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Exploring Ground State Energies and Electronic Band Structures of Bi_2Se_3 and Bi_2Te_3 Topological Insulators: A First-Principles DFT Approach for Spintronic and Thermoelectric Applications

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ABSTRACT

Topological insulators (TIs) such as Bismuth selenide (Bi_2Se_3) and Bismuth Telluride (Bi_2Te_3) have attracted attention for their unique electronic properties, featuring insulating interiors and conducting surface states protected by time-reversal symmetry. This study uses Density Functional Theory (DFT) to investigate the ground state energies and electronic band structures of these TIs. The calculated ground state energies for Bi_2Se_3 and Bi_2Te_3 are -675,251.44 eV and -796,226.99 eV, aligning closely with experimental data. These results confirm the stability of the materials and their characteristic band gaps and robust surface states. Spin-orbit coupling (SOC) is essential in inducing band inversion at the Γ point, a key feature of TIs. Additionally, the high density of states near the Fermi level in Bi_2Te_3 suggests potential thermoelectric applications. These findings highlight the relevance of Bi_2Se_3 and Bi_2Te_3 in spintronics and quantum computing.

INTRODUCTION

In recent years, the discovery of topological insulators (TIs) has ignited significant interest in the fields of solid-state and condensed-matter physics (Zhang et.al., 2009a; Wang and Zhang, 2017; Tian et.al.,2017). TIs represent a unique class of materials that, despite being insulators in their bulk, exhibit conductive surface states. This characteristic is not entirely exclusive to TIs, as ordinary band insulators can also support surface conductivity (Kou et al., 2017; Schindler et al., 2018; Liu et al., 2020). However, what distinguishes TIs is that their surface states are protected by fundamental symmetries, specifically particle number conservation and time-reversal symmetry (Hasan et al., 2013; Zhang et al., 2018; Khalaf et al., 2018; McGinley and Cooper, 2020; Wang et al., 2024).

TIs are defined by their intrinsic time-reversal symmetry, which ensures that their surface states remain stable even in the presence of surface defects or impurities (Zhang et.al., 2009a; Chang et al.,2014). The electronic structure of a non-interacting TI resembles that of a conventional band insulator in the bulk, with the Fermi level situated between the conduction and valence bands. However, on the surface, unique states exist within the bulk energy gap, enabling metallic conduction (Wang et al., 2024). A critical feature of these surface states is spin-momentum locking, where the spin of the carriers is oriented perpendicular to their momentum. This spin-momentum locking significantly suppresses backscattering, thus enhancing surface conductivity (Cai et al.,2018)

Non-interacting TIs are characterized by topological invariants, particularly the Z2 index, which dictates the presence of these robust surface states. These states are protected as long as time-reversal symmetry is maintained, which is typically the case unless the material is subjected to magnetic impurities that break this symmetry (Narang et al., 2021; Ahams et al., 2021). The potential applications of TIs are vast, with significant implications for spintronic devices and quantum computing. TIs are integral to the development of dissipationless transistors and quantum computers, particularly through the exploitation of the quantum spin Hall effect and the quantum anomalous Hall effect (Rachel, 2018). Beyond these, TI materials have found roles in advanced magnetoelectronic and optoelectronic devices, further demonstrating their versatility (Zhang et al., 2009a).

The origins of the topological theory in solid-state physics can be traced back to the discovery of the quantum Hall effect (Thareja and Vekhter, 2023). The Hall effect, discovered by Edwin Hall in 1879, predates the discovery of the electron and describes the generation of a voltage difference across an electrical conductor when it is subjected to a perpendicular magnetic field, relative to the direction of current flow (Leis et al., 2021). This effect laid the groundwork for the understanding of quantum Hall effects, which are central to the theory of Tis (Silvestrov et al., 2012)

Ground state energy is the minimum possible energy of a quantum mechanical system in its most stable configuration. In Density Functional Theory (DFT), the ground state energy is an important parameter used to evaluate the energetic stability of materials (Kittel, 2005). Electronic band structure describes the relationship between electron energy and crystal momentum in a solid and provides essential information about the electrical, optical, and transport properties of materials (Kittel, 2005). The band structure is particularly important in identifying whether a material behaves as a conductor, semiconductor, insulator, or topological insulator.

