$, whose physical and chemical properties are dominated by the spin–orbit interaction. The experimentally reported structure of In$_5$Bi$_3$ is tetragonal with I$4/\text{mcm}$ symmetry (space group 140) and can be described as a commensurate host-guest structure with the host atoms arranged in octagonal channels with guest atomic chains inserted inside them, as shown in figure 1. Using a combination of first principles calculations and low-temperature measurements, we find that In$_5$Bi$_3$ exhibits two interesting features. First, the strong SOC of this material leads to the unusual scenario in which even the macroscopic chemical and structural properties are dominated by relativistic effects. Second, the structure of In$_5$Bi$_3$ can be thought of as an approximant for the incommensurate structure adopted by crystals such as the phase III of bismuth (Bi-III, realised under hydrostatic pressure), which have recently been shown to exhibit strong coupling superconductivity \[21\]. We find that In$_5$Bi$_3$ also exhibits strong coupling superconductivity, and could therefore become a fruitful playground for modelling superconductivity in quasiperiodic crystals.

2. Methods

2.1. Structure

In$_5$Bi$_3$ adopts a tetragonal structure of space group I$4/\text{mcm}$ and 16 atoms in the primitive cell. The lattice parameters $a_p$ of the primitive cell at 195 K are reported as \[22\]:

$$a_{p_1} = (8.48, \ 0.00, \ 0.00), \quad (1)$$

$$a_{p_2} = (0.00, \ 8.48, \ 0.00), \quad (2)$$

$$a_{p_3} = (4.24, \ 4.24, \ 6.30). \quad (3)$$

All our calculations are based on this primitive cell. However, it is customary to construct a conventional tetragonal cell, which in the case of In$_5$Bi$_3$ has supercell lattice parameters $a_s$ given by:

$$a_{s_1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -1 & -1 & 2 \end{pmatrix} a_{p_1} \quad (4)$$

The supercell lattice parameters $a_s$ are used below to report the structural features of In$_5$Bi$_3$ obtained at different levels of theory for ease of comparison with experiment.

2.2. Computational methods

2.2.1. Electronic structure calculations

We have performed our first principles calculations using density functional theory \[23, 24\] with the VASP implementation \[25–28\] of the projector augmented-wave method \[29, 30\]. Convergence tests determine that we use an energy cut-off of 500 eV and Brillouin zone (BZ) Monkhorst–Pack \[31\] $k$-point grids of size $6 \times 6 \times 6$ for In$_5$Bi$_3$, with a primitive cell lattice parameter of 8.48 Å. We also study elemental indium and bismuth for the purpose of calculating the formation energy of In$_5$Bi$_3$, and for these we use an energy cut-off of 500 eV and a finer BZ Monkhorst–Pack $k$-point grid of $12 \times 12 \times 12$, because of smaller primitive cells in

![Figure 1. Crystal structure of In$_5$Bi$_3$ in which the one-dimensional chains are highlighted inside the blue square at the center of the octagonal channels, and their length is perpendicular to the page. The structure has space group I$4/\text{mcm}$ (140) as reported in entry 1244 of the ICSD.](image)
indium and bismuth, with lattice parameters of 3.52 Å and 4.74 Å, respectively. All supercells calculations use commensurate grids. The valence electrons of indium are 4d\(^{10}\)5s\(^{2}\)5p\(^{1}\) and the valence electrons of bismuth are 5d\(^{10}\)6s\(^{2}\)6p\(^{3}\). We have employed the generalized gradient approximation of Perdew–Burke–Ernzerhof (PBE) [32] and the solid modification of PBE (PBEsol) [33] to approximate the exchange-correlation functional. We have included the spin–orbit interaction as a perturbation to the scalar relativistic Hamiltonian, the so-called second variational method [34].

2.2.2. Geometry optimizations
Our geometry optimizations for the internal atomic coordinates have been performed such that the force experienced by all atoms in the cell is lower than 10\(^{-4}\) eV Å\(^{-1}\). For the variable cell geometry optimizations, the stress on the cell has been converged to better than 10\(^{-2}\) GPa.

