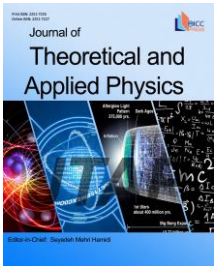

J. Theor. Appl. Phys., 2026; 20(3): 304-309

Journal of Theoretical and Applied Physics (JTAP)

https://doi.org/10.57647/jtap.2026.8598.0301

Research Article

Detailed Analysis of the Electronic and Structural Properties of the New Compound $Tl_{1-x}B_x$ P, Taking into Account the Spin–Orbit Effect Using MBJ-GGA

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Article History:

Received:
26 November 2025

Revised:
25 December 2025

Accepted:
20 January 2026

Published Online:
07 February 2026

Published in Issue:
30 June 2026

Abstract

We report an ab initio study of ternary $Tl_{1-x}B_xP$ alloys (x = 0.25, 0.5) in the zinc-blende structure using DFT with GGA and mBJ-GGA, including spin–orbit coupling (SOC). A 2×2×2 supercell based on TlN was used, where boron atoms were substituted by thallium. Our results show that while BP is an indirect semiconductor and TlN is metallic, $Tl_{1-x}B_xP$ alloys exhibit a semi-metallic character, bridging wide-gap borides and narrow-gap thallium compounds. Increasing boron content reduces the lattice constants and modifies the total energy, enabling precise tuning of electronic properties. This work highlights the stabilizing role of thallium in forming new alloy phases and provides a novel route for band-gap engineering in III–V semiconductors, considering SOC effects. These findings offer guidance for the design of future optoelectronic and electronic devices.

Keywords: Energy gap, Structural properties, DFT, III–V semiconductor, GGA, Ab initio calculations, $Tl_{1-x}B_xP$ alloys, WIEN2k

Cite this article: Abdelali, L., Abed, Z., Lachabi, A., Abid, H., (2026). Detailed Analysis of the Electronic and Structural Properties of the New Compound $Tl_{1-x}B_x$ P, Taking into Account the Spin–Orbit Effect Using MBJ-GGA. *J. Theor. Appl. Phys.,* 20(3), 304-309. https://doi.org/10.57647/jtap.2026.8598.0301

1. Introduction

The continuous quest for novel semiconductor materials with tunable structural and electronic properties has become a major focus of modern materials science due to their wide range of technological applications in optoelectronic and photonic devices [1–3]. In particular, III–V compound semiconductors such as GaAs, InP, and BP have attracted considerable attention because of their favorable electronic band structures, high carrier mobilities, and excellent optical responses [4, 5]. Recent advances in first-principles (ab initio) methods based on Density Functional Theory (DFT) have made it possible to predict and tailor the physical properties of these materials with high accuracy [6, 7].

Within this context, thallium-based III–V compounds have emerged as a promising class of materials owing to the unique electronic characteristics of the Tl 6p orbitals,

which can significantly modify the band gap, band dispersion, and carrier effective masses [8, 9]. Several theoretical studies have investigated binary thallium compounds such as TlN, TlP, and TlAs, reporting a strong dependence of their electronic behavior on chemical composition, crystal structure, and relativistic effects, including a transition from semiconducting to metallic or semi-metallic character [10–12, 21, 22].

In particular, it has been shown that spin–orbit coupling (SOC) plays a crucial role in Tl-based compounds due to the heavy atomic mass of thallium, leading to pronounced modifications of the valence and conduction band edges [23, 24].

On the other hand, boron-based III–V materials such as BN and BP exhibit large band gaps, strong covalent bonding, and excellent chemical and thermal stability, making them attractive candidates for high-power, high-frequency, and optoelectronic device applications [13, 14, 25]. Previous studies on boron-containing III–V alloys have demonstrated that the incorporation of boron can significantly influence the lattice parameters, mechanical rigidity, and electronic band structure through enhanced orbital hybridization and lattice contraction effects [26, 27].

The combination of thallium and boron atoms within the same crystalline matrix therefore offers a unique opportunity for band-gap engineering, allowing a continuous tuning of electronic properties between wide-gap borides and narrow-gap thallium-based compounds.

Despite this potential, systematic studies on ternary $Tl_{1-x}B_xP$ alloys remain very limited, and their structural stability and electronic properties are still not well established in the literature.