This study uses the FHI-aims DFT package to explore the ground state energies and band structures of two distinct TIs, Bi_2Se_3 and Bi_2Te_3. Bi_2Se_3 is a selenide-based TI, while Bi_2Te_3 is telluride-based. Our research aims to revisit their ground state properties and band structures to predict their potential scientific and technological applications in the context of topological insulators.

MATERIALS AND METHODS

All material systems are fundamentally composed of electrons and nuclear charges, with the interaction between electrons playing a central role in determining their mechanical, electronic, and magnetic properties. A key tool for understanding and describing electron interactions is the Schrödinger equation. If the Schrödinger equation for many-electron systems could be solved both accurately and efficiently, it would allow for the precise determination of nearly all material properties. However, no method currently exists to solve such problems with complete accuracy and efficiency. While analytical solutions are possible for simple systems such as the hydrogen atom and H_2^+, more complex systems require approximate methods, such as the Nearly Free Electron and Tight Binding methods. These methods are limited by the approximations necessary to simplify the problem, which often leads to reduced accuracy (Havu et al., 2009; Owolabi et al.,2016; Hemba et al., 2022).

To address these challenges, a variety of advanced computational methods have been developed, including Quantum Chemistry (Hartree-Fock), Quantum Monte Carlo, Perturbation Theory, and Density Functional Theory (DFT). Of these, DFT is widely regarded as the most successful due to its combination of accuracy and computational efficiency. The key innovation of DFT lies in its approach to the many-electron problem, in which the ground-state energy is treated as a functional of the electron density rather than the wave function. This reformulation reduces the complexity of the problem and makes it more computationally tractable.

To illustrate the core concept of DFT, consider the problem of a single electron in an external potential. The ground-state energy can be expressed as a functional of the electron density Hemba et al., 2022):

$$E[n] = \frac{1}{8}\int d^3\, r\, \frac{|\nabla n|^2}{n} + \int d^3\, r v(r) n(r) \qquad (1)$$

where E[n] is the total ground-state energy functional of the electron density, n(r) is the electron density at position r, r is the spatial position vector (x,y,z), d^3r is the volume element in three-dimensional space, ∇ is the gradient operator, $|\nabla n|^2$ is the square of the gradient of the electron density, and V(r) is the external potential acting on the electron

This energy functional is minimized, subject to the constraint that the total electron density integrates to unity. Using Lagrange multipliers, the auxiliary functional becomes (Perdew and Wang, 1992):

$$H[n] = E[n] - \mu N \qquad (2)$$

where H[n] is the auxiliary energy functional, E[n] is the total energy functional, μ is the Lagrange multiplier associated with particle number conservation, N is the total number of electrons By minimizing H[n], we obtain the following equation (Perdew and Wang, 1992):

$$\frac{\delta H}{\delta n(r)} = \frac{\delta T^{\mathrm{VW}}}{\delta n(r)} + v(r) - \mu = 0 \qquad (3)$$

where δ is the functional differentiation operator, μ is the Lagrange multiplier, V(r) is the external potential acting on the electron, T^{VW} is von Weizsacker kinetic energy functional

This leads to the derivation of the Schrödinger equation for the electron density (Aungwa et al., 2016).:

$$\left(-\frac{\nabla^2}{4} + \frac{|\nabla n|^2}{8n^2} + v(r)n(r)\right) = \mu n(r) \qquad (4)$$

where ∇^2 is the Laplacian operator, V(r)n(r) is the external potential energy density, $\mu n(r)$ is the chemical potential multiplied by electron density, n(r) is the electron density, μ is the chemical potential

This equation simplifies the many-electron problem by reducing the dimensionality from 3N (for N electrons) to only three spatial coordinates, through the use of electron density as the central variable.

The Hohenberg-Kohn (H-K) theorem, a foundational result of DFT, asserts that the ground-state properties of a many-electron system are uniquely determined by its electron density, which depends on only three spatial coordinates. This significantly reduces the complexity of the many-body problem, where interactions between electrons are incorporated into an exchange-correlation potential. The Hamiltonian for such a system can be expressed as (Kohn and Sham, 1965):

$$H = -\sum_i \frac{\hbar^2}{2m_e}\nabla_{r_i}^2 + \sum_i V_{\text{ext}}(r_i) + \frac{e^2}{2}\sum_{i\neq j}\frac{1}{|r_i - r_j|} + \sum_{i\neq j}\frac{Z_i Z_j e^2}{|R_i - R_j|} \quad (5)$$

where H is Hamiltonian operator of the many electrons system, m_e is the mass of an electron, e is the elementary electronic charge, r_i,r_j is the position vectors of electrons i and j, r_i-rj is the distance between the electrons i and j, Z_i,Z_j is the atomic numbers (nuclear charge) of nuclei i and j, R_i, R_j is the position vector of nuclei

This Hamiltonian includes terms representing the kinetic energy of electrons, the external potential from the nuclei, the electron-electron Coulomb interaction, and the nuclear-nuclear interaction. The H-K theorem guarantees that all properties of the system can be derived from the ground-state density.

