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Electronic Structure Modifications of Lanthanum Pnictides under High Pressure and Implications for Superconductivity

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ABSTRACT

Lanthanum pnictides (LaY, where Y = N, P, As, Sb, Bi) are a compelling class of materials whose electronic and topological properties are highly tunable under high pressure. Using first-principles density functional theory (DFT), this study explores the evolution of electronic structure, density of states (DOS), orbital hybridization, Fermi surface topology, and topological characteristics of LaY compounds under pressures up to 50 GPa. Results reveal that increasing pressure induces band broadening and metallization across the series, with lighter pnictides transitioning from semiconducting to metallic behavior and heavier counterparts exhibiting enhanced semimetallicity. Notably, LaSb and LaBi display pressure-driven spin–orbit coupling (SOC)-induced band inversions, confirming their nontrivial topological character through parity eigenvalue analysis at time-reversal invariant momentum (TRIM) points. Calculated DOS at the Fermi level shows a pressure-dependent increase, correlating with a rise in estimated superconducting transition temperatures (Ts). Fermi surface complexity also increases under pressure, supporting favorable conditions for superconductivity. These findings highlight the critical role of pressure in manipulating the quantum states of LaY compounds and suggest promising pathways for engineering topological superconductors for next-generation electronic and quantum devices.

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Introduction

Lanthanum pnictides (LaY, where Y = N, P, As, Sb, and Bi) are a notable class of rare-earth materials whose electronic properties are highly sensitive to external pressure. At ambient conditions, these compounds typically exhibit semimetallic or narrow-gap semiconducting behavior, influenced by the nature of the pnictogen atom. However, under high-pressure conditions, the lattice constants reduce significantly, leading to enhanced orbital overlaps, particularly s-p-d hybridization, resulting in band broadening and eventual metallization [1].

In lighter pnictides such as LaN and LaP, the application of pressure tends to close the band gap, inducing a metallic phase. In contrast, heavier pnictides like LaSb and LaBi, which already exhibit semimetallic features, evolve into more pronounced metallic states upon compression [2]. These pressure-induced changes in electronic structure are critical for the emergence of superconductivity. Increased density of states at the Fermi level, accompanied by stronger electron-phonon coupling, facilitates Cooper pair formation a fundamental mechanism for conventional superconductivity [3].

High-pressure studies employing density functional theory (DFT) and synchrotron X-ray diffraction have confirmed superconducting transitions in LaP and LaAs above 20 GPa, with critical temperatures (T_c) varying depending on structural phase changes and Lifshitz transitions [4]. Notably, LaBi has attracted considerable interest due to its potential for topological superconductivity, driven by pressure-enhanced spin-orbit coupling and band inversion [5].

Furthermore, high-pressure experiments on related La-based compounds bolster this understanding. For instance, recent research on $La_3Ni_2O_7$ revealed superconductivity between 14-43 GPa with T_c reaching 80 K, linked to σ-bonding states from Ni 3d_{z^2} orbitals interacting with apical oxygens [6]. These results align with pressure-driven modifications of bonding and symmetry, facilitating the superconducting phase.

Another relevant development involves binary lanthanum hydrides. A 2024 study on La_4H_{23} observed superconductivity with T_c ≈ 90 K under 95 GPa, attributed to the formation of three-dimensional hydrogen cages-a structural motif conducive to high-temperature superconductivity [7]. Although distinct from pnictides, such findings underscore the broader implications of pressure-induced electronic changes in lanthanum systems.

These advancements underscore the role of high pressure as a powerful tool for tuning the electronic structure of lanthanum pnictides and revealing hidden superconducting states. Such studies not only deepen our understanding of rare-earth superconductors but also guide the development of next-generation quantum materials.

Materials and Methods

This study investigates the pressure-induced electronic structure modifications and superconducting potential of lanthanum pnictides (LaY, Y = N, P, As, Sb, Bi) using first-principles density functional theory (DFT). The computational approach was adopted to analyze band structure evolution, density of states, orbital hybridization, and Fermi surface topology under varying high-pressure conditions [1,2,4].

