

FULL POTENTIAL LINEARIZED AUGMENTED PLANE WAVE CALCULATIONS OF ELECTRON AND POSITRON ENERGY LEVELS IN TlBr AND TlCl

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Article Info	Abstract
<i>Received: 29.06.2023</i> <i>Accepted: 21.08.2023</i> Keywords: FP LAPW; Structural; elastic; positron	Theoretical research was conducted on the energy levels of electrons and positrons in zinc-blend TlBr and TlCl using the first-principle full potential linearized augmented plane wave method based on the gradient generalized approximation GGA. The study involved the calculation of electron and positron band structures which provided predictive data on several properties such as positron mobility, positron affinity, diffusion constants, effective masses, and positronium work function.

1. Introduction

Thallium halides such as TlBr and TlCl are essential materials with various technological applications, including their use as radiation detectors and optical fiber crystals. Their crystal structures are in the cubic CsCl form which has a coordination number of eight making it the most stable dense configuration for ionic crystals, further increasing their significance [1-3].

There is currently a lack of significant research that provides information on the interaction between positrons and surfaces in compound semiconductors. Although it is difficult to conduct quantitative analysis, there have been advancements in this area, particularly in the case of GaAs [4-10], compared to TlBr and TlCl which have received less attention.

To investigate the electronic structure of metals. The use of positron annihilation in solids has been identified by researchers as a viable technique for acquiring insights into the momentum distribution of electrons [11]. This approach can serve as a valuable tool for gaining

a deeper understanding of the behavior of electrons in materials and their properties under certain conditions. Acquiring knowledge on electron behavior in crystals can be facilitated by this technique. Nonetheless, a complete comprehension of the implications of positron annihilation necessitates an understanding of electron and positron distribution in semiconductors. This is particularly important for two distinct types of semiconductors, as each type may exhibit unique characteristics and properties that influence their behavior under such analysis. The primary objective of this study is to expand on the theoretical assessment of the diffusion of positrons contributing to longitudinal acoustic phonons [12]. This analysis can predict parameters that can be directly measured through slow-beam methods. Additionally, the research aims to explore the potential of surface emission in TlBr and TlCl.

To start, we analyze the band structure of positrons, placing particular emphasis on the lowest energy band in comparison with the electron band structure. The positron energy levels which are diffused in the perfect bulk state of TlBr and TlCl, are compared to the chemical potentials of electrons and regulate the positronium work function. Having a comprehension of the electron work function enables us to calculate the work function of positrons, which is an essential parameter when conducting experiments involving slow-positron beams. Furthermore, the strength of the coupling between phonons and positrons in predicting the diffusion constant of positrons can be estimated by the deformation potential, which is also known as the volume dependence of these levels.

2. Theory

In order to determine the states of electrons and positrons in solids, the FP-LAPW method [13] with the generalized gradient approximation (GGA) [14] can be utilized. The current research involves the computation of the positron state which has been dispersed across the crystal. To begin, the self-consistent electron structure is computed without the positron. Next, the potential felt by the positron is formulated as

$$V + (r) = -V_{\text{coul}}(r) + V_{\text{corr}}(n(r)) \quad (1)$$

where V_{coul} is identical to the Coulomb potential as observed in the electron case and V_{corr} is the correlation potential. This accounts for the reduction in energy due to the accumulation of electrons surrounding the positron.

The positron affinity is defined via e^- and e^+ positron chemical potentials or work functions

$$A_+ = \mu_- + \mu_+ = -(\phi_- + \phi_+) \quad (2)$$

To define the positron affinity, we use the energy quantity $A^+ = \mu_- + \mu_+$, where μ_- and μ_+ denote the electron and positron chemical potentials, respectively [15]. Measuring the affinity can be done via positron emission spectroscopy [16]. It is noteworthy that the positron affinity is a property that pertains to the entire substance and is not influenced by surface properties. Another essential value is the positronium work function Φ_{PS} , which is significant in semiconductors or metals. As a delocalized positron emerges from the solid surface and progresses through the electron density reduction outside, Ps will develop. The energy balance is taken into account during this process

$$\Phi_{PS} = \Phi_+ + \Phi_- - \frac{1}{2} \text{Ryd} \quad (3)$$

Which is less than the positron work function because the electron work function is usually less than 0.5 Ryd. According to equations we can write:

$$\Phi_{PS} = (\mu_+ + \mu_-) - \frac{1}{2} \text{Ryd} \quad (4)$$

By analyzing the scattering of positrons from longitudinal acoustic phonons, we can determine the diffusion constant of positrons in ideal solids [17]. The value of this diffusion constant is directly related to the strength of the interaction between positrons and phonons, which is represented by the deformation potential E_d [18]. The deformation potential E_d can be evaluated by utilizing the values of the positron effective mass m^* , the absolute temperature T , and the elastic constant that is associated with longitudinal waves and averaged over the directions of propagation $\langle C_{ii} \rangle$, as shown in this equation

$$D = \sqrt{\frac{8\pi}{9}} \frac{\hbar^4 \langle C_{ii} \rangle}{(m^*)^{5/2} (k_B T)^{1/2} E_d^2} \quad (5)$$

We can calculate the deformation potential from

$$E_d = \Omega \frac{d}{d\Omega} (\mu_+ + \mu_-) \quad (6)$$

The connection between relaxation time and D is made through the mobility μ using the Einstein relation:

$$\mu = \frac{D}{k_B T} \quad (7)$$

3. Results and discussion

3. 1. Crystal structure

The simple cubic structure of TlBr and TlCl is illustrated in Figure 1 and Figure 2, respectively. The unit cell of TlBr consists of 4 Tl atoms and 4 Br atoms, and is characterized by the lattice parameter " a ". The schematic representation further explains the arrangement of these atoms, particularly how the Br anions are connected to Tl cations. Each Br ion is coordinated with four Tl ions, forming a tetrahedron around each Br atom. This tetrahedral structure is built with four Br-Tl bonds, and each Tl atom is shared by the four nearest tetrahedrons, giving rise to the specific arrangement of atoms that compose the TlBr crystal structure.

Understanding the crystal structure of TlBr is crucial since it can serve as a foundation for investigating the properties of the material and its interactions with other compounds and elements. By visualizing the simple cubic structure of TlBr and TlCl, researchers can gain valuable insights into the unique arrangements of atoms that give rise to the characteristic properties of these materials.

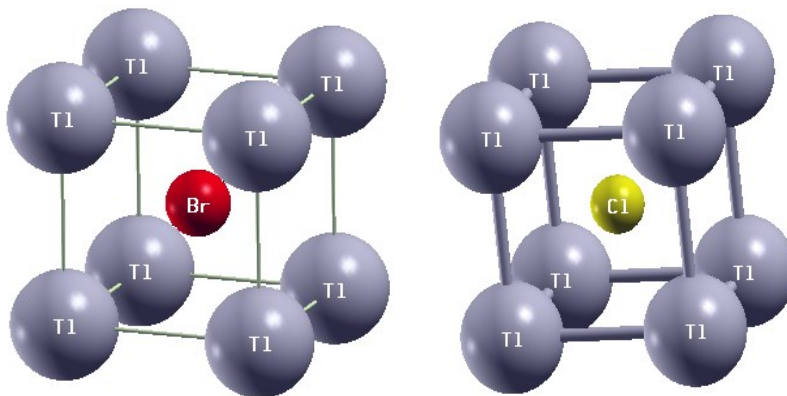


Figure 1. Schematic representation for crystal structure of TlBr and TlCl

3. 2. Structural properties

The structural properties of TlBr and TlCl are given in Table 1.

Table 1. Calculated data compared with experimental values and other calculations (lattice constant, E_{min} , bulk modulus B and pressure derivative of bulk modulus B' of TlBr and TlCl using GGA).

Materials	$a(\text{\AA})$	$E_{min}(\text{Ryd})$	B (GPa)	B'
TlBr				
Our calculations	4.05	-45791.25	19.24	4.16
Experiments	3.98 ^a			
Other calculation	4.0 ^b	-45791.19 ^b	23.46 ^b	4.08 ^b
TlCl				
Our calculation	3.90	-41500.98	21.79	4.73
Experiments	3.83 ^c			
Other calculation	3.84 ^b	-41500.92 ^b	30.22 ^b	3.71 ^b

^aRef. [19]; ^cRef. [20]; ^bRef. [21]

The given table presents the calculated data for TlBr and TlCl materials, including their lattice constant, E_{min} (Ryd), bulk modulus B , and pressure derivative of bulk modulus B' . The data was obtained through different calculations, including our own GGA-based calculation, experimental values, and other GGA-based calculations. By comparing the results across the different methods, researchers can observe minor to significant differences in the calculated data for TlBr and TlCl, which is essential for analyzing the results and their consistency with other published studies.