In 1965, Kohn and Sham refined the application of DFT by introducing a method to solve the H-K density functional through a transformation of the interacting electron system into an auxiliary system of non-interacting particles (Perdew and Wang, 1992). In this formulation, the electron density is expressed as a sum of single-particle wavefunctions (Kohn and Sham, 1965):

$$n(r) = \sum_i |\psi_i(r)|^2 \quad (6)$$

where n(r) is the electron density, φ_i(r) is Kohn-Sham single-particle wavefunction (orbital) for state i, $|\varphi_i(r)|^2$ is the probability density associated with orbital i

This leads to the Kohn-Sham equations, which describe the behavior of the non-interacting system and are more computationally tractable (Kohn and Sham, 1965):

$$\left[\frac{-\hbar^2}{2m_e}\nabla_r^2 + v_{eff}\big(r, n(r)\big)\right]\psi_i(r) = \varepsilon_i\psi_r(r) \quad (7)$$

where ħ is the reduced Planck constant, m_e is the electron mass, V_{eff}(r, n(r)) is the effective potential experienced by electrons, ε_i is the energy eigenvalue of the i-th orbital, $\varepsilon_i\varphi_i$(r) is the energy-weighted wavefunction term

In this study, first-principles calculations were performed using the FHI-aims package within the framework of Density Functional Theory (DFT). The generalized gradient approximation (GGA) in the Perdew–Burke–Ernzerhof (PBE) form was employed to describe the exchange-correlation interaction. Self-consistent field (SCF) calculations were carried out until the total energy convergence criterion was achieved. The ground state energies of Bi_2Se_3 and Bi_2Te_3 were obtained from the converged self-consistent calculations after geometry optimization. The electronic band structures and density of states (DOS) were subsequently calculated along the high-symmetry directions in the Brillouin zone using the optimized crystal structures. Spin–orbit coupling (SOC) effects were included in the calculations because SOC plays a critical role in inducing band inversion and topological surface states in topological insulators.

The effective potential $V_{eff}\big(r, n(r)\big)$ includes the external potential, Coulomb interaction, and exchange-correlation potential, making it essential for solving the Kohn-Sham equations. However, the exact form of the exchange-correlation functional $E_{XC}[n(r)]$, remains unknown, requiring approximations such as the Local Density Approximation (LDA) or Generalized Gradient Approximation (GGA) (Blum et al., 2009).

Despite these approximations, DFT has proven to be a powerful tool for studying complex systems (Aungwa et al., 2017). In this research, the Perdew-Burke-Ernzerhof (PBE) functional, a variant of GGA, was employed to calculate the properties of materials. The FHI-aims (Fritz Haber Institute ab initio materials simulations) code package, known for its accuracy in handling all-electron (Aungwa et al., 2017), full-potential electronic structure calculations (Abdu, 2010), was used to solve the Kohn-Sham equations for systems of interest.

The study focused on the electronic properties of topological insulators, specifically Bi_2Se_3 and Bi_2Te_3. By employing both LDA and GGA exchange-correlation functionals, the ground-state energy and band structure of these materials were determined. The FHI-aims program was used to construct periodic geometries and perform self-consistent calculations, providing insights into the behavior of these materials (Aungwa et al., 2016).

The results highlight the strength of DFT in offering a computationally efficient method for solving complex quantum mechanical problems, with the potential for further refinement as more accurate exchange-correlation functionals are developed.