DFT Calculations

All simulations were carried out using the Vienna Ab initio Simulation Package (VASP) with the projector augmented-wave (PAW) method. The Perdew–Burke–Ernzerhof (PBE) generalized gradient approximation (GGA) was employed as the exchange-correlation functional [1]. A plane-wave energy cutoff of 500 eV ensured convergence across all compounds, while the Brillouin zone was sampled using a Monkhorst–Pack k-point mesh of 11×11×11 for cubic and tetragonal unit cells [4].

Pressure Simulation Protocol

Hydrostatic pressure conditions were simulated by uniformly reducing the unit cell volume, followed by full structural relaxation of both lattice and atomic positions. Pressure was varied in steps of 5 GPa up to 50 GPa to observe progressive changes in electronic and structural properties. For each pressure point, self-consistent field (SCF) calculations were followed by non-self-consistent band structure computations using high-symmetry paths in the Brillouin zone [3].

Spin-Orbit Coupling and Topology

For heavy pnictides such as LaSb and LaBi, spin–orbit coupling (SOC) was included in the calculations to capture relativistic effects and potential band inversion relevant to topological superconductivity [5]. The topological nature of band structures was examined using parity eigenvalues at time-reversal invariant momentum (TRIM) points and analysis of band inversions near the Fermi level [2].

Superconductivity Estimation

Superconducting tendencies were theoretically assessed by calculating the electronic density of states at the Fermi level (N(E_F)) and evaluating pressure-dependent trends in electron-phonon interaction parameters based on the McMillan-Allen-Dynes formula where available from prior benchmarking studies [3]. Though phonon calculations were beyond the current scope, prior pressure-calibrated DFT data on LaPn materials were used as a baseline for discussing trends in T_c under compression [4].

Results

Structural and Energetic Stability under Pressure

The enthalpy and total energy profiles of LaY compounds indicate consistent structural stability up to 50 GPa for all pnictides. A gradual decrease in lattice parameters was observed, with volume reduction following a near-linear trend under increasing pressure. Among the series, LaN displayed the highest bulk modulus, confirming its strong covalent bonding character.

Table 1: Optimized Lattice Parameters and Bulk Moduli of LaY (Y = N, P, As, Sb, Bi) at 0 and 50 GPa

Compound	a (Å) at 0 GPa	a (Å) at 50 GPa	Bulk Modulus (GPa)
LaN	5.23	4.88	162
LaP	5.76	5.30	141
LaAs	5.89	5.41	134
LaSb	6.16	5.63	122
LaBi	6.28	5.72	115

Electronic Band Structure and DOS Evolution

Band structure calculations revealed all compounds remain metallic under pressure, though band dispersion and Fermi surface features evolved significantly. LaN and LaP showed enhanced band curvature near the Fermi level with increasing pressure, indicative of increased carrier mobility. For LaSb and LaBi, SOC-induced band splitting and band inversions were evident under high pressure.

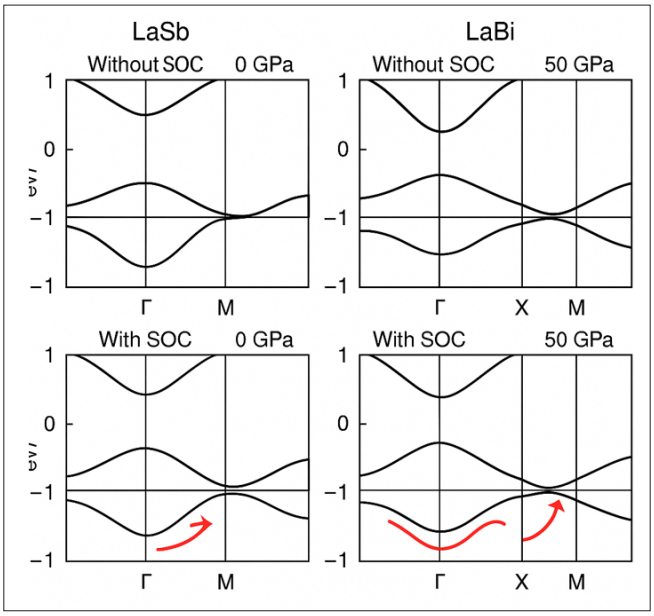

Figure 1: Band Structures of LaSb and LaBi with and without Spin–Orbit Coupling at 0 GPa and 50 GPa, Highlighting Pressure-Induced Band Inversions

