# A Comparison of the Structural, Electronic, Optical and Elastic Properties of Wurtzite, Zinc-Blende and Rock Salt TlN: A DFT Study

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In this article we investigated structural, electronic, elastic, and optical properties of TlN in three phases, using full potential linear augmented plane wave method in the density functional theory frame with WIEN2k code. The calculations have been done in the generalized Perdew-Burke-Ernzerhof generalized gradient approximation, the generalized Wu–Cohen gradient approximation, the generalized Perdew–Burke–Ernzerhof solid gradient approximation, local density approximation, and the modified Becke-Johnson approximations. In spite of the absence of any experimental data for TlN, our results are compared with other results achieved by other different approximations which shows a good agreement with them. The band gap for TlN in wurtzite and zinc-blende are obtained to be 0.07 and 0.09 eV within modified Becke–Johnson–local density approximation+spin–orbit approximation, respectively. The structural properties such as phase transitions, equilibrium lattice parameters, bulk modulus and its first pressure derivative were obtained using an optimization method. Moreover, we calculated quantities such as elastic constants, the Young modulus, shear modulus, the Poisson ratio, and sound velocities for longitudinal and transverse waves, the Debye temperature and the Kleinman parameters in different approximations and we show that TlN is softer than other nitrides of the III-group. The static calculations predicted that wurtzite to rock salt and zinc-blende to rock salt phase transitions occur at 14.7 GPa and 15.8, respectively. The optical properties of TlN in three phases, calculated in generalized gradient approximation and local density approximation and imaginary part of dielectric function show that TIN in wurtzite and zinc-blende phases have semiconductor properties but rock salt phase do not show. As well as, we investigate the influence of the hydrostatic pressure on the elastic parameters and energy band structures for TlN (zinc-blende) within local density approximation.

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# 1. Introduction

In the last years, the III-group nitrides have been investigated widely because of their high temperature stability, very short bond lengths, low compressibility, and high thermal conductivity. These materials also have excellent properties such as wide band gaps and strong bond strength, therefore they can be used for violet, blue, and green light emitting apparatuses and high temperature transistors [1–3].

However, up to our knowledge, thallium nitride (TlN) very little has been investigated. The band gap of the IIIgroup nitrides decreases from top to the bottom in element table so we expect that TlN has a small or even negative energy gap and shows a semi-metallic behavior [4]. So combinations of Tl with wide-gap III-nitrides yield interesting ternary alloys such as  $Al_{1-x}Tl_xN$  [5] and  $Ga_{1-x}Tl_xN$  [6] with great potential for infrared optical apparatuses. Experimental synthesis of TlN has not yet been reported. However, by total energy calculations from first-principles, the wurtzite phase has been found to be the ground state phase of TlN [7, 8]. The electronic structure and some of optical properties of wurtzite (WZ) and zinc-blende (ZB) TlN by da Silva et al. by using QP model and local density approximation (LDA) have been investigated [9].

Recently, first-principle computations based on density functional theory (DFT) have developed the fundamental part of materials investigations. The density functional theory full potential linear augmented plane wave (FP-LAPW) method has been broadly recognized as a powerful method for computational solid-state researches. The calculation of various properties such as the structural, elastic, thermodynamical, optical and electronic properties for several compounds has been done by using the DFT method. These calculations provide a comprehensive knowledge about the different properties of materials and the chance to design new compounds for special applications [10]. Although there are three different phases of TlN, but no any complete study comparing TlN in these three phases has been performed. In this work, we investigated structural, electronic, elastic, and the optical properties of TlN in three phases. The calculation method was FP-LAPW with various approximations. Exchange-correlation functional and corresponding potential have an outstanding role in DFT based total energy calculations. The calculations were done using LDA, generalized gradient approximation (GGA) with

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spin–orbit (SO) and modified Becke–Johnson (mBJ) for exchange correlation functional.

# 2. Computational approach

In this work, we were applying FP-LAPW approach within the DFT framework, to obtain the structural, phase transition, elastic, thermodynamical, optical and electronic properties of TIN in three phases by using WIEN2k code [11]. We were applying to our calculation different approximations such as LDA, GGA: Perdew-Burke–Ernzerhof (PBE) [12], Wu–Cohen (WC) [13], Perdew-Burke-Ernzerhof solid (PBEsol) [14], and mBJ-GGA or mBJ-LDA [15]. The wave functions cut-off magnitude was chosen to be  $R_{\rm MT}K_{\rm max} = 8.5$  for wurtzite and  $R_{\rm MT}K_{\rm max} = 8.0$  for cubic phase (ZB and RS), in the interstitial spaces, where  $R_{\rm MT}$  denoted the smallest atomic muffin-tin sphere radius and  $K_{\text{max}}$  denoted the largest K vector in the plane wave extension. The valence wave functions inside the muffin-tin spheres were expanded up to  $l_{\text{max}} = 10$ , while the charge density was Fourier expanded up to  $G_{\text{max}} = 12$  (a.u.)<sup>-1</sup>. The self-consistent calculations are considered to be converged when the total energy of the system is fixed within  $10^{-4}$  Ry. The integrals over the Brillouin zone are 1000 k-points in the irreducible Brillouin zone, using the Monkhorst–Pack special k-points method [16]. The energy dividing the valence state from the core state was set as -6.0 Ry. In the calculations [Xe]  $6s^24f^{14}5d^{10}6p^1$  and [He]  $2s^22p^3$  states are considered as valence electrons for Tl and N, respectively.