Address this gap, the present work provides a comprehensive ab initio investigation of $Tl_{1-x}B_xP$ (x = 0.25 and 0.5) alloys in the zinc-blende structure, employing Density Functional Theory within the Generalized Gradient Approximation (GGA), as implemented in the WIEN2k code.

The effects of boron concentration and thallium incorporation on the lattice parameters, energetic stability, and electronic band structure are systematically analyzed, offering new insights into the design of tunable III–V semiconductor alloys for future optoelectronic and electronic applications.

2. Computational details

All calculations were performed using the full-potential linearized augmented plane wave (FP-LAPW) method as implemented in the WIEN2k code [15]. This approach is based on Density Functional Theory (DFT), which provides an accurate description of the ground-state electronic structure of solids and has been successfully applied to a wide range of III–V semiconductor compounds [21].

The exchange–correlation potential was treated within the Generalized Gradient Approximation (GGA) formulated by Perdew, Burke, and Ernzerhof (PBE) [16]. To obtain a better estimation of the electronic band gaps, we also employed the modified Becke–Johnson (mBJ-GGA) potential [17].

Furthermore, the spin–orbit coupling (SOC) was included in all calculations, as it plays a significant role in systems containing heavy elements such as thallium (Tl) and phosphorus (P).

The choice of the GGA-PBE exchange–correlation functional is motivated by its well-established reliability in describing structural properties and ground-state energetics of III–V semiconductors. However, it is well known that conventional GGA tends to underestimate the electronic band gap.

To overcome this limitation, the modified Becke–Johnson (mBJ) potential was employed, as it has been shown to provide significantly improved band-gap values for a wide range of semiconductors without the high computational cost of hybrid functionals.

Furthermore, spin–orbit coupling (SOC) was explicitly included due to the presence of the heavy Tl atom, for which relativistic effects strongly influence the electronic band structure and band splitting. In the FP-LAPW framework, the unit cell is divided into two regions:

(i) non-overlapping muffin-tin spheres surrounding each atomic site with radii (Rmt), and (ii) the interstitial region between these spheres.

Inside the muffin-tin spheres, the Kohn–Sham wave functions are expanded in spherical harmonics up to (lmax = 10), while in the interstitial region they are represented as plane waves with a cutoff parameter defined by (Rmt•Kmax = 7), where Kmax is the maximum value of the reciprocal lattice vector used in the plane-wave expansion.

The self-consistent field (SCF) cycles were iterated until the total energy convergence criterion was better than 0.1 mRy per formula unit.

On average, seven iterations were required to reach full convergence.

The k-point mesh used for the Brillouin zone integration was determined after several convergence tests, ensuring that the total energy variation became negligible with increasing number of k-points. The electronic configurations of the constituent atoms were defined by treating only the valence electrons as active states, while the core electrons were considered frozen. For the alloyed systems $Tl_{1-x}B_xP$ (x = 0.25 and 0.5), a 2×2×2 supercell was generated based on the zinc-blende BP structure, where

thallium atoms were substituted for boron atoms to simulate the desired compositions.

The equilibrium lattice parameters were optimized by fitting the total energy–volume data to the Murnaghan equation of state, allowing the determination of the lattice constants, bulk modulus, and total energy for each configuration.

Although the present work focuses primarily on the structural stability and electronic band structure of $Tl_{1-x}B_xP$ alloys, the calculation of carrier effective masses, which is essential for a deeper understanding of charge transport properties, will be addressed in a separate forthcoming study.

3. Results and discutions

3.1. Structural properties

3.1.1. *Vegard's law analysis of structural parameters*

The lattice parameters and mechanical properties of $Tl_{1-x}B_xP$ are strongly influenced by the boron concentration (x), due to the smaller atomic size and higher electro negativity of boron compared to thallium. Investigating the lattice constant as a function of x provides insight into the structural evolution and atomic interactions within the crystal, while the bulk modulus reflects the material's resistance to volume compression and overall mechanical stability. Studying these variations with boron content is essential for understanding the structure–property relationships in this ternary system.

Typically, increasing the boron fraction reduces the lattice volume due to the substitution of smaller B atoms for Tl, which can simultaneously affect the elastic response and cohesive energy of the crystal. Such trends are crucial for predicting the material's suitability for optoelectronic and thermoelectric applications, where both structural stability and precise lattice tuning are required [24, 25].

This work provides a new insight into how boron incorporation tunes the structural and mechanical properties of $Tl_{1-x}B_xP$ alloys, which has not been extensively studied in previous literature.