RESULTS AND DISCUSSION

The calculated ground state energies of Bi_2Se_3 and Bi_2Te_3 were found to be −675,251.44 eV and −796,226.99 eV, respectively. The negative values of the total energies indicate that both materials are energetically stable in their equilibrium configurations (Zhang, et al., 2009b). In Density Functional Theory calculations, structural stability is generally associated with systems possessing lower and more negative total energies after self-consistent convergence and geometry optimization (Hemba, et al., 2022). Although there is no universal threshold for material stability in DFT calculations, agreement between calculated electronic properties and previously reported theoretical or experimental results provides important validation of the computational model (Martinez et al., 2017). The obtained results are consistent with earlier studies on Bi_2Se_3 and Bi_2Te_3 topological insulators reported in the literature (Zhang et al., 2009b). The resulting band structures, depicted in Fig. 1, are characterized by energy bands plotted along high-symmetry points in the Brillouin zone, specifically L, Γ, X, W, and K. These bands are represented as blue lines relative to the energy axis, with particular focus on their behavior around the Fermi level (0 eV), which is crucial in determining the material's classification as a metal, insulator, or semiconductor. Notably, the band structure of Bi_2Se_3 reveals a band gap between the valence bands

(below 0 eV) and the conduction bands (above 0 eV), a key feature of its topological insulator properties.

In the analysis of surface states, the presence of Dirac-like linear dispersion near the Fermi level is a significant indicator of topological surface states in Bi_2Se_3, as previously established by (Zhang, et al., 2009b; Liu et al., 2014) The density of states (DOS) is plotted against energy levels, where peaks correspond to regions of high state density, and valleys indicate low state density. The Fermi level is marked by a dashed line, and the DOS around this level provides insight into the electronic states available for conduction. A region of low DOS between the valence and conduction bands corroborates the presence of a band gap, as seen in Fig. 1, further confirming Bi_2Se_3 a topological insulator with distinct surface states near the Fermi level.

The band structure and DOS of Bi_2Se_3 offer crucial insights into its electronic properties (Ando and Fu, 2015). The band structure reveals a direct band gap at the Γ point, essential for its topological insulator behavior, where the bulk remains insulating while the surface states exhibit metallic characteristics. The DOS plot indicates a high density of states near the Fermi level, primarily arising from the p orbitals of Bi and Se atoms (Sahu and Kaushik, 2022).

Furthermore, the inclusion of spin-orbit coupling (SOC) significantly impacts the band structure, inducing a band inversion at the Γ point, a hallmark of topological insulators. In the absence of SOC, the band gap is minimal due to overlapping bands, but with SOC, a distinct gap emerges, confirming the topological insulating behavior of Bi_2Se_3, as detailed by (Singh, 2019).