2.2.3. Lattice dynamics
We have performed the lattice dynamics calculations using an in-house code that implements the finite displacement method [35, 36] in conjunction with nondiagonal supercells [37]. We note that software to construct nondiagonal supercells was published together with [37]. To sample a coarse 2 × 2 × 2 \(q\)-point grid in the vibrational BZ, we use three different supercells constructed with the following supercell matrices:

\[
\begin{pmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
1 & 1 & 2
\end{pmatrix},
\begin{pmatrix}
1 & 0 & 1 \\
0 & 2 & 1 \\
0 & 0 & 1
\end{pmatrix},
\begin{pmatrix}
1 & 0 & 1 \\
1 & 1 & 0 \\
0 & 1 & 1
\end{pmatrix}.
\] (5)

all of which provide access to the (0, 0, 0) \(q\)-point, and then the first one provides access to the (0, 0, 1/2) \(q\)-point, the second one to the (0, 1/2, 0) point, and the third one to the (1/2, 1/2, 1/2) point. All other \(q\)-points on the 2 × 2 × 2 grid are related to these four by symmetry and therefore explicit calculations are not necessary. From these supercell calculations we have constructed the matrix of force constants, and then calculated and diagonalized the dynamical matrix along high-symmetry lines of the BZ to construct the phonon dispersion.

2.3. Experimental methods
We obtained samples of In\(_5\)Bi\(_3\) by radio frequency induction melting. High purity In and Bi were first etched with diluted acid and vacuum melted separately several times to remove surface oxidation. A stoichiometric combination of In and Bi was then melted together on a water-cooled copper boat under ultra-high vacuum and cooled down slowly by switching off the heater power. We measured the low temperature electrical resistivity \(\rho\) and the heat capacity \(C\) in a quantum design physical properties measurement system (PPMS) using a standard four-point AC technique and a pulse-relaxation method, respectively. The room temperature resistivity was scaled to published values [38].

3. Equilibrium properties

3.1. Formation energy
We calculate the static lattice formation energy per atom of In\(_5\)Bi\(_3\) according to:

\[
\Delta U_{\text{In}_5\text{Bi}_3} = \frac{U_{\text{in}_{N_{\text{In}}}} + U_{\text{Bi}_{N_{\text{Bi}}}}}{N_{\text{In}} + N_{\text{Bi}}},
\] (6)

where \(U_A\) denotes the internal energy of compound A, and \(N_A\) denotes the number of atoms of compound A. We have used the experimentally reported structures for both indium and bismuth as a starting point for our first principles geometry optimizations. Indium crystallizes in a structure of tetragonal I\(_4\)/mmm symmetry with 1 atom per primitive cell [39], and bismuth crystallizes in a structure of trigonal R\(_3\)m symmetry with 2 atoms per primitive cell [40].

Table 1 summarises the formation energy of In\(_5\)Bi\(_3\) at different levels of theory. In the non-relativistic limit, we obtain a positive formation energy of +28 meV/atom at the PBE level, and of +19 meV/atom at the PBEsol level, indicating that In\(_5\)Bi\(_3\) is chemically unstable to decomposition into elemental indium and bismuth. Interestingly, when we repeat the formation energy calculations including the relativistic SOC, we obtain lower formation energies of +6 meV/atom at the PBE level (still slightly unstable to decomposition), but of −1 meV/atom at the PBEsol level (resulting in a chemically stable composition). The latter results indicate that relativity drives the chemical stability of this compound. Inspection of the separate contributions from indium and bismuth reveals that the SOC is almost entirely dominated by bismuth.

Analogous calculations for In\(_5\)Sb\(_3\), which has been experimentally reported to have the same structure as In\(_5\)Bi\(_3\) [41], give a very similar picture in which relativistic SOC enhances chemical stability (see table 1). However, due to the weaker SOC present in antimony compared to bismuth, the change in formation energy is
smaller in In₅Sb₃. We note that antimony has the same structure as bismuth, crystallising in a rhombohedral lattice [42].

### 3.2. Structural parameters

There are multiple experimental reports of the structural cell parameters of In₅Bi₃ [22, 43], and we compare them with our calculated values in table 2. Our calculations based on the PBE exchange-correlation functional lead to an overestimation of the volume when compared with experiment. Remarkably, the values calculated with and without SOC differ significantly, with the a lattice parameter increasing by more than 3% and the c lattice parameter decreasing by more than 5% with the inclusion of relativistic corrections. The better agreement with experiment is only obtained with the inclusion of SOC. Repeating the calculations using the PBEsol functional instead again shows that the inclusion of SOC significantly improves the agreement with experiment.

For the subsequent calculations reported in this work, and unless otherwise stated, we use the lattice parameters of In₅Bi₃ reported in [22] as measured at 195 K (see table 2), and only optimize the internal atomic coordinates.

### 4. Lattice dynamics

#### 4.1. Non-relativistic limit

Figure 2(a) shows the phonon dispersion calculated without SOC. Two imaginary phonon modes appear at the Γ-point of the BZ, indicating that the experimentally reported I₄/mcm structure of In₅Bi₃ is dynamically unstable at the PBE level of theory.