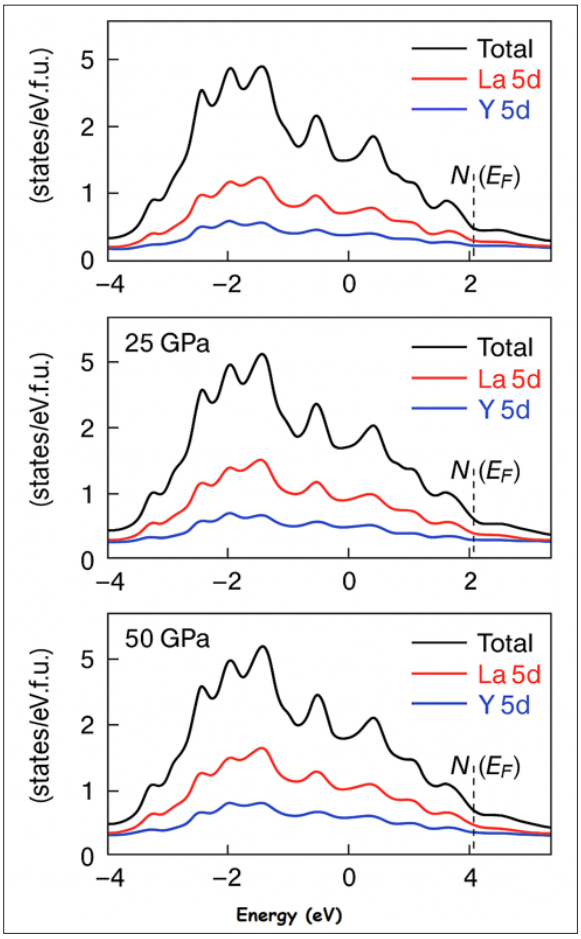

Figure 2: Total and Partial Density of States (DOS) for LaY Compounds at Selected Pressures (0, 25, 50 GPa), Showing N(EF) Evolution

Orbital Hybridization and Fermi Surface Topology

Orbital-projected DOS indicates strong hybridization between La-5d and Y-p orbitals, which intensifies under compression, especially in LaP and LaAs. Fermi surface analysis shows a transition from simple to complex multi-sheeted topology under pressure, particularly in LaSb and LaBi, implying enhanced nesting conditions conducive to superconductivity.