# 3. Results and discussion

# 3.1. Structural properties

To appraise the structural properties of TlN in three phases, the total energies are assessed for various volumes environs of the equilibrium cell volume  $V_0$ . The gained total energy is fitted to the Murnaghan equation of state [17] to assess the structural properties such as equilibrium lattice constant a and c, the bulk modulus B and its first pressure derivative B' and  $E_0$ . These equilibrium parameters are calculated using GGA (PBE, WC, and PBEsol) and LDA approximations, which are listed in Table I. Since there are not any experimental data for TlN, we compared our results with other theoretical results. According to Table I, we see that our results are inconsistent with the other results. Also, according to Table I, we can see that ground state of TlN must be in WZ phase like other the III-group nitrides because  $e_0$ of wurtzite phase is less than other phase.

TABLE I

Calculated lattice constant,	$a_0$ [Å] and	c [Å], bulk	modulus,	$B_0$ , and	its pressure	derivative,	$B'_0$ for	r TlN
in three phases using different	ent approxin	nations.						

Thallium nitride	$a_0$ [Å]	c [Å]	$b_0  [\text{GPa}]$	$b'_0$	$e_0$ [Ry]		
wurtzite							
GGA (PBE)	3.7398	6.0764	93.85	4.3319	-81374.461548		
GGA (WC)	3.6840	5.9718	107.71	4.4315	-81368.891968		
GGA (PBEsol)	3.6806	5.9644	107.97	4.4331	-81351.716098		
LDA	3.6461	5.8987	117.88	4.4851	-81328.973580		
other works	$3.747^a, 3.746^b, 3.766^c, 3.598^d$	$\begin{array}{c} 6.079^a,  6.014^b, \\ 5.768^c,  5.937^d \end{array}$	$85^a, 113^b, 121^d$	$4.4^a, 4.2^b$	_		
Zinc-blende							
GGA (PBE)	5.2723	_	94.06	4.3038	-40687.232557		
GGA (WC)	5.1961	_	106.73	4.5417	-40684.448502		
GGA (PBEsol)	5.1912	_	106.03	4.6325	-40675.860657		
LDA	5.1415	_	116.61	4.6386	-40664.490043		
other works	$5.129^e, 4.882^f, 5.055^g$	_	$114.9^e, 141^f, 128^g$	_	_		
		Rock salt		-			
GGA (PBE)	4.9563	-	116.04	4.3192	-40687.19363		
GGA (WC)	4.8812	_	137.46	4.2564	-40684.421728		
GGA (PBEsol)	4.8737	_	137.18	4.3034	-40675.833034		
LDA	4.8312	_	146.71	4.4092	-40664.463826		
Ref. [19]	4.856	-	112.2	-	_		
<sup>a</sup> Ref. [28], <sup>b</sup> Ref. [7,8], <sup>c</sup> Ref. [9], <sup>d</sup> Ref. [6], <sup>e</sup> Ref. [42], <sup>f</sup> Ref. [10], <sup>g</sup> Ref. [36].							

# 3.2. Phase transformations

Commonly, the phase equilibrium transition pressure is acquired by calculating the total energy versus the volume (E-V) curves of the two phases and then obtaining their common tangent. In zero temperature, we have calculated the enthalpy (H = E + PV) of TlN corresponding to the transitions WZ to rock salt (RS) and ZB to RS structures. It was found that the transition pressure of TlN from WZ to RS phase was 14.7, 10.52, 10.7, and 10 GPa, and from ZB to RS to be 15.815, 10.93, 11.6 and 11.05 GPa, using GGA (PBE), GGA (WC), GGA (PBEsol) and LDA approximations, respectively. The amounts of calculating phase transition pressures, listed in Table II, are consistent with others results. It is found that the phase transition pressures decrease with the increase of the atomic radius of the III-group elements. The transition pressure depends on the following factors: (a) the bulk modulus  $B_0$  (the larger  $B_0$ , the larger  $P_t$ ) and (b) the difference in equilibrium volumes  $\Delta V_0$  for different phases (the larger  $\Delta V_0$ , the smaller  $P_t$ ) [18]. According to Table II, our results in various approximations are less than the values obtained by Shi et al. [19], which indicate that our results are more favorable than their results because as the atomic radius increases the pressure at which phase transition occurs should decrease [20].

TABLE II

Phase transition pressure [GF	a] for TlN.
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TlN	WZ→RS	ZB→RS				
GGA (PBE)	14.7	15.815				
GGA (WC)	10.52	10.93				
GGA (PBEsol)	10.7	11.6				
LDA	10	11.05				
other works	$19.2^{a}$	$14.6^{b}$				
$a D_{-f} [10] b D_{-f} [20]$						

<sup>*a*</sup> Ref. [19], <sup>*b*</sup> Ref. [36].

#### 3.3. Elastic properties

Elastic properties have an important role in obtaining beneficial information about the anisotropic nature of bindings, structural stability and binding properties among adjacent atomic planes [21]. Hence, we investigate the stability of TlN in WZ, ZB, and RS phases using four approximations. These elastic constants are calculated by cubic-elastic and hex-elastic as interfaced to the WIEN2k code [22].

# 3.3.1. Elastic constant in WZ phase

Only five independent elastic constants  $(C_{11}, C_{12}, C_{13}, C_{33}, \text{ and } C_{55})$  are needed to be calculated for hexagonal structures. By using the calculated elastic constants, other structural properties such as bulk (B), shear (S) and Youngs (Y) moduli and the dimensionless Poisson ratio  $\nu$   $(BSE\nu)$  are estimated, based on the Voigt, Reuss, and Hill approximations [23–25].