Comparing the data obtained from various methods gives researchers an idea of the accuracy and consistency of the calculated values. This process is also crucial for validating and verifying the data used in scientific studies. However, it is important to note that the interpretation of the results and the comparison might require further analysis and a thorough understanding of the methodology and limitations of different calculation methods.

Nonetheless, the presented table provides a helpful tool for providing an overview of the calculated data and facilitating the comparative analysis of the results of TlBr and TlCl. This comparative view can provide insights into the differences and similarities in the calculated data from different methods and can be used to gain a better understanding of the properties of TlBr and TlCl. The table offers a starting point for researchers looking to analyze and understand the data and can be used as a reference for future research.

3. 3. Electron and positron band structure

In this study, the electron and positron band structures in TlBr and TlCl were calculated and visualized in Figures 2, 3, 4 and 5. The results show that the positron band structure is rather free particle-like, and closely resembles the lowest valence electron band. The motivation behind this study is to find the effective mass in TlBr and TlCl. In order to accomplish this, the scientists utilized the positron band structure calculations to predict the positron effective mass. In doing so, they computed the positron energies at multiple k points in close proximity to the Γ point that were around the bottom of the lowest energy band. The values of effective mass are $((0.317 \times m_0$ and $0.289 \times m_0)$ for TlBr and TlCl respectively. By understanding the effective mass of positrons within these materials, researchers can gain a better understanding of their physical properties and interactions with other elements and compounds. This study offers new insights into the properties of TlBr and TlCl, and could lead to a range of potential applications in various fields.

