First Principles Studies of Electronic and Superconducting Properties of The Simple Cubic Phase of Alpha –Polonium

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Abstract— **The electronic and superconducting properties of alpha-polonium under pressure have been investigated theoretically using the first principles tight-binding linear muffin-tin orbital method within atomic sphere approximation (ASA). The studies on electronic properties such as energy band structure , density of states , Fermi energies and bulk modulus have been carried out from the self-consistent TB - LMTO method. Calculations on superconducting properties like Debye temperature, electron-phonon coupling constant and superconducting transition temperature have been obtained from the electronic band structure studies. The theoretically calculated values of T_C are compared with the available results of literature data.**

Keywords: First-Principle Study, Fermi Energy, Debye Temperature, Superconductivity

I. INTRODUCTION

Polonium is named after Poland , the Native Country of Marie Curie , who first isolated the element [1]. The polonium with atomic number 84 is the only element which forms a simple cubic lattice at an ambient conditions. Crystal structure of polonium was first measured by Beamer and Maxwell and later by Desando et al [2]. At higher temperatures > 348K the structure changes into a rhombohedral beta form. The radioactive chemical element is formed by the disintegration of radium. It is a rare metal with 33 different isotopes of the element and all of the isotopes are radioactive. The isotope in mass number 209 has the longest half life of 103 years. Polonium has variety of applications such as heat source for thermoelectric power devices for space, as a natural tracer of environmental process in biological and used in static eliminator [3]. There are several theoretical investigations have been studied on this cubic phase polonium [4-6]. To the best of our knowledge, there is no experimental verifications on the superconducting behaviour of this nonferrous metal. Chang- Jong Kang et al [7] investigated the phonon softening and superconductivity in cubic α- polonium and the results on superconducting transition temperature have predicted to be approximately 4K. The above interesting physical properties make us to view and analysing the electronic and superconducting properties of α -polonium.

II. COMPUTATIONAL DETAILS

Cubic alpha-polonium is a chalcogen with an atomic number 84. Space Group is Pm3m (no.221). The electronic configuration of the element is Po: [Xe] $4f^{14}$ $5d^{10}$ $6s^2$ $6p^4$. Desando et al determined the cubic structure of alpha-polonium with a lattice parameter as 3.359Å as taken to be the reference in our study. Energy bands of alpha-polonium in the simple cubic phase are obtained by means of the TB-LMTO method within the atomic sphere approximation (ASA) [8]. Tetrahedron method is employed to obtain the total and partial density of states, with 512 k-points were for the convergence of the density of states at E_f [9]

III. RESULTS AND DISCUSSION

The total energy is plotted for various volume compressions and shown in Fig.1 Using these results, the total energy has been computed and the equation of state studies have been carried out by using the Birch-Murnaghan method [10]. The minimum energy value corresponds to volume from which the equilibrium lattice constant calculated for alpha-polonium is 3.302Å and the bulk modulus is to be 53.25GPa. The present

calculated values of lattice parameter are in good agreement with the compared results from experimental and the theoretical studies reported earlier.

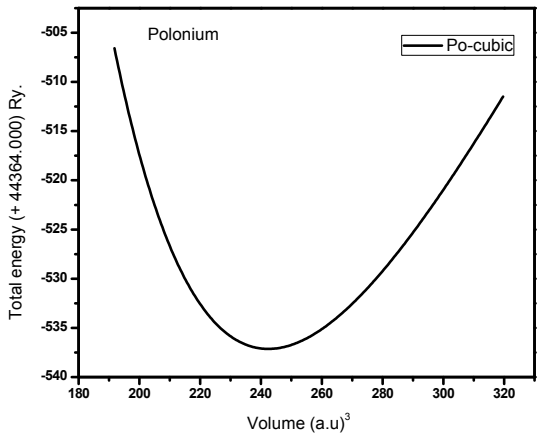

Figure 1. Total Energy Vs Volume for alpha-Polonium

The band structure along the high symmetry directions at ambient pressure for alpha-polonium is presented in Fig.2.The lowest energy bands are due to s-state electrons and the next higher energy bands occur in the conduction region. The calculated Fermi energy is 5.28eV.At the Fermi level, the bands from the conduction region is found dispersing down to the valence region along M, X-symmetry point which is mainly due to the p-state electrons of alpha-polonium atom and also shows its metallic behaviour which is evident from density of states (DOS) results at Fermi level (E_f) for the alpha-polonium under ambient conditions and it is shown in Fig.3.