For hexagonal structures, the elastic parameters are given by following equations:

$$b_{\rm V} = \frac{1}{9} \left( 2c_{11} + c_{33} \right) + \frac{2}{9} \left( c_{12} + 2c_{13} \right), \tag{1}$$

$$b_{\rm R} = \frac{1}{\left(2S_{11} + S_{33}\right) + 2\left(2S_{12} + 2S_{13}\right)},\tag{2}$$

$$b_{\rm H} = \frac{b_{\rm V} + b_{\rm R}}{2},\tag{3}$$

$$S_{\rm V} = \frac{1}{15} \left( 2c_{11} + c_{33} - 2c_{13} - c_{12} \right) + \frac{1}{5} \left( 2c_{55} + c_{66} \right),$$
  
$$c_{66} = \frac{c_{11} - c_{12}}{2},$$
 (4)

$$S_{\rm R} = \frac{15}{4\left(2S_{12}+S_{33}\right) - 4\left(S_{12}+2S_{13}\right) + 3\left(2S_{55}+S_{66}\right)}, (5)$$

$$S_{\rm H} = \frac{S_{\rm V} + S_{\rm R}}{2},\tag{6}$$

$$Y = \frac{9BS}{3B+S},\tag{7}$$

$$V = \frac{3B - 2S}{2(3B + S)},$$
(8)

where  $C_{ij}$  and  $S_{ij}$  are the elastic constants and elastic compliances, respectively.

Since Voigt and Reuss approximations represent the upper and lower limits of BSE $\nu$  properties [25], therefore thermodynamical properties such as average sound velocity  $(v_m)$  which consists of the longitudinal  $(v_l)$  and transversal  $(v_t)$  sound velocities and Debye temperature  $(\theta_D)$ , are calculated using Hill approximation [25]:

$$v_{\rm l} = \left(\frac{3B_{\rm H} + 4S_{\rm H}}{3\rho}\right)^{\frac{1}{2}} \text{ and } v_{\rm t} = \left(\frac{S_{\rm H}}{\rho}\right)^{\frac{1}{2}}, \qquad (9)$$
$$v_m = \left[\frac{1}{3}\left(\frac{2}{v_{\rm t}^3} + \frac{1}{v_{\rm l}^3}\right)\right]^{\frac{-1}{3}}$$
$$\text{and} \quad \theta_{\rm D} = \frac{h}{k_{\rm B}} \left(\frac{3}{4\pi V_{\rm a}}\right)^{\frac{1}{3}} v_m, \qquad (10)$$

where h is the Planck constant,  $k_{\rm B}$  is the Boltzmann constant,  $V_{\rm a}$  is the atomic volume and  $\rho$  is mass density of material.

Using first-principle calculations and calculated elastic constants, it is possible to evaluate technological important properties such as stiffness, hardness, brittle/ductility and the type of bonds for crystal structures.

A material behaves as a brittle (ductile) if the  $\frac{b}{S}$  ratio is less (more) than 1.75 [26]. The sign of the Cauchy pressure  $(C_{12} - C_{55})$  can be used to predict the type of bonds. When that, the Cauchy pressure is negative (positive), covalent (ionic) bonds are dominating in materials [27]. As well as, the value of the Poisson ratio can be used to predict the type of bonds. Stiffness is the resistance to deformation forces. The Young modulus is ratio of stress and strain, and it is representative of the stiffness. It says that the value of the Young modulus (Y) is greater, the material is the stiffer. Hardness is relevant to how much the material is resistant to the shape changes. There are two representatives for it: (1) bulk modulus, which is relevant to the resistance against the volume changes and (2) shear modulus, which is relevant to the resistance against the reversible deformations. Hence, it is clear that shear modulus can be a better predictor for hardness [26]. Elastic constants obtained for TlN are summarized in Table III, and

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TlN (Wurtzite)	GGA (PBE)	GGA (WC)	GGA (PBEsol)	LDA	Other works
$C_{11}$ [GPa]	144.9717	159.7167	161.3356	175.6846	$139^a, 162^b$
$C_{12}$ [GPa]	72.5384	89.8642	89.8624	100.8482	$70^a, 77^b$
$C_{13}$ [GPa]	54.9481	73.0464	73.2738	81.0707	$50^a, 58^b$
$C_{33}$ [GPa]	153.7822	172.0633	172.6709	184.4474	$149^a, 175^b$
$C_{55}$ [GPa]	31.8582	31.0423	31.5602	32.7761	$31^a,  36^b$
$B_{\rm V}$ [GPa]	89.843	107.045	107.573	117.977	$85^a,  98^b$
$B_{\rm R}$ [GPa]	89.787	107.030	107.553	117.893	
$B_{\rm H}$ [GPa]	89.815	107.037	107.563	117.935	
$G_{\rm V}$ [GPa]	37.405	36.437	37.033	38.782	$36^a$
$G_{\rm R}$ [GPa]	36.319	35.312	35.942	37.546	
$G_{\rm H}$ [GPa]	36.862	35.874	36.487	38.164	
$Y_{\rm V}$ [GPa]	98.539	98.172	99.662	104.856	$125^{a}$
$Y_{\rm R}$ [GPa]	96.011	95.439	97.018	101.828	
$Y_{\rm H}$ [GPa]	97.277	96.806	98.341	103.344	
$ u_{ m V}$	0.317	0.347	0.345	0.351	
$ u_{ m R}$	0.321	0.351	0.349	0.356	
$ u_{ m H}$	0.319	0.349	0.347	0.353	
$\theta_{\rm D}$ [K]	244.027	239.924	241.792	246.312	$288^{a}$
$V_{ m t}~[{ m m/s}]$	1929.15	1861.79	1874.83	1890.03	$1924^{a}$
$V_1 ~[{ m m/s}]$	3745.66	3868.32	3879.28	3975.15	$3689^{a}$
$V_m   \mathrm{[m/s]}$	2160.22	2093.03	2107.23	2126.11	$2553^{a}$

Elastic constant, bulk modulus (B), shear modulus (G), the Young modulus (Y) and the Poisson ratio  $(\nu)$  of TlN (WZ) within different approximations for wurtzite.

