ELECTRONIC AND STRUCTURAL PROPERTIES OF Bi ADSORBED $TlInTe_2$

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The results of calculations using density functional theory (DFT) of the crystal structure and electronic properties of Bi adsorbed on the $TlInTe_2$ structures were investigated. The research was carried out by computer modeling using the Atomistic Toolkit software. Adsorbing Bi can increase the cell parameters, cell asymmetry and band gap. We have obtained a different value of the band gap for adsorption Bi on the $TlInTe_2$ surface in the different temperature values. The band gap of single crystal $TlInTe_2$⟨Bi⟩ relative to $TlInTe_2$ decreases at 300 K.

Keywords: $TlInTe_2$ structure, Bi adsorption, DFT.
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INTRODUCTION

Nowadays, there is a significant need for the alternatives of the energy using because of the depletion of the energy resources on our planet. Thermoelectric materials, which can realize the energy conversion between heat and electricity, might be potential candidates. Although practical applications for thermoelectric devices became feasible only after mid twenty century because of advancements in the semiconductor technologies. The structural and electronic properties of the $TlInTe_2$ are investigated experimentally [1] and theoretically [2,3,4]. Have been shown [5] that the deviation from linearity can be unprecedently large in incommensurate phases as exemplified by archetypal Zintl-like semiconductor $TlInTe_2$. This happens because two mutually incompatible translational symmetries allow spatially and temporally varying phase shifts, thus giving rise to two new heat-carrying modes: phasons and amplitudons. TlInTe2 has a multivalley band structure [6]. This structure contributes to the high Seebeck coefficients and thermoelectric figure of merit of $TlInTe_2$. Zintl compounds such as InTe [7], TlSe [8], and $TlInTe_2$ [9] exhibit both covalent (stronger) and ionic (weaker) substructures within them. The presence of such hierarchically bonded sublattices makes Zintl compounds Ideal for intrinsically ultra-low thermal conductivity. The [10] work demonstrates that the stoichiometric excess of the additive atom in the TlInTe2 crystal with a chain structure allows to purposeful control the anisotropic properties of materials. The work [11] includes models of the studied objects, along with tables presenting the adsorption energy and the magnitude of the distance between the adsorbate and the atoms.

The aim of this investigation is the first-principles calculation of the energy of Bi adsorption by the surface of $TlInTe_2$ supercells. Theoretical research on the adsorption of Bi on the $TlInTe_2$ surface reveal that the calculated band structure depend on several factors, including the calculation technique, adatom structure, the bond distance and the nature of the interaction between the adatom and the $TlInTe_2$ structure.

COMPUTATIONAL DETAILS

Crystal structure and electron band structure for Bi adsorbed on $TlInTe_2$ are performed within the framework of DFT using Perdew–Zunger (PZ) exchange correlation functional, as implemented in the Atomistix ToolKit. The kinetic cut-off energy is set to 150 Ry. During the structure optimization, the reciprocal space is sampled by a 5x5x5 k-point mesh. The primitive cell of $TlInTe_2$ was relaxed and optimized with force and stress tolerances of 0.01eV/Å and 0.01eV/Å3, respectively.

RESULT AND DISCUSSION

$TlInTe_2$ belongs to the TlSe-family and has a simple tetragonal crystal structure with the space group I4/mcm. Fig.2 (a) presents the atomic structure of $TlInTe_2$ and (b) corresponds to the adsorption sites of Bi adsorbed on $TlInTe_2$. The relaxed lattice parameters are a = 8.7Å and b= 7.33Å, in agreement with previous calculations and experimental measurements [12]. Due to the sp3 hybridized In, $TlInTe_2$ adopts a Zintl-like structure and exhibits semiconducting properties.

The band structure of Bi adsorbed on $TlInTe_2$ in the different temperature values is displayed in Table. The influence of Bi adsorbed on the electronic structure of $TlInTe_2$ material was calculated using DFT. As presented in Figure 1, the obtained band structure of $TlInTe_2$ reveals a band gap of 0.61eV, which is consistent with the experimental results of 0.65eV [14-15].