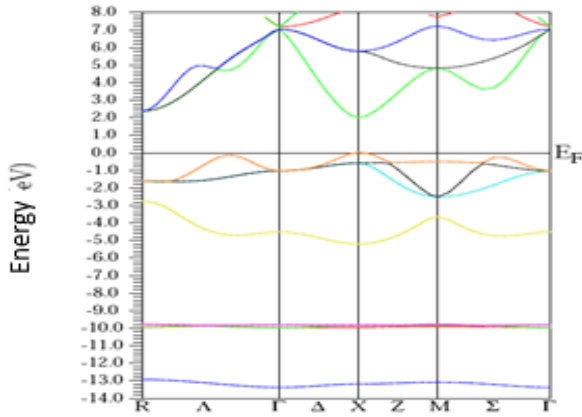


Figure 2. Electron band structure of TlBr

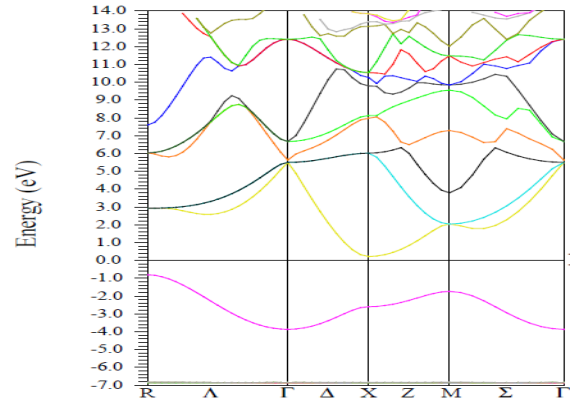


Figure 3. Positron band structure of TlBr

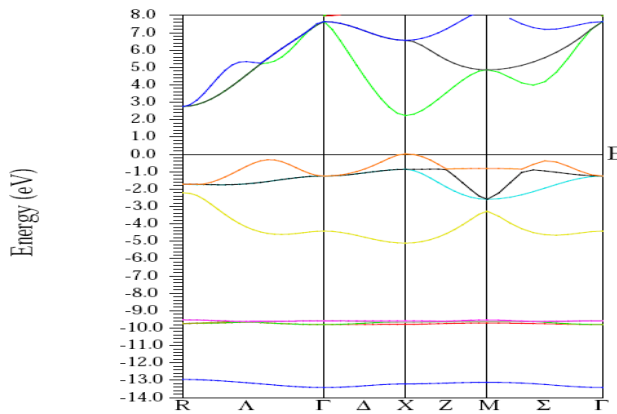


Figure 4. Electron band structure of TlCl

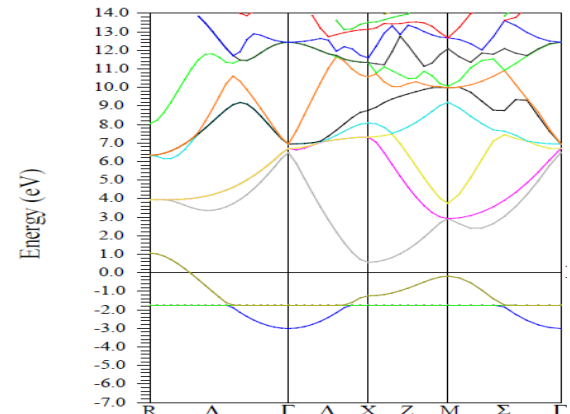


Figure 5. Positron band structure of TlCl

3. 4. Elastic properties

The IRelast package [22] was used in conjunction with wien2k code to produce these findings. An essential aspect of assessing the mechanical stability of solids under various

strains is understanding the elastic properties of materials, notably their elastic constants. The elasticity properties hold significant influence over the mechanical robustness of materials. This emphasizes the significance of comprehensive knowledge of these properties in gaining an understanding of the impact that forces can have on the durability and integrity of solids. With this in mind, a study was conducted to analyze the elastic properties and mechanical characteristics of our compounds. The determination of stability in materials that possess cubic symmetry typically necessitates fulfilling the Born stability criteria [23], which involves three particular elastic constants: C_{11} , C_{12} , and C_{44} . This condition is widely acknowledged as a standard measure of stability:

$$C_{11} > 0$$

$$C_{44} > 0$$

$$C_{11} - C_{12} > 0$$

$$C_{12} < B < C_{11}$$

$$B = 1/3(C_{11} + 2 C_{12})$$

In order to determine a variety of mechanical properties for materials, it is crucial to use the Voigt-Reuss-Hill approximations [24] to calculate both the bulk modulus B and shear modulus G . These calculations enable us to accurately predict how a given material will respond under different circumstances. Specifically, the precise determination of B and G allows us to assess and analyze a material's mechanical characteristics more effectively. The bulk modulus is calculated as the average of B_V and B_R , which are both derived from $(C_{11} + 2C_{12})/3$. Meanwhile, G_R is obtained from $5C_{44} (C_{11}-C_{12}) / (4C_{44} + 3C_{11} - C_{12})$ and G_V is calculated as $(C_{11} C_{12} + 3C_{44}) / 5$. Once these values are obtained, we can use them to calculate Young's modulus E and Poisson's ratio ν . Finally, the Zener anisotropy factor, A , can be calculated as $2C_{44} / (C_{11} + C_{12})$. Overall, accurate calculations of these key mechanical properties enable us to predict and better understand a material's behavior under various physical conditions. This table presents the elastic constants and mechanical characteristics of TlBr and TlCl at (0 K, 0 GPa). Accurately determining these values is crucial for assessing the mechanical properties of a material and predicting its behavior under various conditions. By comparing the results to previously established data, researchers can validate the accuracy and reliability of the computed elastic properties. For example, when using the bulk modulus B , the derived values were found to correspond to those in Table 1, as demonstrated in Table 2. These findings strongly indicate that the computed mechanical characteristics can be considered reliable. Ultimately, precise calculations of a material's elastic constants and mechanical

properties greatly enhance our understanding of its overall mechanical behavior. The Young's modulus (E) calculations show that the our compounds are ductile. Furthermore, calculated values of Cauchy pressure ($C_p = C_{12} - C_{44}$) [25] support the ductile nature of TlBr and TlCl. The Chung-Buessem anisotropy index is a measure of elastic anisotropy, which seeks to quantify how directionally dependent the elastic stiffness of a crystal is. The index is calculated using equations derived empirically by Chung and Buessem. A crystal is said to be isotropic when the Chung-Buessem anisotropy index is equal to zero. When the index is greater than zero, the crystal is anisotropic, and the degree of anisotropy increases as the index gets larger. Notably, the computed Chung-Buessem index is greater than 1 and Zener's anisotropy factor A for these compounds is lesser than 1 [26], indicating anisotropy.