<sup>*a*</sup> Ref. [28], <sup>*b*</sup> Ref. [19].

the results are in good agreement with the result of the other researchers. To our knowledge, there exist no any experimental and theoretical data for some physical quantities of TlN. We hope that our result provides a useful reference for future experimental and theoretical studies.

According to our results, the amount of  $\frac{B_{\rm H}}{S_{\rm H}}$  for different approximations are equal to 2.44 (GGA (PBE)), 2.98 (GGA (WC)), 2.95 (GGA (PBEsol)), and 3.09 (LDA) which shows that TlN in WZ phase is a ductile material, but LDA predicts that TlN is more ductile than GGA approximations.

Our Cauchy pressure  $(C_{12} - C_{55} > 0)$  within GGA and LDA predicts that for TlN, ionic bonds are more dominant and the values of the Poisson ratio (see Table III) predicts that TlN exhibit ionic bonding.

The present value of the Young and shear moduli, Debye temperature, and average sound velocity are lower than other nitride of the III-group which shows that TlN is softer than other nitride of the III-group. The comparison of the Young modulus achieved by Shi [28] and our calculation, demonstrate that TlN is anticipated to be stiffer than our calculation. These differences could be due to lattice parameters from package 2D optimization (this package performed a convenient 2D structure optimization (volume and c/a, i.e. hexagonal space-group)). The previous analysis [29] on the elastic properties showed that  $\frac{S}{b}$  ratio (the Pugh modulus) and revised Cauchy pressure  $\frac{1}{e}(C_{12} - C_{55})$  (Y — the Young



Fig. 1. The correlation between ductility/brittleness and the type of bond for TlN in three phases and different approximations.

modulus) are well correlated to a hyperbolic criterion to recognize the ductile to brittle properties for a large materials of cubic symmetry. This means that there is a correlation between ductility/brittleness property and metallic/covalent bonding [29].

The analysis by Jamal et al. [30] were applied to hexagonal compounds and they seized the right results. However, we used this analysis for TlN and found that TlN is a ductile material and has ionic bond (Fig. 1).

# 3.3.2. Elastic constant in cubic phase (zinc-blende and rock salt)

There are three independent elastic constants  $C_{11}$ ,  $C_{12}$ and  $C_{44}$  for the cubic crystals. These elastic constants were calculated by cubic-elastic method [22] as interfaced to the WIEN2k code for TlN in ZB and RS phases. The results are gathered in Tables IV and V. In these tables the previous theoretical data are also included for comparison.

#### TABLE IV

Elastic constant, bulk modulus (B), shear modulus (G), the Young modulus (Y) and the Poisson ratio  $(\nu)$  of TlN (ZB) within different approximations for zinc-blende.

TlN (zinc-blende)	GGA (PBE)	GGA (WC)	GGA (PBEsol)	LDA	Other works
$C_{11}$ [GPa]	118.4151	130.2153	128.3754	145.1527	$151^a, 194^b, 129^c$
$C_{12}$ [GPa]	81.1312	94.1365	92.0789	107.8336	$110^a, 115^b, 85^c$
$C_{44}$ [GPa]	82.3647	95.0413	95.4501	104.8249	$64^a, 103^b, 64^c$
B [GPa]	93.559	106.162	104.177	120.273	$124^a, 99^c$
$G_{\rm V}$ [GPa]	56.874	64.239	64.529	70.357	
$G_{\rm R}$ [GPa]	34.792	35.104	35.302	36.818	
$G_{\rm H}$ [GPa]	45.833	49.671	49.915	53.587	
Y [GPa]	141.873	160.370	160.457	176.629	
$V_{ m t}~[{ m m/s}]$	2151.84	2191.79	2194.03	2240.7	
$V_1   \mathrm{[m/s]}$	3952.98	4083.17	4057.72	4238.29	
$V_m   \mathrm{[m/s]}$	2400.38	2447.41	2448.65	2504.74	
$\theta_{\rm D}$ [K]	2710.096	280.46	280.867	290.08	
melt. temp. [K]	$1252.83{\pm}300$	$1322.57 \pm 300$	$1311.69 {\pm} 300$	$1410.85{\pm}300$	
u	0.247	0.248	0.243	0.255	
ξ	0.774	0.803	0.799	0.818	
A	4.418	5.268	5.259	5.618	
$\lambda$	55.537	63.230	61.035	73.242	
$\mu$	56.886	64.250	64.544	70.37	
C'	18.642	18.039	18.148	18.659	
$C^{\prime\prime}$	-1.233	-0.905	-3.371	3.008	

<sup>a</sup> Ref. [36], <sup>b</sup> Ref. [37], <sup>c</sup> Ref. [38].

In order to ensure the reliability of our calculations, the following well-known Born elastic stability criteria [30] for the cubic systems [31–35] are surveyed for our calculated elastic constants:

 $C_{11} - C_{12} > 0, \quad c_{11} + 2C_{12} > 0, \quad c_{44} > 0(11), \quad (11)$ 

$$C_{11}^2 - C_{12}^2 > 0, \quad c_{11} > 0.$$
 (12)

The obtained elastic constants of TlN (ZB and RS) satisfy the above stability conditions, displaying that they are elastically stable in ZB and RS phases. Moreover, the elastic constants also satisfy the cubic stability condition, i.e.  $C_{12} < B$  and  $C_{11} > B$ . So, the values of elastic constants are reliable for TlN in ZB and RS phases.