The results show that the lattice constant decreases with increasing boron concentration (x) (Figure 1), due to the smaller atomic size of boron compared to thallium, which is in good agreement with Vegard's law. Conversely, the bulk modulus gradually increases with higher boron content, indicating a stiffer lattice and enhanced resistance to volume compression (Figure 2). These observations confirm that boron incorporation improves the structural stability and allows precise tuning of lattice properties, which is particularly relevant for electronic and optoelectronic applications.

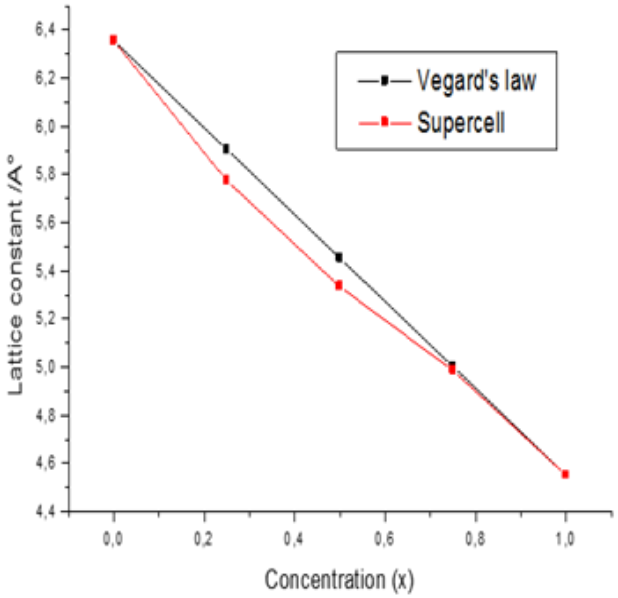

Figure 1. Composition dependence of the calculated lattice constant of Tl1-xBxP alloy compared with Vegard's law

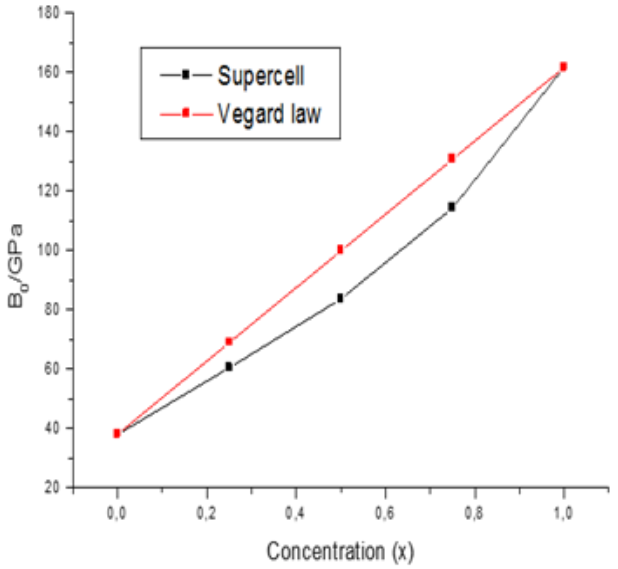

Figure 2. Composition dependence of the calculated bulk modulus of $Tl_{1-x}B_x$ As alloy compared with Vegard's law

4. Electronic properties

The electronic band structure and density of states (DOS) calculations are essential for understanding the fundamental electronic behavior of the $Tl_{1-x}B_xP$ alloys and for elucidating how boron incorporation modifies their band characteristics. These calculations were performed using three different exchange–correlation approaches: the generalized gradient approximation (GGA), the modified Becke–Johnson potential (mBJ-GGA), and the mBJ-GGA including spin–orbit coupling (SOC).

Such a combination of computational schemes provides a comprehensive evaluation of the band-gap nature and magnitude, since GGA is known to underestimate the

energy gap, whereas mBJ yields a more accurate correction closer to experimental values [17, 18]. The inclusion of SOC is particularly important in thallium-based systems because the heavy atomic mass of Tl induces strong relativistic effects, which significantly influence the valence and conduction band edges [19].

In the case of the $Tl_{1-x}B_xP$ alloy, substituting thallium atoms with boron is expected to modify the hybridization between the Tl-6p, B-2p, and P-3p orbitals, leading to noticeable shifts in the position and curvature of the electronic bands. As the boron concentration increases, the lattice constant decreases, enhancing the orbital overlap and altering the dispersion of the bands near the Fermi level. Consequently, both the energy gap and its nature (direct or indirect) vary with composition, reflecting the interplay between structural contraction and electronic localization [20].

