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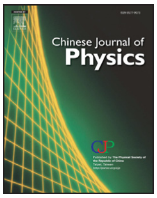

# Pressure and temperature dependence of the structural, elastic and thermodynamic properties of potassium telluride: First-principles calculations

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ABSTRACT

The structural, elastic and thermodynamic properties of $K_2Te$ have been studied by the FP-APW+lo method as implemented in the WIEN2k code. The exchange-correlation potential is treated by the generalized gradient approximation within the scheme of Perdew, Burke and Ernzerhof (GGA-PBE). The structural parameters are in good agreement with the available experimental and theoretical results. The Young's and shear modulus, and Poisson ratio have been calculated. The elastic constants and thermodynamic quantities under pressure and temperature are also calculated and elaborated.

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## 1. Introduction

Alkali metal telluride $K_2Te$ can crystallize into anti-fluorite (anti-$CaF_2$) structure type [1,2] (space group no. 225) at room temperature. The calcium fluoride $CaF_2$ crystal is one of the most common ordered crystal types found in nature; it is often referred to as the fluorite type structure. $CaF_2$ has a basic structure that can be described as a face-centered cubic packing of cations, with anions in all the tetrahedral holes. In contrast to the $CaF_2$ structure, the anti-$CaF_2$ structure has a basic face-centered cubic packing of anions, with cations at the tetrahedral holes. In the $K_2Te$ compound, the metal atoms (K) are located at the (1/4, ¼, 1/4) and (3/4, ¾, 3/4) positions, whereas the tellurium atoms (Te) are located at the (0, 0, 0) position. These materials $K_2X$ (X=O, S, Se and Te) are potential candidates for use in power sources, fuel cells, gas-detectors and ultraviolet space technology devices. These materials will be used as power sources for portable electronics devices such as laptops, cellular phones and digital cameras [3–7]. These ionic compounds also play an important role in the development of photocathode, in supporting catalytic reactions and in enhancing oxidation of semiconductor surfaces [8–11]. Most of the theoretical studies for alkali metal tellurides have been dedicated to their structural properties, such as the lattice constants and bulk modulus [12–16] or to the phase diagrams of these materials [17–20].

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The electronic band structures of some $M_2Te$ (M: Li, Na, K and Rb) compounds have been predicted by Eithiraj et al. [21] and Seifert-Lorenz and Hafner [22] using the Tight-Binding Liner Muffin-Tin Orbitals (TB-LMTO) method and the pseudopotential method, respectively, in the framework of density functional theory (DFT). Alaye-Abbas and Shaukat [23] have studied the structural, electronic, and optical properties of alkali metal tellurides $M_2Te$ using the full potential augmented plane wave (FP-LAPW) method. Alkali metal telluride has received less attention from researchers. For these compounds, most of the work done by researchers has been confined to studying their cohesive energies [12–15], elastic properties [13] and bulk modulus [14,15]. So far, only photoemission studies are reported for $K_2Te$ [24]. From the theoretical viewpoint, the linearized augmented-plane wave method (LAPW) approach has been reported for a series of tellurides with the anti-fluorite structure, to study the diffusivity of alkali metals [25]. Using the Vienna ab initio simulation package (VASP), lattice parameter, bulk modulus, and band gap calculation are performed for $K_2Te$ [26].

To the best of our knowledge, there is a real lack of knowledge of the elastic properties, and thermodynamics properties of $K_2Te$ under pressure and temperature effects up to now. This lack has prompted us to investigate them. This work aims to present a first-principles study of the structural, electronic, elastic and thermodynamic properties under pressure and temperature of $K_2Te$ in the anti-fluorite phase, using the full potential (linear) augmented plane wave plus local orbital (FP-APW+lo) method within the density functional theory based on the Perdew–Burke–Ernzerhof (PBE) functional. We describe the computational method used in this work in Section 2. The results are discussed in Section 3. Finally, a summary of the work is given in Section 4.

## 2. Computational method

The full-potential (linear) augmented plane waves plus local orbital (FP-APW+lo) method [27,28] as implemented in the WIEN2k [29] code based on the density functional theory DFT [30] is used to describe the ground state. We used the Perdew, Burke and Ernzerhof (PBE) generalized gradient approximation [31,32] (GGA) to bring the calculated properties into closer agreement with the experimental values. In this method, the unit cell is divided into non-overlapping spheres centered at atomic sites with a fixed radius and an interstitial region. The APW+lo method expands the Kohn–Sham orbitals in an atom like Muffin-tin spheres and plane waves in the interstitial region. The basis set inside each Muffin-tin sphere is split into core and valence subsets. The core states are treated within the spherical part of the potential only, and are assumed to have a spherically symmetric charge density totally confined inside the Muffin-tin spheres [27,28,33]. The valence part is treated within a potential expanded into spherical harmonics up to $l = 4$. The valence wave functions inside the spheres are expanded up to $l_{\max} = 10$. A plane-wave expansion with $R_{mt}\ K_{\max} = 9$, and k sampling with $8 \times 8 \times 8$ k-point mesh in the full Brillouin zone turns out to be satisfactory. The k integration over the Brillouin zone is performed using the Monkhorst and Pack mesh [34]. The energy separating the valance state from the core state has been chosen to be $-6.0$ Ryd. The leakage electrons from the Muffin-tin radius are found to be less than 0.0001.

In order to obtain the thermodynamic properties of $K_2Te$, the quasi-harmonic Debye model [35] is introduced, in which the non-equilibrium Gibbs function $G^*(V, P, T)$ takes the form of

$$G^*(V, P, T) = E(V) + PV + A_{vib}(\theta(V), T), \tag{1}$$

where $E(V)$ is the total energy per unit cell of $K_2Te$, $PV$ corresponds to the constant hydrostatic pressure condition, $\Theta(V)$ is the Debye temperature as a function of $V$, and $A_{vib}$ is the vibrational Helmholtz free energy which can be expressed as [36]

$$A_{vib}(\theta, T) = n\,k_B\,T\left[\frac{9\theta}{8T} + 3\ln(1 - e^{-\theta/T}) - D(\theta/T)\right], \tag{2}$$

where $D(\theta/T)$ is the Debye integral, and is defined as

$$D(\theta/T) = \frac{3}{(\theta/T)^3}\int_0^{e/T}\frac{x^3}{e^x - 1}dx, \tag{3}$$

where $n$ represents the number of atoms per formula unit, $\theta$ is the Debye temperature that is expressed as [36-38]

$$\theta = \frac{\hbar}{K}\left[6\pi^2 V^{1/2} n\right]^{1/3} f(\sigma)\sqrt{\frac{B_s}{M}}, \tag{4}$$

where $M$ is the mass of per formula unit, $\sigma$ is the Poisson ration and $B_S$ is the adiabatic bulk modulus that is approximated as

$$B_s \cong B(V) = V\left(\frac{d^2E(V)}{dV^2}\right) \tag{5}$$

and the $f(\sigma)$ is given by

$$f(\sigma) = \left\{3\left[2\left(\frac{2(1+\sigma)}{3(1-2\sigma)}\right)^{3/2} + \left(\frac{1+\sigma}{3(1-\sigma)}\right)^{3/2}\right]^{-1}\right\}^{1/3}. \tag{6}$$

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