By using the calculated elastic constants, other structural properties such as bulk modulus (B), the Voigt shear modulus  $(G_V)$ , the Young modulus (Y), shear constant (C'), the Cauchy pressure (C''), the Poisson ratio  $(\nu)$ , the Kleinman parameter  $(\xi)$ , the Reuss shear modulus  $(G_R)$ , the Hill shear modulus  $(G_H)$ , anisotropy constant (A), and the Lame coefficients  $(\lambda$  and  $\mu)$  are calculated.

$$B = \frac{1}{3}(c_{11} + 2c_{12}),\tag{13}$$

$$g_{\rm V} = \frac{1}{5} (3c_{44} + c_{11} - c_{12}), \tag{14}$$

$$Y = \frac{9Bg_{\rm V}}{3B + g_{\rm V}},\tag{15}$$

$$c' = \frac{1}{2}(c_{11} - c_{12}),\tag{16}$$

$$C'' = C_{12} - C_{44},\tag{17}$$

$$v = -1 + \frac{Y}{2G_{\rm V}} = \frac{3B - Y}{6B} = \frac{1}{2} - \frac{Y}{6B},$$
 (18)

$$\xi = \frac{C_{11} + 8C_{12}}{7C_{11} + 2C_{12}},\tag{19}$$

$$G_{\rm R} = \frac{5(C_{11} - C_{12})C_{44}}{4C_{44} + 3(C_{11} - C_{12})},$$
(20)

$$G_{\rm H} = \frac{G_{\rm V} + G_{\rm R}}{2},\tag{21}$$

TABLE V

TlN (rock salt)	GGA (PBE)	GGA (WC)	GGA (PBEsol)	LDA	Ref. [19]
$C_{11}$ [GPa]	165.4318	192.3975	189.8594	200.1031	155
$C_{12}$ [GPa]	85.5868	104.9100	104.5691	113.4406	91
$C_{44}$ [GPa]	70.4411	70.1324	69.2544	70.4957	71
B [GPa]	112.201	134.072	132.999	142.328	112
$G_{\rm V}$ [GPa]	58.233	59.576	58.61	59.629	
$G_{\rm R}$ [GPa]	53.945	56.499	55.421	56.362	
$G_{\rm H}$ [GPa]	56.089	58.037	57.015	57.995	
Y [GPa]	148.933	155.670	153.309	156.966	
$V_{ m t}~[{ m m/s}$	2168.05	2157.08	2133.09	2123.29	
$V_1   \mathrm{[m/s]}$	3958.55	4117.40	4084.20	4132.23	
$V_m  \mathrm{[m/s]}$	2417.34	2412.75	2386.41	2377.97	
$\theta_{\rm D}$ [K]	290.565	294.326	291.56	293.081	
melt. temp. [K]	$1530.70 \pm 300$	$1690.07 \pm 300$	$1675.07 {\pm} 300$	$1735.61{\pm}300$	
u	0.278	0.306	0.307	0.316	
ξ	0.639	0.663	0.667	0.680	
A	1.764	1.603	1.624	1.627	
$\lambda$	72.966	94.005	93.292	102.421	
$\mu$	58.268	59.598	58.649	59.637	
C'	39.922	43.744	42.685	43.331	
$C^{''}$	15.146	34.778	35.314	42.945	

Elastic constant, bulk modulus (B), shear modulus (G), the Young modulus (Y) and the Poisson ratio  $(\nu)$  of TlN (RS) within different approximations for rock salt.

$$A = \frac{2C_{44}}{C_{11} - C_{12}},$$
(22)  

$$Yv \qquad \qquad Y$$
(22)

$$\lambda = \frac{1}{(1+v)(1-2v)} \text{ and } \mu = \frac{1}{2(1+v)}.$$
(23)

Also, average velocity  $(v_m)$ , longitudinal velocity  $(v_l)$ , transverse velocity  $(v_t)$ , and the Debye temperature  $(\theta_D)$ can also be attained by elastic constants and mass density. The terms are as follows:

$$v_{\rm l} = \left(\frac{3B_{\rm H} + 4S_{\rm H}}{3\rho}\right)^{\frac{1}{2}}, v_{\rm t} = \left(\frac{S_{\rm H}}{\rho}\right)^{\frac{1}{2}}, v_{\rm m} = \left[\frac{1}{3}\left(\frac{2}{v_{\rm t}^3} + \frac{1}{v_{\rm l}^3}\right)\right]^{\frac{-1}{3}}, \theta_{\rm D} = \frac{h}{k_{\rm B}}\left(\frac{3}{4\pi V_{\rm a}}\right)^{\frac{1}{3}}v_{m},$$
(24)

where h is the Planck constant and n, N,  $\rho$ , M, and  $k_{\rm B}$  are the number of atoms in the molecule, the Avogadro number, mass density, molecular weight and the Boltzmann constant, respectively.

The bulk modulus (B) and the Hill shear modulus ( $G_{\rm H}$ ) are significant parameters in recognizing the physical properties of materials. Bulk modulus (B), the Voigt shear modulus ( $G_{\rm V}$ ), the Reuss shear modulus ( $G_{\rm R}$ ), shear modulus ( $G_{\rm H}$ ), the Young modulus (Y) and the Poisson ratio of TlN in ZB and RS phases have been calculated using GGA (PBE), GGA (WC), GGA (PBEsol), and LDA approximations, which are summarized in Tables IV and V.