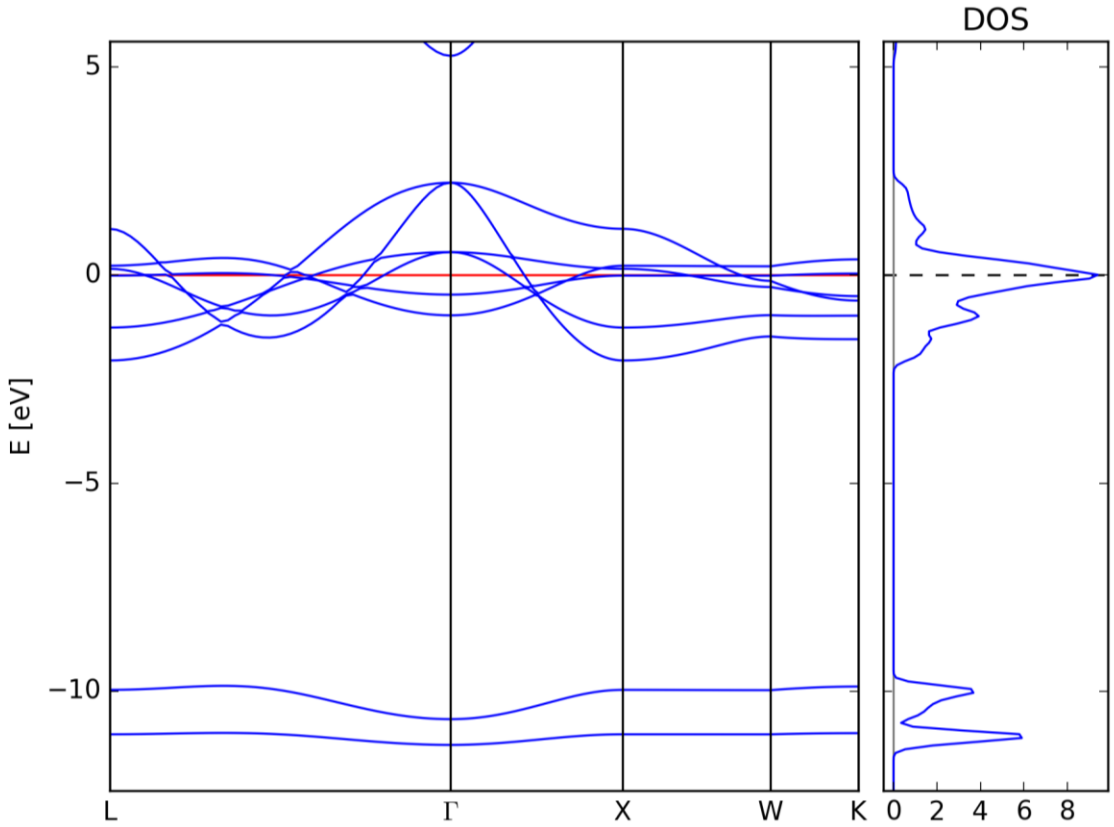

Figure 1: Band Structure and Density of States of the (Bi_2Se_3) as generated by the 'aimsplot.py.' script

Bismuth telluride (Bi_2Te_3) is a well-studied material recognized for its unique electronic properties, particularly its role as a topological insulator and its thermoelectric applications (Pandey et al., 2021). The electronic band structure and density of states (DOS) are crucial for understanding these properties.

The band structure of Bi_2Te_3, as depicted in Figure 2, is calculated along high-symmetry points in the Brillouin zone (L, Γ, X, W, K). The energy levels, represented on the Y-axis in electron volts (eV), show the distribution of electronic bands, with the Fermi level (EF) set at 0 eV (indicated by the red line).

A notable feature of Bi_2Te_3's band structure is the direct band gap observed at the Γ point. This band gap is critical for the material's topological insulating properties (He et al., 2019). The band inversion at the Γ point, where the conduction band minimum and valence band maximum swap places due to strong spin-orbit coupling, is a hallmark of topological insulators. This inversion leads to

the emergence of robust surface states that are protected against scattering by time-reversal symmetry.

The density of states (DOS), plotted alongside the band structure, provides additional insight into the electronic characteristics of Bi_2Te_3. The DOS plot, with the X-axis representing the density of states and the Y-axis representing energy levels (eV), shows a significant concentration of states near the Fermi level.

The peaks in the DOS near the Fermi level are primarily due to the p orbitals of bismuth (Bi) and tellurium (Te) atoms. These sharp peaks indicate the presence of localized states, which are crucial for the topological surface states characteristic of Bi_2Te_3. The high density of states near the Fermi level also suggests an enhanced thermoelectric effect, as these states contribute to the material's high Seebeck coefficient and low thermal conductivity, making Bi_2Te_3 a promising candidate for thermoelectric applications.

The calculated electronic properties of Bi_2Se_3 and Bi_2Te_3 demonstrate their suitability for advanced spintronic and thermoelectric applications. The SOC-induced band inversion and topologically protected surface states support efficient spin transport with reduced backscattering, making these materials promising candidates for low-power spintronic devices and quantum information technologies (Hasan and Kane,2010). Furthermore, the high density of states near the Fermi level in Bi_2Te_3 contributes to enhanced thermoelectric performance through improved Seebeck coefficient and reduced thermal conductivity (He et al., 2019). These properties make Bi_2Te_3 highly attractive for thermoelectric energy conversion applications.