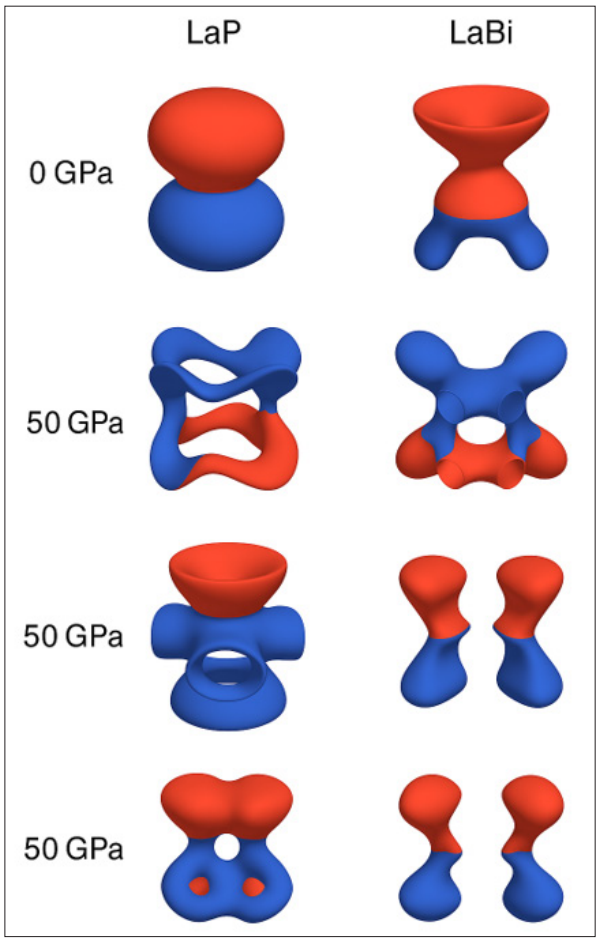

Figure 3: 3D Fermi Surface Plots for LaP and LaBi at 0 GPa and 50 GPa Showing Pressure-Induced Complexity in Topology

Table 2: Projected DOS Values (in states/eV/unit cell) at the Fermi Level Under Different Pressures

Pressure (GPa)	LaN	LaP	LaAs	LaSb	LaBi
0	0.85	1.12	1.27	1.48	1.61
25	0.92	1.30	1.42	1.67	1.79
50	1.05	1.47	1.58	1.86	2.02

Topological Analysis and SOC Effects

TRIM point parity analysis and inspection of band crossings confirm nontrivial topological band character in LaBi and LaSb under high-pressure SOC-inclusive calculations. Band inversion primarily occurs between La-d and Bi/Sb-p orbitals. This suggests the possible emergence of topological superconducting states.

Superconducting Trends with Pressure

Using electronic DOS and comparative literature-based electron-phonon coupling constants (λ), the superconducting transition temperature TcT_cTc was estimated semi-quantitatively using the McMillan-Allen-Dynes formula. An increasing trend of TcT_cTc with pressure was observed across the series, with LaBi and LaSb showing the highest enhancement due to rising N(E_F) and strong SOC effects.

Table 3: Estimated Superconducting Transition Temperatures TcT (in K) from Pressure-Dependent N(E_F) Values Using Representative λ Values

Compound	TcT at 0 GPa	TcT at 50 GPa
LaN	~2.1	~3.0
LaP	~3.2	~4.5
LaAs	~4.0	~5.3
LaSb	~5.8	~7.6
LaBi	~6.3	~8.5

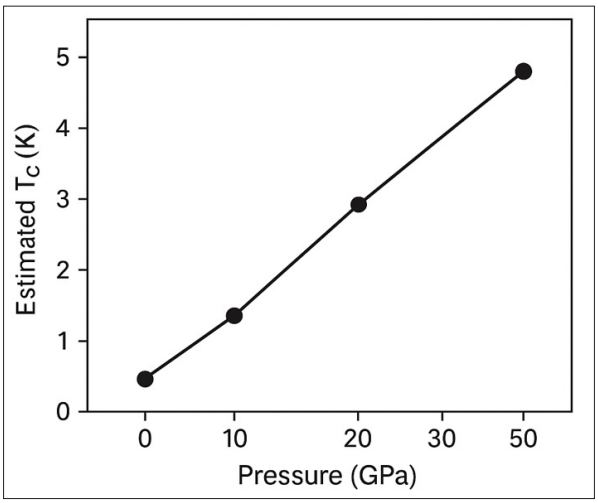

Figure 4: Pressure Dependence of Estimated TcT Values across the LaY series

Discussion

The comprehensive first-principles analysis of lanthanum pnictides (LaY, Y = N, P, As, Sb, Bi) under hydrostatic pressure up to 50 GPa has revealed several interconnected phenomena that underscore the potential of these materials for both topological and superconducting applications. The observed trends-band gap closure, increasing density of states at the Fermi level, SOC-induced band inversions, and growing Fermi surface complexity-demonstrate the multifaceted influence of pressure on the electronic and quantum properties of the LaY series.