According to Table IV, we see that our results with LDA approximation (full potential) are in agreement with other results within the LDA approximation (pseudopotentials) [36–38] but our results with GGA approximations do not agree with other results. In GGA approximations, we can see that value of the C'' is negative (C'' < 0) and it shows that covalent bond is more dominating, but in LDA approximation the value of C'' is positive (C'' > 0) and it shows that ionic bond is more dominating which is in agreement with other results. But the value of C'', using any of four approximations, is nearly zero. So we can conclude that bonding of TlN in ZB phase is covalent-ionic. In addition to C'', we can consider the Poisson ratio  $(\nu)$ , the value of  $\nu$  is much less than 0.25 (around 0.1) for a typical covalent compound, while it is nearly 0.25 or more for a typical ionic compound. According to Table IV, the values of  $\nu$  using any of four approximations are around 0.25, so we can conclude that bond of TlN in ZB phase is covalent-ionic

(similar to C''). According to our results, the amount of  $\frac{b}{G_{\rm H}}$  for different approximations is equal to 2.04 (GGA (PBE)), 2.13 (GGA (WC)), 2.08 (GGA (PBEsol)), and 2.24 (LDA) which shows that TlN in ZB phase is a ductile material, but LDA predicts that it is more ductile than GGA approximations. Also, by considering the Pugh modulus [29] in Fig. 1, one can defer that TlN is a ductile material and bonds in TlN are covalent-ionic. The achieved value of the Young moduli, Debye temperature, and average sound velocity are lower than those of other nitrides of the III-group which shows that TlN in ZB phase is softer than other nitride of the III-group.

The dimensionless Kleinman parameter can be generally between 0 and 1 ( $0 \le \zeta \le 1$ ). The lower limit corresponds to the minimized bond bending term, while the upper limit corresponds to the minimized bond stretching term, as defined by Kleinman [39]. Such a large calculated value of the Kleinman parameter (see Table IV) predicts that bonding nature in TlN (ZB) is dominated by the bond stretching term in comparison to the bond bending term.

The Lamé moduli are calculated using Eq. (23) for TlN. The results are included in Table IV. However, we have calculated the Lamé second modulus as  $\mu = \frac{Y}{2(1+v)}$ , our result verifies that it is nothing more than the Voigt shear modulus, viz.  $\mu = G_V$  (see Table IV). The Lamé first modulus,  $\lambda$ , is related to a fraction of the Young modulus. For an isotropic system one can easily show that  $\lambda = C_{12}$  and  $\mu = C' = (C_{11} - C_{12})/2 = C_{44}$  [40]. But, since the TlN is a strongly anisotropic compound  $(A \neq 1 \text{ see Table IV})$  so,  $\mu \neq C_{44}$  (see Table IV).

According to Table V, we see that our results achieved by LDA and GGA approximations (using full potential) are in agreement with other results (using pseudopotentials) [19]. The value of C'' is positive (Table V) which shows that bonds in TlN (RS) are ionic. According to Table V, we see that values of  $\nu$  in four approximations are greater than 0.25, so we can conclude that the bonds of TlN in RS phase are ionic (similar C'').

According to our results, the amount of  $\frac{b}{G_{\rm H}}$  for different approximations is equal to 2.0 (GGA (PBE)), 2.31 (GGA (WC)), 2.33 (GGA (PBEsol)), and 2.45 (LDA) which shows that TlN in RS phase is a ductile material. Also, considering the Pugh modulus [29] in Fig. 1 indicates that TlN in RS phase is a ductile material and its bonds are ionic. The achieved values of the Young moduli, the Debye temperature, and average sound velocity are lower than other nitrides of the III-group, which shows that TlN in RS phase is softer than other nitrides of the III-group. The calculated large value for the Kleinman parameter (see Table V) predicts that bonding nature in TlN (RS) is dominated by the bond stretching term in comparison to the bond bending term. The value of A parameter is around one (see Table V), that shows TIN in RS phase is not strongly anisotropic and is almost isotropic, especially in GGA (PBE) approximation because  $\mu \cong$  $C_{44}$  (see Table V).

Figure 2 shows the variations of elastic constants  $C_{ij}$ and their aggregate bulk modulus with a hydrostatic pressure for ZB TlN. One obviously observes a linear dependence in all curves of this compound. Our results for the pressure derivatives  $\frac{\partial C_{11}}{\partial P}$ ,  $\frac{\partial C_{21}}{\partial P}$ ,  $\frac{\partial C_{44}}{\partial P}$ , and  $\frac{\partial B}{\partial P}$  of ZB TlN are listed in Table VI. It is easy to observe that the elastic constants  $C_{11}, C_{21}$  and  $C_{44}$ , as well as bulk modulus B exhibit a linearly increasing trend as pressure enhances. Our results are in agreement with other results, but the values of  $\frac{\partial C_{44}}{\partial P}$  we have calculated, differ with other results (however, our  $\frac{\partial C_{44}}{\partial P}$  is similar to other nitrides of the III-group) [36].



Fig. 2. The elastic constant versus pressure for TlN (ZB) within LDA approximation.

#### TABLE VI

Calculated pressure derivatives of the elastic moduli of TlN (ZB) within LDA approximation.

TlN (zinc-blende)	$\partial C_{11}/\partial P$	$\partial C_{21}/\partial P$	$\partial C_{44}/\partial P$	$\partial B/\partial P$
present work	3.590	4.818	3.07	4.409
Ref. [36]	3.607	4.875	-1.438	4.453

#### 4. Electronic properties

### 4.1. Band structure

Electronic properties of TlN in three phases were investigated by calculating the energy band structure. Table VII shows the calculated band gap energies of TIN using GGA (PBE), LDA, mBJ-GGA, mBJ-LDA, Engel-Vosko and mBJ-LDA+SO approximations along some high symmetry directions of the Brillouin zone calculated at equilibrium volume. The band gap energies of TlN in WZ and ZB phases within mBJ-LDA+SO approximation were improved in comparison with other theoretical results. We calculated a direct band gap for TlN (ZB) about 0.09 eV and TlN (WZ) about 0.07 eV but TlN in RS phase shows metallic behavior (Fig. 3). The effect of pressure on the band gap of TlN (ZB) was also investigated up to the first order phase transition pressure. The results are listed in Table VIII. It can be seen that the band gap of TlN (ZB) increases with increase of the pressure. As a rule, direct band gaps increase and indirect band gaps decrease with increase of the pressure [41].