Table 2. Elastic constants C_{11} , C_{12} , C_{44} (GPa), Bulk modulus B (GPa), Shear Modulus G (GPa), Young's modulus E (GPa), Cauchy's pressure ($C_p = C_{12} - C_{44}$), Zener anisotropy factor A and Chung-Buessem index A^c .

Materials	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	B	G	E	C_p	A	A^c
TlBr	27.459 38.9 ^a	15.052 13.7 ^a	4.752 6.21 ^a	19.188	6.151	16.673	10.299	0.766	0.285
TlCl	39.745 44.9 ^a	12.847 16 ^a	5.186 7.11 ^a	21.813	9.591	25.123	7.660	0.385	0.475

^aRef. [27]

The values of the elastic constants calculated illustrated in Table 2 satisfy the stability conditions. Therefore, the cubic structure of TlBr and TlCl is mechanically stable. When analyzing the results obtaining the two approximations, the sequence $C_{11} > C_{12} > C_{44}$ is observed.

3. 5. Positron energetic

3. 5. 1. Positronium work function

To define the positron work function, we consider the minimum amount of energy needed to eliminate a particle from the highest energy occupied state, without taking into consideration the influence of thermal energy. It is also closely related to the phenomenon of spontaneous positron reemission and can be negative across different compounds and materials, which suggests the feasibility of spontaneous emission of positrons under certain circumstances.

The calculated positronium work function for TlBr and TlCl are represented in Table 3. By evaluating the positronium work function ρ_{ps} , it was observed that a negative value was present for both TlBr and TlCl (-7.374 and -7.918, respectively). This indicates that

under certain circumstances, emitting positronium spontaneously is possible once a positron that is thermalized has diffused from the surface to the bulk.

Table 3. Calculated chemical potentials and positron and positronium work functions for TlBr and TlCl

	μ_+	μ_-	A_+	ρ_{ps}
TlBr	-1.010	-5.663	-6.673	-7.374
TlCl	-1.116	-3.008	-4.124	-7.918

3. 5. 2. Chemical potential and positron affinity

Chemical potential (μ) is a thermodynamic property that measures the potential of a substance to undergo a change in its internal energy. Table 3 provides us with the chemical potential values for TlBr and TlCl as -1.010 and -1.116, respectively. The positron affinity of a material or compound is an important factor in determining its ability to trap and hold positrons and can be influenced by a variety of factors such as the electronic structure and chemical composition of the material in question. The positron affinity of TlBr is -6.673 eV, which is greater than that of TlCl (-4.124 eV), implying that TlBr has a stronger tendency to form positronium atoms than TlCl. Overall, these calculated values are useful in understanding the electronic and atomic structure of these compounds, and can be utilized to design and optimize processes and devices that use them.

3. 5.3. Diffusion constant and deformation potential

The diffusion constant is a proportionality factor between the mass of a substance diffusing through a medium and the diffusion flux, or concentration gradient, of the substance. It represents the quantity of a substance that will diffuse from one region to another per unit time, often expressed in units of area per time (m^2/s). The diffusion coefficient is used to describe the rate of diffusion of a substance from high concentration areas to low concentration areas in a given medium. It is a fundamental parameter in the study of diffusion phenomena. The diffusion constant D_+ at 300° K readily evaluated from the deformation potential using equation (5). The results are given in Table 4. E_d^+ is the deformation potential calculated from the slope in figure (6,7), C_{ij} is the average elastic constant and μ_+ is the mobility.