The imaginary phonon modes have Eₜ symmetry and correspond to a distortion of the linear chains in which the atoms move in a direction perpendicular to the chain length, with the lighter indium atoms exhibiting the largest distortion. The octagonal channels also distort to accommodate the displaced chain atoms. The displacement pattern corresponding to one of the imaginary phonon modes is shown in the inset of figure 3, where the relative arrow lengths indicate the relative displacement amplitudes of the individual atoms.

We show the total energy as a function of phonon mode amplitude for one of the Γ-point imaginary modes in figure 3. The violet circles show the calculations without spin–orbit coupling (NSOC) and the potential exhibits a double-well shape indicating that the distortion associated with the depicted Eₜ phonon mode is an energy-lowering distortion of the I₄/mcm structure. Starting from one of the two equivalent minima of the double well, we have allowed the In₅Bi₃ structure to freely relax, arriving at a new monoclinic structure of space group Cm that is 7.6 meV per cell lower in energy than the experimentally reported I₄/mcm structure.

Overall, our lattice dynamics calculations at the PBE level of theory suggest that the experimentally reported I₄/mcm structure of In₅Bi₃ is dynamically unstable, and that a structure of space group Cm is the ground state of In₅Bi₃ at this level of theory.
Figure 2. Phonon dispersion of In$_5$Bi$_3$ calculated using the PBE exchange-correlation functional (a) without SOC and (b) with SOC. The results without SOC are also included in (b) as purple lines to facilitate comparison.

Figure 3. Total energy as a function of amplitude for one of the two degenerate $E_u$ modes. The inset shows the displacement pattern associated with this phonon mode, with red arrows corresponding to indium atoms, and green arrows to bismuth atoms. Note that when multiple arrows appear to emerge from a single atom, these in fact correspond to different atoms located exactly underneath the atom shown in the picture.
We re-emphasize that the results discussed in this section correspond to a calculation in which the cell volume and shape of In$_5$Bi$_3$ have been fixed to those reported experimentally in [22]. If instead we relax the cell volume and shape consistently using PBE (as reported in table 2), we still obtain an imaginary phonon mode at the $\Gamma$-point, but in this case it has $A_{2u}$ symmetry and is singly degenerate.

To further cross-check the validity of our calculations, we have repeated the calculations reported in this section using the CASTEP package [44] with both finite displacements and density functional perturbation theory [45, 46] for the lattice dynamics, and using both norm-conserving [47] and ultrasoft [48] pseudopotentials. The results obtained using CASTEP agree with those obtained using the method described in section 2.2, and therefore all results reported in this work have been obtained using the latter approach.

4.2. Spin–orbit coupling

Figure 2(b) shows the phonon dispersion of In$_5$Bi$_3$ calculated using the PBE exchange–correlation functional and with the inclusion of SOC (red lines), while also including the results obtained without SOC (purple lines) for comparison. The phonon dispersions are largely similar, with the high energy modes slightly softer and the low energy modes slightly harder in the SOC case. However, the most remarkable difference between the two dispersions is that the imaginary modes at the $\Gamma$-point disappear if SOC is included in the calculations.

The doubly degenerate modes that are imaginary at the PBE level of theory become real at the PBE+SOC level of theory. Their frequency is only 0.8 meV, but, as shown in figure 3, the distortion associated with these modes no longer lowers the energy of the system. Instead, the potential well has a strong anharmonic quartic nature that indicates the presence of soft vibrations along the direction perpendicular to the chain. The presence of low-frequency lattice vibrations could lead to strong coupling superconductivity, as recently reported for the related incommensurate Bi-III phase [21].

5. Structural distortion suppressed by spin–orbit

The results presented in section 4 show that relativistic SOC is central in stabilizing the crystal structure of In$_5$Bi$_3$. In order to understand the microscopic origin of this effect, we plot the calculated electronic band structure and density of states in figure 4 both with and without SOC. Both calculations show metallic behaviour, as expected for a superconducting material, and they also show a similar bandwidth. Figure 4(a) shows that SOC raises some degeneracies in bands near the Fermi energy, for example between the X and P points (highlighted with a blue square). To quantify this effect, figure 4(b) shows that for an energy between about 1 eV below the Fermi energy up to the Fermi energy itself (highlighted with an orange band), the density of states calculated without SOC is larger than the corresponding density of states calculated with SOC. This indicates that SOC suppresses the density of states near the Fermi energy, thus lowering the electronic energy of the system. Projecting the electronic states near the Fermi energy onto atomic orbitals reveals that they are dominated by bismuth $p$ states (see figure 4(b)), explaining the strong effect of SOC.