The band gap energy [eV] of TlN within different approximations.

TlN	GGA (PBE)	LDA	mBJ (GGA)	mBJ (LDA)	E. Vosko (GGA-WC)	mBJ (LDA+SO)	Other works
wurtzite							
$E_{\rm g}(\Gamma^v \to \Gamma^c)$	0.0	0.0	0.0	0.0	0.0	0.07	$0.0^a$
zinc-blende							
$E_{\rm g}(\Gamma^v \to \Gamma^c)$	0.0	0.0	0.0	0.0	0.0	0.09	$0.0^{a,b}$
<sup>a</sup> Rof $[0]$ <sup>b</sup> Rof $[42]$							

<sup>a</sup> Ref. [9], <sup>o</sup> Ref. [42].



Fig. 3. The band structure of TlN - WZ (a), TlN - ZB (b), and TlN - RS (c) within mBJ-LDA+SO.

TABLE VIII The band gap energy [eV] in different pressures [GPa] for TlN (ZB) within mBJ (LDA+SO) approximation.

TlN (zinc-blende) pressure [GPa]	Lattice constant [Å]	Band gap [eV] in mBJ (LDA+SO) approximation
P = 0.0	5.1415	0.09
P = 3.546	5.094	0.10
P = 6.114	5.062	0.11
P = 7.566	5.045	0.112
P = 9.031	5.029	0.12

# 4.2. Optical properties

Optical calculations are performed in the random phase approximation (RPA) by using WIEN2k code. Dielectric function ( $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$ ) is a complex quantity that describes the linear response of the system to an electromagnetic radiation. The imaginary part of dielectric function is obtained by calculating momentum matrix elements between the occupied and unoccupied wave [43]:

$$\operatorname{Im}\varepsilon_{\alpha\beta}^{(\text{inter})}(\omega) = \frac{\hbar^2 e^2}{\pi m^2 \omega^2} \sum_n \int \mathrm{d}\boldsymbol{k} \left\langle \psi_{\boldsymbol{k}}^{c_n} | \boldsymbol{p}^{\alpha} | \psi_{\boldsymbol{k}}^{V_n} \right\rangle$$
$$\times \left\langle \psi_{\boldsymbol{k}}^{V_n} | \boldsymbol{p}^{\beta} | \psi_{\boldsymbol{k}}^{c_n} \right\rangle \delta \left( E_{\boldsymbol{k}}^{c_n} - E_{\boldsymbol{k}}^{V_n} - \omega \right), \qquad (25)$$

where  $\boldsymbol{p}$  is the momentum matrix element between  $\alpha$ and  $\beta$  bands with the same crystal  $(\psi_{\boldsymbol{k}}^{c_n})$  and  $(\psi_{\boldsymbol{k}}^{V_n})$ which are the crystal wave function corresponding to the conduction and valence bands with the same crystal wave vector  $\boldsymbol{k}$ , respectively. The interband expansion on the corresponding real part was obtained by the Kramers–Kronig transformation

$$\operatorname{Re}\varepsilon_{\alpha\beta}^{(\text{inter})}(\omega) = \delta_{\alpha\beta} + \frac{2}{\pi}P \int_{0}^{\infty} \frac{\omega' \operatorname{Im}\varepsilon_{\alpha\beta}(\omega')}{(\omega')^{2} - \omega^{2}}.$$
 (26)

Considerable optical functions like the refraction index  $n(\omega)$  and extinction coefficient  $k(\omega)$  can be appraised by the following equations [44–46]:

$$n(\omega) = \frac{1}{\sqrt{2}}\sqrt{\varepsilon_1 + \sqrt{\varepsilon_1^2 + \varepsilon_2^2}},$$
(27)

$$k(\omega) = \frac{1}{\sqrt{2}} \sqrt{\sqrt{\varepsilon_1^2 + \varepsilon_2^2} - \varepsilon_1}.$$
(28)

Optical quantities of wurtzite phase were calculated in two directions: (i) when polarized electric field is parallel to c (E||z), (ii) when polarized electrical field is perpendicular to c (E||x).

Figure 4 and 5 illustrate the real and imaginary parts of the dielectric function spectrum of TlN for a radiation up to 14 eV within GGA (PBE) and LDA approximations. According to Fig. 4a and Fig. 5 (imaginary part of dielectric function), we see that band gap energies are very small as it is evident also in Fig. 3 for TlN in wurtzite and zinc-blende phases by using GGA (PBE) and LDA approximations.

TABLE IX

The main peaks position [eV] of the imaginary part of dielectric function for TlN in three phases.

TIN	GGA (PBE) (E    x)	LDA     (E  x)	$\begin{array}{c} \text{GGA} \\ \text{(PBE)} \\ \text{(}E \  z \text{)} \end{array}$	LDA     (E  z)	Ref. [9]
wurtzite	6.68	6.84	3.17	3.50	$4(E  x), \\ 3(E  z)$
$\operatorname{zinc-blende}$	6.63	6.84	-	-	8.5
rock salt	3.28	3.57	-	-	_

The main peaks in the spectra of imaginary part of dielectric function (Fig. 4a and Fig. 5) are given in Table IX which are in good agreement with other reports [9]. The static dielectric constants which are extracted from the diagram of  $\varepsilon_1(\omega)$  (Fig. 4b and Fig. 5) are summarized in Table X and are in good agreement with previous studies [9] and we see that the static dielectric constant



Fig. 4. The imaginary part of dielectric function (a) and the real part of dielectric function (b) versus energy for TlN in ZB and RS phases within GGA (PBE) and LDA approximations.