The following figures Figures 3, 4, and 5 illustrate the calculated band structures of the $Tl_{1-x}B_xP$ alloys at compositions x = 0.25, 0.5, and 0.75, respectively, obtained using the GGA, mBJ-GGA, and mBJ-GGA + SOC approaches.

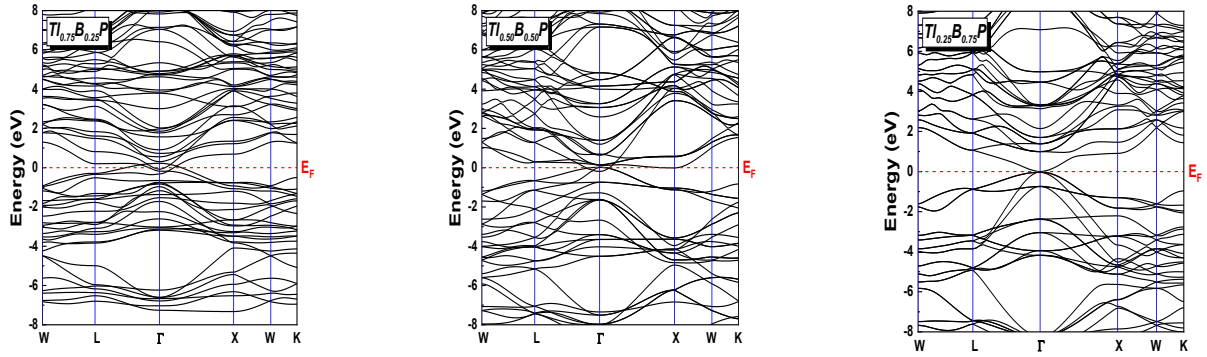

Figure 3. Calculated electronic band structure of $Tl_{1-x}B_xP$ alloy at different compositions (x = 0.25, 0.5, and 0.75) within the GGA approximation

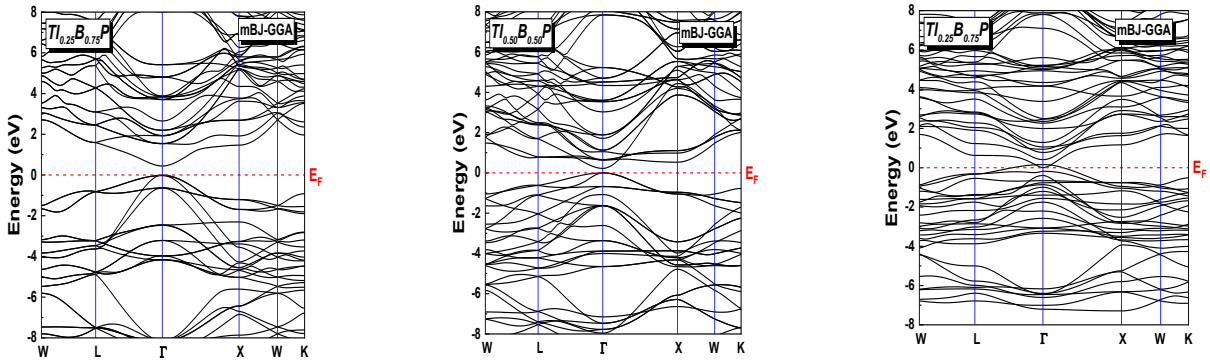

Figure 4. Calculated electronic band structure of $Tl_{1-x}B_xP$ alloy at different compositions (x = 0.25, 0.5, and 0.75) within the Mbj-GGA approximation