In the absence of SOC, the structural distortion described in section 4 lowers the overall energy of the system by reducing the density of states at the Fermi energy. This is similar to the well-known Peierls instability in one-dimensional atomic chains, but we emphasise that this distortion is not observed experimentally. When SOC is included, this relativistic interaction already lowers the density of states at the Fermi energy as shown in figure 4, thus rendering the structural distortion unnecessary. Our results suggest that this is sufficient to stabilize the I4/mcm structure of In$_5$Bi$_3$, and thus explain the experimentally observed phase.

An analogous spin–orbit mechanism to the one described here has been recently proposed to explain the structural stability of monolayer jacutingaite [49]. This material is a Dirac semimetal without the inclusion of SOC, and it undergoes a structural distortion that opens a trivial gap thus reducing the density of states at the Fermi energy. With the inclusion of SOC, a topologically non-trivial gap opens, thus rendering the structural distortion unnecessary. The only difference with the In$_5$Bi$_3$ system is that the latter remains metallic even in the presence of SOC. Put together, these results suggest that the spin–orbit interaction could play a major role in stabilizing high–symmetry crystal structures in metallic or semimetallic materials containing heavy ions.

We also note that the incommensurate nature of related materials such as Bi-III could also arise from the energetics near the Fermi energy, as has been discussed for a variety of other incommensurate crystals that exhibit a reduced density of states compared to commensurate counterparts, thus providing an alternative mechanism for reducing the energy of the system [50–52]. We therefore speculate that in materials like In$_5$Bi$_3$ or Bi-III there is a competition between a symmetry–lowering structural instability, an incommensurate instability, and the spin–orbit interaction, and their relative strength determines the eventual crystal structure of the system. For completeness, we remark that the Stoner instability provides an additional mechanism for reducing the density of states at the Fermi energy by inducing magnetic order, although this mechanism is unlikely to play a role in the class of materials studied here.
6. Superconductivity

Resistivity measurements confirm the high quality of our samples of In$_5$Bi$_3$, with a residual resistivity ratio of $\rho_{300\text{ K}} / \rho_0 \approx 33$ (figure 5). They display a sharp superconducting transition below $T_c \approx 4.17$ K, which shifts in moderate applied magnetic field (inset of figure 5). The mid-point transition temperatures can be used to extract an extrapolated upper critical field of just under 0.3 T for $T \to 0$ (inset of figure 6), which corresponds to a coherence length of $\xi \approx 330$ Å. These findings are consistent with earlier reports [38], which classed In$_5$Bi$_3$ as a type-II superconductor.

The low temperature heat capacity $C$ displays a temperature dependence that cannot solely be attributed to an electronic term $(\gamma T)$ plus an acoustic phonon term $(\beta T^3)$, as demonstrated by plotting $C/T$ versus $T^2$ in figure 6. Including an additional Einstein phonon contribution of the form

$$nR \left( \frac{\hbar \omega_0}{k_B T} \right)^2 \frac{e^{\hbar \omega_0/(k_B T)}}{\left( e^{\hbar \omega_0/(k_B T)} - 1 \right)^2}$$

produces a fit curve that follows the measured data closely (blue line in figure 6). Here, $n = (1.91 \pm 0.05)$ f.u. is the spectral weight attributed to this Einstein contribution, in number of modes per formula unit, $R$ is the molar gas constant, and $\omega_0 = \frac{\omega}{2\pi} = \frac{1}{2} (30.5 \pm 0.2)$ K is the frequency of the Einstein mode. We also find $\gamma = (16.7 \pm 0.9)$ mJ mol$^{-1}$ K$^{-2}$ and $\beta = (7.8 \pm 0.2)$ mJ mol$^{-1}$ K$^{-4}$, corresponding to a Debye temperature of $\theta_D = \left( \frac{12 \pi \alpha R}{5 \beta} \right)^{1/3} \approx 126$ K, where $n_a = 8$ is the number of atoms per formula unit of In$_5$Bi$_3$. 