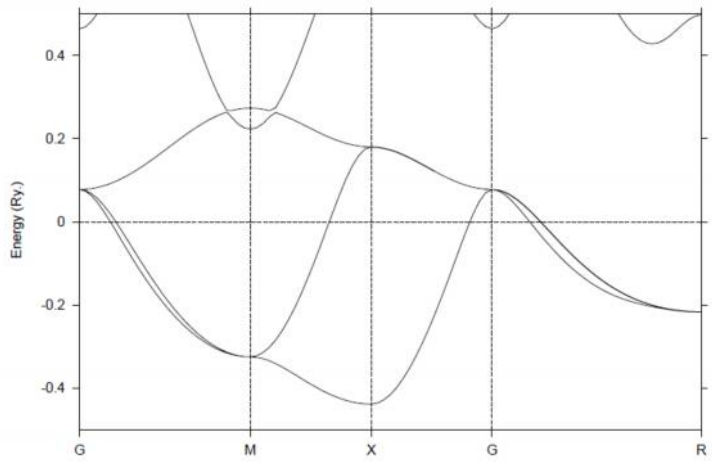

Figure 2. Band structure of alpha-Polonium along symmetry directions

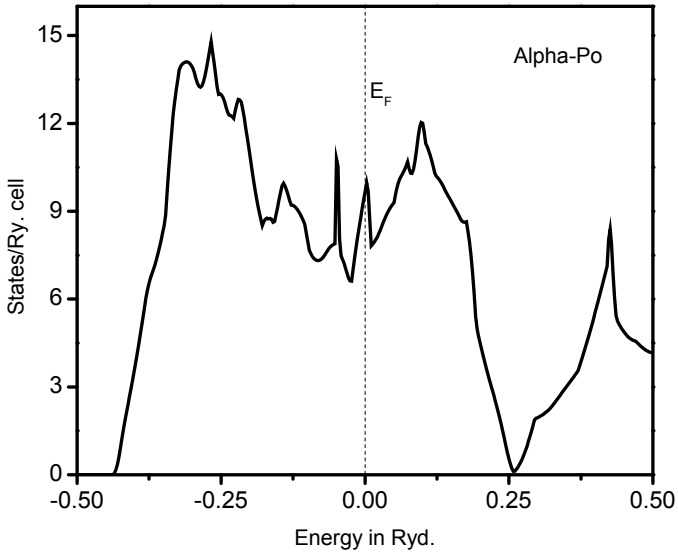

Figure 3. Total DOS of alpha-Polonium.

The bulk modulus B_0 is extracted from the Murnaghan equation of state and is used to calculate the Debye temperature by following Moruzzi et al [11] for the cubic alpha-polonium

$$\theta_D = 41.63\sqrt{\left(\frac{r_0 B0}{M}\right)} \qquad (1)$$

where B_0 is the bulk modulus in kbar evaluated at the equilibrium Wigner-Seitz sphere r_0 in a.u. and M is the average atomic mass of cubic alpha-polonium (209). The calculated value of θ_D is found to be 116 K, where r_0 = 3.07227 a.u. good agreement with the available literature data. The electron-electron interaction constant μ^* is obtained from the empirical relation given by Bennemann and Garland [12].

$$\mu^* = \frac{0.26\, N(E_F)}{1+ N(E_F)} \qquad (2)$$

The superconducting transition temperature is calculated using McMillan as [13].

$$T_c = \frac{\theta_D}{1.45} \exp\left\{\frac{-1.04\,(1+\lambda)}{\lambda-\mu^*(1+0.62\lambda)}\right\} \qquad (3)$$

Where θ_D the Debye temperature, λ is the electron-phonon coupling constant and μ^* electron-electron interaction parameter can be written by the theory of Gaspari and Gyorffy (GG)

$$\lambda = \frac{N(E_F)\langle I^2\rangle}{M\langle\omega^2\rangle} \qquad (4)$$

Where M is the atomic mass, $<\omega^2>$ an average squared phonon frequency [14]. and $<I^2>$ is the square of the electron-phonon matrix element averaged over the Fermi surface [15]. $<I^2>$ can be written in (Rydberg units)

$$\langle I^2\rangle = 2\sum_l \frac{(l+1)}{(2l+1)(2l+3)} M^2_{l,l+1} \frac{N_l(E_F) N_{l+1}(E_F)}{N(E_F) N(E_F)} \qquad (5)$$

Where $M_{l,l+1}$ is the electron –phonon matrix element which can be expressed in terms of the logarithmic derivatives D_l

$$M_{l,l+1} = -\phi_l(E_F)\phi_{l+1}(E_F)\left[(D_l(E_F) - l)(D_{l+1}(E_F) + l + 2) + \left(E_F - V(S)\right)S^2\right] \quad (6)$$

Where V(s) is the one electron potential and φl, the sphere boundry at E_f. N_l in equation is the partial density of states function for the angular momentum quantum number l. The necessary parameters to calculate $M_{l,l+1}$ are taken from the bandstructure results. The matrix elements are calculated as per the earlier work [16-18]. and the average of the square of the phonon frequency $<\omega^2>$ given by $<\omega^2> = 1/2\theta_D^2$ where θ_D is in energy units. The present calculated values of λ and T_C are 1.1 and 3.6K . The values estimated by the present work for the cubic alpha-polonium which is in close agreement with the available literature values [7].

IV. CONCLUSIONS

The electronic band structure studies of cubic alpha-polonium are carried out by using the self –consistent tight-binding linear muffin-tin orbital method. The electronic total energy values are obtained for various unit cell volumes and fitted Birch-Murnaghan equation of state. The ground state properties such as, equilibrium lattice parameter, primitive cell volume, bulk modulus has been obtained. The density of states at the Fermi energy is found to be strongly influenced by the p-states electrons in cubic alpha-polonium and it is also evident in the band structure results. The calculated results are observed to be in good agreement with the available results existing in the literature. The calculated values of Debye temperature, electron-electron interaction constant, electron-phonon coupling constant and superconducting transition temperature are observed to be in excellent agreement with the available literature data. Thus the present studies provide the basic knowledge of understanding the electronic and superconducting properties of the cubic alpha-polonium.

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