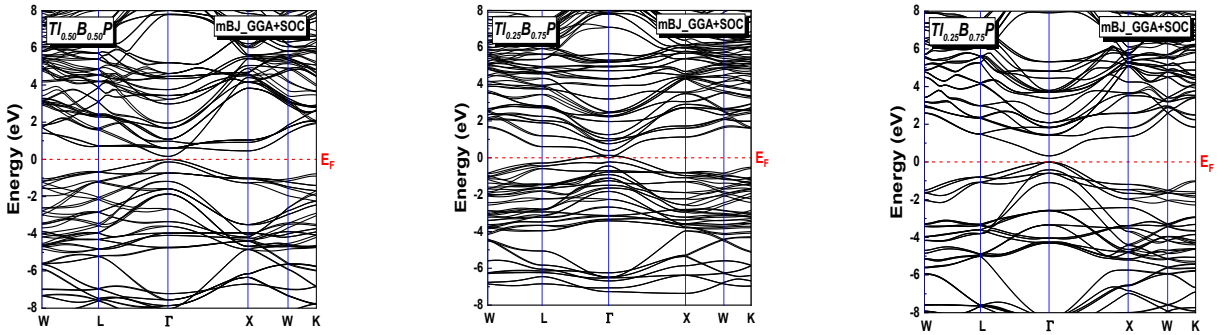

Figure 5. Calculated electronic band structure of $Tl_{1-x}B_xP$ alloy at different compositions (x = 0.25, 0.5, and 0.75) within the Mbj-GGA+SOC approximation

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Table 1. Calculated Band Gaps of $Tl_{1-x}B_xP$ Using GGA, Mbj-GGA, and Mbj-GGA+SOS approximations

Calculated band gap	concentration		
	x=0.25	x=0.5	x=0.75
GGA	metal	metal	metal
Mbj-GGA	metal	0.22 eV	0.44 eV
Mbj-GGA+SOS	metal	0.15 eV	0.32 eV

The electronic properties of $Tl_{1-x}B_xP$ alloys were systematically investigated at compositions x = 0.25, 0.5, and 0.75** using the GGA, mBJ-GGA, and mBJ-GGA + SOC approaches (Table 1). The GGA results indicate metallic behavior at all compositions, reflecting its well-known tendency to underestimate the energy gap in Tl-based compounds. In contrast, the mBJ-GGA calculations reveal a gradual transition from metallic to semiconducting behavior: at x = 0.25, the alloy remains metallic, while at x = 0.5 and x = 0.75, it exhibits a direct band gap of 0.22 eV and 0.44 eV, respectively. These values highlight the effect of boron incorporation, which reduces the influence of Tl-6p states and enhances B-2p and P-3p orbital hybridization. Including spin–orbit coupling (SOC) in the mBJ-GGA calculations slightly decreases the band gap due to the strong relativistic effects associated with thallium. Specifically, at x = 0.25, the alloy remains metallic, at x = 0.54 the direct band gap is 0.157 eV, and at x = 0.75 it increases to 0.32 eV. This trend shows that SOC has a more pronounced effect at low Tl content and becomes less significant as boron concentration increases. Overall, the results demonstrate a clear composition-dependent evolution of the electronic structure, with the alloy transitioning from metallic to direct-gap semiconducting behavior as the boron content rises. Such tunable electronic properties make $Tl_{1-x}B_xP$ a promising candidate for band-gap engineering in optoelectronic and infrared devices.
It is worth noting that this alloy is studied here for the first time, so a direct comparison with previous works is not possible; however, the observed trends are consistent with similar alloys, supporting the reliability of the obtained results.

5. Conclusion

The electronic properties of $Tl_{1-x}B_xP$ alloys were systematically investigated at different compositions (x= 0.25, 0.5, 0.75) using GGA, mBJ-GGA, and mBJ-GGA + SOC approaches. The results reveal a gradual transition from metallic to direct-gap semiconducting behavior with increasing boron content, while the effects of SOC are more pronounced at lower thallium concentrations. As this ternary alloy is examined here for the first time, direct comparison with previous studies is not feasible; nevertheless, the observed trends align with similar systems, supporting the reliability of our findings. Overall, this work provides clear insights into the tunable electronic structure and band-gap engineering of $Tl_{1-x}B_xP$, underscoring its potential for future semiconductor and optoelectronic applications.

Acknowledgment

I am honored to dedicate this work to my supervisor, Professor Lachabi Abdelhadi, whose valuable guidance and support were crucial for the completion of this study. I also dedicate this work with respect to Professor Hamza Abid, the head of the laboratory I belong to, in appreciation of his role in providing a supportive scientific environment for the accomplishment of this research.

Authors Contribution
All the authors have participated sufficiently in the intellectualcontent, conception and design of this work or the analysis andinterpretation of the data (when applicable), as well as the writingof the manuscript.

Availability of data and materials
The data that support the findings of this study are available fromthe corresponding author, upon reasonable request.

Conflict of interests
The authors declare that they have no known competing financialinterests or personal relationships that could have appeared toinfluence the work reported in this paper.

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