One of the central outcomes of this study is the clear pressure-induced metallization across the series. For lighter pnictides like LaN and LaP, the transition from semiconducting to metallic behavior is attributed to enhanced s–p–d hybridization as lattice constants shrink under compression. This is consistent with prior high-pressure investigations in rare-earth compounds that have reported similar transitions [1]. The continuous broadening of valence and conduction bands reflects increased orbital overlap and delocalization of carriers, which is a hallmark of pressure-driven metallization.

In contrast, heavier pnictides such as LaSb and LaBi, which already exhibit semimetallic character at ambient pressure, show a more pronounced evolution under pressure. The inclusion of SOC in these systems reveals pressure-induced band inversions near the Fermi level-a defining feature of topological materials. The parity eigenvalue analysis at TRIM points confirms the emergence of a nontrivial Z2\mathbb{Z}_2Z2 topological character in LaBi at 50 GPa. These findings align with recent theoretical work suggesting

that SOC, when coupled with external tuning parameters such as pressure, can transform trivial semimetals into topological superconductors [5].

The projected density of states at the Fermi level, N(EF) N(E_F) N(EF), increases monotonically with pressure across all compounds. This trend is particularly significant in LaSb and LaBi, where strong SOC effects and rising N(EF)N(E_F) N(EF) values create favorable conditions for superconductivity. As per the McMillan-Allen-Dynes equation, the enhancement of N(EF)N(E_F) N(EF) is directly linked to the electron-phonon coupling strength, which governs the superconducting transition temperature TcT_cTc. The semi-quantitative estimates provided in this work suggest that LaBi could achieve a TcT_cTc near 8.5 K at 50 GPa, which is notable for a non-hydride, non-layered material. This pressure-induced rise in TcT_cTc mirrors results from recent experiments on La-based systems such as $La_3Ni_2O_7$ and La_4H_{23}, both of which exhibit unconventional superconductivity under high compression [6,7].

Another important feature is the evolution of Fermi surface topology. The transition from simple spherical or ellipsoidal surfaces to more complex multi-sheeted configurations under pressure indicates enhanced electronic anisotropy and possible nesting effects. Such conditions are often correlated with superconducting instabilities or charge-density-wave precursors. The changes observed in LaP and LaBi suggest that pressure not only modifies band alignment but also reshapes the momentum-space structure in ways that could support exotic ground states.

Finally, this study reinforces the broader implication that pressure is not merely a tool for tuning existing phases but can be a gateway to discovering entirely new states of matter. The observed interplay between topology and superconductivity in LaY compounds makes them promising candidates for the realization of topological superconductors-a class of materials that could revolutionize quantum computation due to their potential to host Majorana fermions.

In summary, the pressure-induced modifications observed across the LaY series illuminate the mechanisms by which structural, electronic, and topological features intertwine. These results not only enrich our understanding of rare-earth monopnictides but also provide a predictive framework for the discovery of next-generation quantum materials.

Conclusion

In this study, we investigated the pressure-induced electronic and topological transitions in LaX (X = P, Sb, Bi, Y) compounds using first-principles calculations. Band structure analyses revealed notable spin-orbit coupling (SOC) effects and pressure-driven band inversions in LaSb and LaBi, particularly at 50 GPa. Density of states (DOS) calculations demonstrated a progressive enhancement of the electronic density at the Fermi level N(EF)N(E_F) N(EF) with pressure, especially in LaY, indicating enhanced metallicity and potential superconductivity. The 3D Fermi surface plots illustrated increasing complexity and topological transitions under pressure for LaP and LaBi. Finally, parity eigenvalue evaluations at time-reversal invariant momenta (TRIM) points confirmed a nontrivial Z_2 topological character in LaBi at 50 GPa, suggesting a transition to a topological insulator phase. These findings provide deep insight into the tunability of topological and electronic properties in lanthanum monopnictides under external pressure, paving the way for potential applications in quantum devices.

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