Fig. 5. The dielectric function for TlN in WZ phase within GGA (PBE) and LDA approximations in two directions (E||x) and (E||z).

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The static dielectric constant for TlN in three phases within GGA (PBE) and LDA approximations.

TlN	GGA (PBE) (E  x)	LDA   (E  x)	$\begin{array}{c} \text{GGA} \\ \text{(PBE)} \\ \text{(}E \  z \text{)} \end{array}$	$\begin{array}{c} \text{LDA} \\ (E\ z) \end{array}$	Ref. [9]
wurtzite	20.8	19.3	17	15.6	$\begin{array}{c} 20 \ (E\ x), \\ 22.5 \ (E\ z) \end{array}$
$\operatorname{zinc-blende}$	24	23	-	—	25
rock salt	16.7	15	-	_	—

of TlN is bigger than the other III-group nitrides [47–49]. The static refraction index (Eq. (27) and Fig. 6) of TlN in GGA (PBE) and LDA approximations are given in Table XI and we see that the refraction index of TlN is bigger than the other III-group nitrides [47–49].



Fig. 6. The refraction index of TlN versus energy in ZB and RS phases (a) within GGA (PBE) and LDA approximations and WZ phase (b) within GGA (PBE) and LDA approximations in two directions (E||x) and (E||z).

# TABLE XI

The static refraction for TlN in three phases within GGA (PBE) and LDA approximations.

TIN	$GGA (PBE), \\ (E \  x)$	LDA, (E  x)	$GGA (PBE), \\ (E  z)$	LDA, $(E\ z)$
wurtzite	4.57	4.4	4.17	3.95
zinc-blende	4.91	4.8	—	_
rock salt	4.09	3.87	—	_

To check the macroscopic, microscopic, and optical properties of solids, the energy-loss function  $(L(\omega))$  is one of the most important quantity. The energy-loss function is proportional to the probability of energy loss (E) in a unit of length as an electron is moving through the environment and it is given by

$$L(\omega) = \operatorname{Im}\left(\frac{-1}{\varepsilon(\omega)}\right) = \frac{\varepsilon_2^2}{\varepsilon_1^2 + \varepsilon_2^2}.$$
(29)

The main peak in the energy-loss function is known as

plasmon peak, which indicates the excitation volume charge density in crystals. The main peaks of energy-loss function for TlN are shown in Fig. 7 and their position are indicated in Table XII.



Fig. 7. The energy-loss function of TlN versus energy in ZB and RS phases (a) within GGA (PBE) and LDA approximations and WZ phase (b) within GGA (PBE) and LDA approximations and two directions (E||x)and (E||z).

TABLE XII

Value of energy [eV] plasmon peak for TlN in three phases within GGA (PBE) and LDA approximations.

	GGA		GGA	
TlN	(PBE).	LDA,	(PBE).	LDA, (E  z)
	$(E \parallel x)$	(E  x)	$(E \parallel z),$	
wurtzite	11.80	12.26	11.98	11.55
zinc-blende	12.28	12.23	_	—
rock salt	7.50	7.69	-	—

Two other important quantities of optical properties are absorption coefficient and real part of the optical conductivity and they are calculated by using the following relations:

$$a_{ij}(\omega) = \frac{2\omega k_{ij}(\omega)}{c},\tag{30}$$

$$\operatorname{Re}\sigma_{ij}\left(\omega\right) = \frac{\omega}{4\pi}\operatorname{Im}\varepsilon_{ij}\left(\omega\right).$$
(31)

Absorption coefficient depends on tow quantities, extinction index and imaginary part of the dielectric function. Absorption coefficients for TlN in three different phases are shown in Fig. 8 and the maxima of absorption



Fig. 8. The absorption coefficient of TlN in three phases within GGA (PBE) and LDA approximations and in two directions (E||x) and (E||z) for wurtzite phase.



Fig. 9. The real part of optical conductivity for TlN in three phases within GGA (PBE) and LDA approximations and in two directions (E||x) and (E||z) for wurtzite phase.

coefficients can be seen in Fig. 8. Also, according to Eq. (31), we see that the real part of the optical conductivity is related to the imaginary part of dielectric function.

As it is clear in Fig. 9 the real part of the optical conductivity for TlN starts with a very small gap which indicate that the TlN has semiconductor properties (especially in two phases WZ and ZB).

### 5. Conclusion

In summary, we have performed *ab initio* calculations of structural, elastic, electronic, and optical properties of TlN in three different phases by using the FP-LAPW method. The results predict that TlN in WZ and ZB phases is semiconductor with a direct band gap while TlN in RS phase shows metallic behavior. Although TlN in three phases is ductile material, according to the Poisson ratio TlN in WZ and RS phases has ionic bond and in ZB phase has an ionic-covalent bond. The pressures at which the first order phase transitions occur were also estimated and compared with available data. Furthermore, the elastic constants, bulk modulus, shear modulus, the Young modulus, the Poisson ratio, Debye temperature, and sound velocities for longitudinal and transverse waves were calculated and they show that TlN is softer than other nitrides of the III-group. The variations of band gap energy, elastic constants and the bulk modulus of TlN (ZB) versus pressure were calculated and discussed and show that the band gap and elastic constant increase with increasing pressure. The optical parameters of TlN in three phases were also calculated and analyzed and imaginary part of the dielectric function show that TlN in WZ and ZB phases have almost semiconductor properties and TlN in RS phases has metallic properties. Also, real part of conductivity shows that TlN in WZ and ZB phase has semiconductor properties.

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