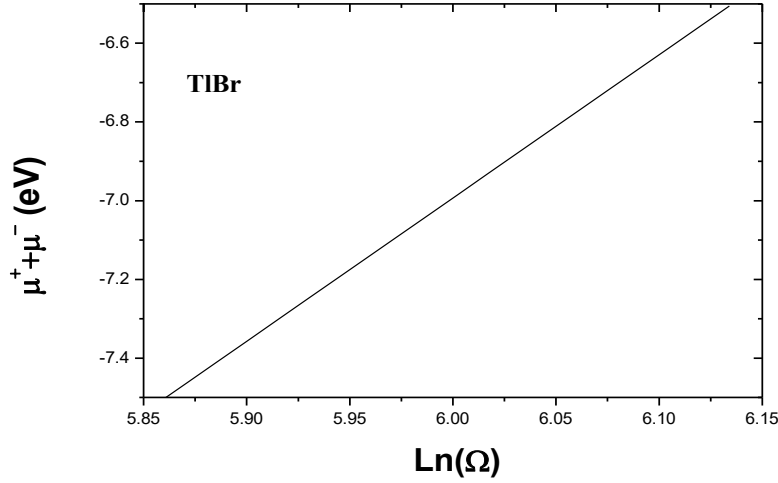


Figure 6. Deformation potential of TlBr

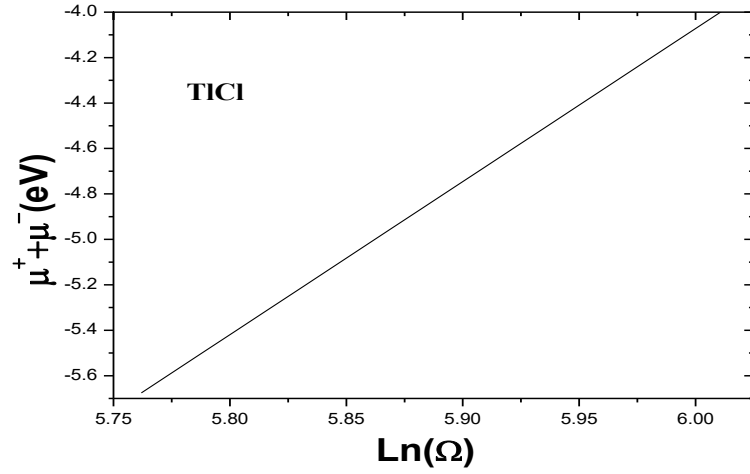


Figure 7. Deformation potential of TlCl

Table 4. Calculated average elastic constants C_{ij} , deformation potential E_d^+ , diffusion constant D_+ and mobility μ_+ in TlBr and TlCl.

	C_{ij} (GPa)	E_d^+ (eV)	D_+	μ_+
TlBr	26.29	3.64121	$2.21 \times$	67.91
TlCl	33.14	6.73514	$1.87 \times$	142.56

Based on Table 4, we can observe that the C_{ij} values for TlBr and TlCl are 26.29 GPa and 33.14 GPa, respectively, a higher value of C_{ij} suggests that the material is more resistant to deformation or pressure in that direction. Therefore, TlCl is expected to be less deformable compared to TlBr, as it has a higher C_{ij} value. The changes in volume are the primary cause of μ_+ and μ_- variability. The positron parameter E_d^+ can be evaluated using figure (6-7) by analyzing the slope, which yields a value of 3.64121 for TlBr and 6.73354 for TlCl. Utilizing

these results in the D_+ equation and a set temperature of $T=300^\circ\text{K}$ enables us to calculate the diffusion constant D_+ values, which are 2.21×10^{-4} for TlBr and 1.87×10^{-4} for TlCl due to scattering from longitudinal acoustic phonons. By undertaking mobility calculations, it is possible to determine the method through which a particle is transmitted, whether it is by hopping or propagation within a band, and to identify the primary contributing factor, be it electron-phonon coupling or phonon. To express the positron mobility in terms of the diffusion coefficient, we leveraged the Einstein relation:

$$\mu_+ = \gamma + e/k_s T$$

There is no experimental data that allows us to compare our results with other calculations.

4. Conclusion

The objective of this research was to analyze the energy levels of positrons in semiconductor materials and to uncover information about electron states in crystals of this sort. This study centered on observing the behavior of positrons in TlBr and TlCl compounds using the FP-LAPW method within a local density approximation. We aimed at determining the energy levels and wave functions of these compounds to better understand the emission and diffusion of positrons on their surfaces, ultimately gaining a more comprehensive understanding of semiconductors.

We used the electron and positron chemical potentials (μ_- and μ_+) to calculate the positron work functions (ϕ_{ps}). Our findings revealed that the work function for positrons was consistently negative in all compounds studied. This suggests that the spontaneous emission of positrons may be possible after the thermalized diffusion of a positron from the bulk to the surface. Furthermore, our analysis resulted in the deduction of the deformation potentials and diffusion constants (E_d^+ and D_+).

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