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**Figure 4.** (a) Band structure of In$_5$Bi$_3$ calculated without (NSOC) and with SOC. (b) Top: electronic density of states of In$_5$Bi$_3$ calculated without (NSOC) and with SOC. The Fermi energy is indicated by the vertical dashed line. We also show the partial density of states for the case with SOC for bismuth p-states (orange dashed line) and indium s states (blue dashed line). Bottom: ratio of the electronic density of states calculated without and with SOC. The orange band indicates the energy range below the Fermi energy in which SOC suppresses the density of states.
Subtracting the estimated lattice contribution from the experimental heat capacity reveals the underlying electronic contribution near the superconducting transition (right inset of figure 6). This data closely follows a BCS form with a gap \( \Delta(T) \) enhanced over the standard BCS gap by 22%, giving \( 2\Delta(0) = 4.28 \, k_B T_c \), which suggests strong coupling superconductivity. The relative jump height at \( T_c \), i.e. the difference between superconducting and normal state heat capacities, divided by the normal state heat capacity, is \( \frac{C_s - C_n}{C_n} = \frac{2.09}{2.09} \), again significantly enhanced over the BCS value of 1.43.

We can apply Carbotte’s relations [53] linking the logarithmically averaged phonon frequency \( \omega_{ln} \) as introduced by Allen and Dynes [54], to the gap size and the jump height, with \( x = \frac{\hbar \omega_{ln}}{(k_B T_c)} \):

\[
\frac{2\Delta(0)}{k_B T_c} = 3.54(1 + 12.5x^{-2}\ln(x/2)) \approx 4.28, \tag{8}
\]

\[
\frac{C_s - C_n}{C_n} = 1.43(1 + 53x^{-2}\ln(x/3)) \approx 2.09. \tag{9}
\]

Inverting these relations graphically produces estimates for \( \hbar \omega_{ln} \) between 41 K (from equation (8)) and 55 K (from equation (9)). These values are consistent with the estimates obtained from the analysis of the temperature

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**Figure 5.** Temperature dependence of the electrical resistivity of In\(_5\)Bi\(_3\), showing a rapid increase at low temperature \( T \) and saturation near room temperature. A superconducting transition is observed at \( T_c \approx 4.17 \) K. The inset shows the effect of applied magnetic field on the superconducting transition.

**Figure 6.** Sommerfeld ratio of the heat capacity \( C/T \) of In\(_5\)Bi\(_3\) versus \( T^2 \) (main panel), showing the heat capacity anomaly for zero applied field (red symbols) at the transition temperature \( T_c \), as well as the normal state data in 0.5 T applied field (blue symbols). The line shows the result of fitting the normal state data to \( C/T = \gamma T + \beta T^3 + C_{Einstein}/T \) (see text). The left inset shows the upper critical field versus temperature, as extracted from the mid-points of the resistive transitions shown in figure 5. The line shows the Werthamer–Helfand–Hohenberg clean-limit curve [55]. The right inset shows the Sommerfeld ratio of the electronic contribution to the specific heat, obtained by subtracting the fitted phonon terms from experimental data. The line shows the expectation from BCS theory for a zero-temperature gap magnitude of \( 2\Delta/(k_B T_c) = 4.28 \).
dependence of the resistivity in [21], which gave an electron–phonon coupling constant of $\lambda \approx 1.25$, a gap magnitude of $2\Delta(0)/(k_B T_c) = 4.2$ and a logarithmically averaged phonon energy of $\hbar \omega_{\text{an}} \approx 45$ K.

7. Conclusions

In summary, we have investigated the chemical, structural, and superconducting properties of In$_5$Bi$_3$. Our first principles calculations show that the spin–orbit interaction plays a central role in determining the composition and crystal structure of this material. In$_5$Bi$_3$ dissociates into elemental indium and bismuth at the non-relativistic level, but the inclusion of relativistic spin–orbit coupling chemically stabilizes the material. Furthermore, an energy-lowering structural distortion develops in the absence of relativistic effects, but this distortion disappears with the inclusion of the spin–orbit interaction and the material adopts a tetragonal I4/mcm structure. The microscopic mechanism driving this stabilization is a suppression of the electronic density of states near the Fermi energy by the spin–orbit interaction. We have also measured the resistivity of In$_5$Bi$_3$ as a function of temperature and magnetic field to determine a superconducting critical temperature of 4.2 K and a superconducting critical field of 0.3 T.

These findings make In$_5$Bi$_3$ an interesting material in which to explore exotic physics. First, it could be used as a model system to study the nature of strong coupling superconductivity in incommensurate crystals because its structure is an approximant for the incommensurate structure of superconductors like Bi-III. Second, In$_5$Bi$_3$ might be a viable candidate superconductor for combination with ferromagnetic atomic chains for the realisation of Majorana quasiparticles, using a strategy analogous to that in [56], and exploiting the host-guest nature of the material. Overall, we hope that our work will motivate further studies of the physical properties of In$_5$Bi$_3$.

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