The conduction band minimum and the valence band maximum are both located at the Γ point. The $TlInTe_2$ band gap can be engineered by creating lattice defects, such as vacancies, substitutions, and interstitial spaces, which in turn change its electrical, thermal, and optical properties.

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Table

Calculated band gap of Bi adsorbed on $TlInTe_2$

Structure	Band gap, eV	temperature, K
$TlInTe_2$	0.61eV	300K
$TlInTe_2\langle Bi\rangle$	0.46eV	300K
$TlInTe_2\langle Bi\rangle$	0.413eV	400K
$TlInTe_2\langle Bi\rangle$	0.406eV	550K

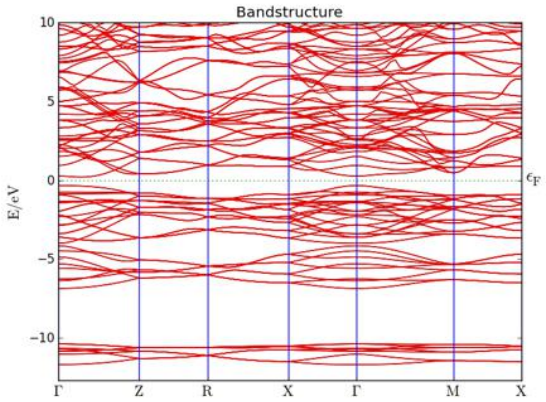
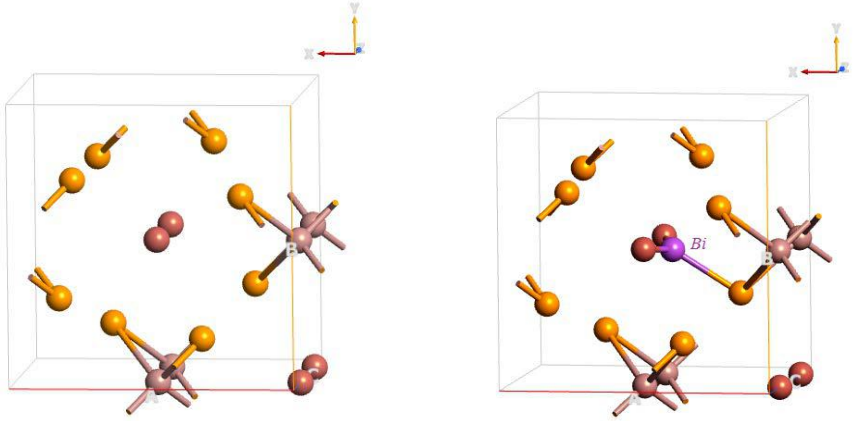


Fig.1: Band structure of Bi adsorbed $TlInTe_2$



a) b)

Fig. 2. Atomic structure of (a) $TlInTe_2$ and (b) Bi adsorbed on $TlInTe_2$

The influence of Bi adsorbong on the electronic structure and optical properties of $TlInTe_2$ is systematically studied. It can be seen that the for band gap of $TlInTe_2$ is obviously smaller after Bi doping.

In Figure 2, the structure of (a) $TlInTe_2$ and (b) Bi adsorbed on $TlInTe_2$ are shown. The Bi atom is at the center of the structure. When Bi atom is adsorbed on the $TlInTe_2$ structure Bi-Te bond length is $3.219A^0$, Bi-In bond length is $3.044A^0$ respectively. The band gap decreases when Bi adsorbed on the $TlInTe_2$ structure. Our calculations indicate that the band gap of Bi adsorbed on $TlInTe_2$ is 0.46eV, 0.413eV, and 0.406eV at respective temperatures described in the Table. As the temperature increases, the band gap value of this structure also changes.

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