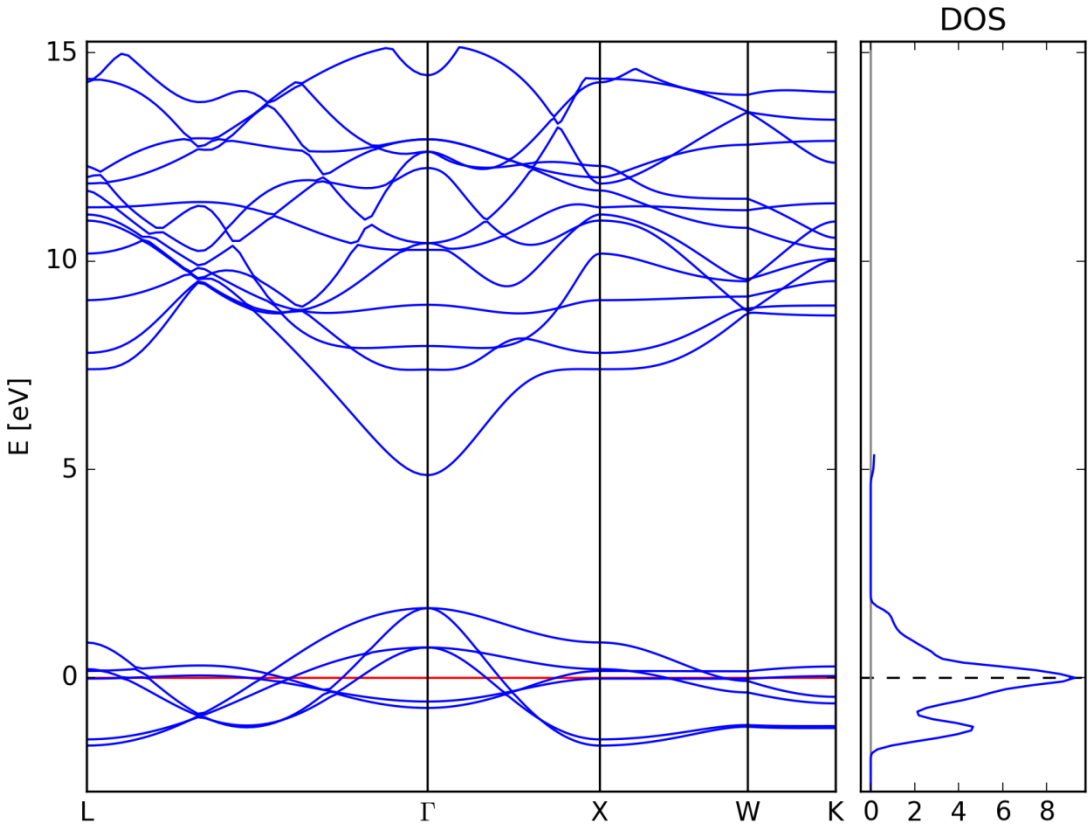

Figure 2: Band Structure and Density of States of the (Bi_2Te_3) as generated by the 'aimsplot.py.' script

The detailed analysis of the ground state energies, band structures, and density of states (DOS) of Bi_2Se_3 and Bi_2Te_3 has provided substantial insights into their electronic properties, crucial for their classification as topological insulators and their potential applications in thermoelectric.

For Bi_2Se_3, the band structure reveals a distinct band gap between the valence and conduction bands, with a notable direct gap at the Γ point. This band gap, along with the observed Dirac-like linear dispersion near the Fermi level, is indicative of the topological surface states that are characteristic of topological insulators. The DOS further confirms this behavior, showing a low DOS region corresponding to the band gap, and peaks near the Fermi level that arise from the p orbitals of Bi and Se atoms. The inclusion of spin-orbit coupling (SOC) plays a critical role in inducing the band inversion at the Γ point, a key feature of topological insulators, where the bulk remains insulating while the surface states are metallic.

Bi_2Te_3 exhibits similar topological insulator behavior, with a direct band gap at the Γ point and a high DOS near the Fermi level. The band inversion at the Γ point, driven by strong SOC, underscores its topological nature. The high density of states near the Fermi level, mainly due to the p orbitals of bismuth and tellurium, suggests enhanced thermoelectric properties, making Bi_2Te_3 a promising material for thermoelectric devices. The sharp peaks in the DOS near the Fermi level indicate the presence of localized states, which are essential for the topological surface states and contribute to the material's low thermal conductivity and high Seebeck coefficient.

CONCLUSION

Both Bi_2Se_3 and Bi_2Te_3 exhibit the hallmark features of topological insulators, with their electronic structures dominated by SOC-induced band inversions at the Γ point. The high density of states near the Fermi level in Bi_2Te_3 further enhances its suitability for thermoelectric applications. These findings align with previous studies, solidifying the role of these materials in advancing topological insulator research and thermoelectric technologies. In addition to its thermoelectric potential, Bi_2Te_3 also exhibits significant promise for spintronic applications due to its strong spin–orbit coupling and topologically protected surface states. The spin-momentum locking mechanism present in Bi_2Te_3 enables efficient spin transport with reduced energy dissipation, making the material suitable for next-generation spin-based electronic and quantum computing devices.

List of abbreviations

TIs Topological insulators
DFT Density Functional Theory
SOC Spin-orbit coupling
DOS Density of State
H-K Hohenberg-Kohn
LDA Local Density Approximation
GGA Generalized Gradient Approximation
PBE Perdew-Burke-Ernzerhof
FHI-aims Fritz Haber Institute ab initio materials simulations

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