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Electronic and Structural Properties of Ba_2HgCuO_4: A Density Functional Theory Study

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Abstract: The highest Tcs superconductors are made up of intricated homologous series of the compound $HgBa_2Ca_{n-1}Cu_nO_{2n+2+\delta,}$. For n=1, $HgBa_2CuO_{4+\delta}$ have raised a Tc of up to 97K, displaying the highest critical temperature for related compounds result a single copper layer. The compound Mercury Dibarium Copper oxide belongs to space group of 123 of cuprate based superconductor. The compound $HgBa_2CuO_4$ has reported electronic structure using LDA. The cuprate material has the only band crossing the E_f is the Cu-O which has derived antibonding state characteristic of HTSC. From these lines, we can conclude that the compound is Mott insulator and the excess oxygen contributes to conduct superconductivity. In working with this paper, we have been finding about the crystal structure, band structure, Density of states (DOS) using the first principal theory i.e. popularly known as DFT (Density Functional Theory). The band structure and DOS diagram of compound Mercury DiBarium Copper oxide is existed by LSDA and LSDA+U.

Keywords: Density Functional Theory, Electronic band structure, Density of state

1. INTRODUCTION

$HgBa_2CuO_{4+\delta}$ where δ can be stimulated by controlling oxygen on both underdoped and over doped [1]. Up to n=3 the Tc becomes 133K for the compound will be $HgBa_2Ca_2Cu_3O_{8+\delta}$ [2, 3] and n=4 the compound will be isolated [4]. From Fig. 1 we came to the conclusion that it has layers (HgO_δ) (Bao)(CuO_2) (BaO) covering the c-axis of the tetragonal unit cell. HgO and CuO_2 layers reflect both the Ba and O atoms in the BaO layer

are displaced =0.9Å from one another in the direction of the c-axis due to the interaction of these atoms with the neighboring layers. BCS coworker explains the working of the electrons in superconducting material with the help of the namesake theory that electrons present in the superconducting material form copper pair below the critical temperature [5].In the meanwhile, in nearly about 20s centuries a new type of superconductor was discovered that performs superconductivity in higher temperatures generally named cuprates [6].The development of the cuprate has been intensive for more than thirty years. Newly, APRES had given the accuracy of spin-charge separation, leading to the growth of $Ba_2HgCuO_{4+\delta}$. $Ba_2HgCuO_{4+\delta}$ was contributed by S.N. Putilin et al 1993[7].The subject of the effective model for curates can be constructed solely on the $d_{x^2-y^2}$ band structure. ARPES observation of a second band $d_{x^2-y^2}$ hybridizing with $d_{x^2-y^2}$ orbital in over-doped LSCO has recently challenged this latter assumption. The development the cuprates has been intensive for more than three decades. Newly, APRES had provided the accuracy of spin-charge separation leading to the growth of Ba_2HgCuO_4. [8-10]. The apical oxygen in the Cu plane is greater than the CuO bond due to the John Teller effect and interlayer Coulomb interaction [11]. For the low doping region Tc, proven to the Mott insulator with antiferromagnetic order [12,13]. The critical value when exceeds form the 0.77 i.e. Pmax then Tc vanishes in over the doping region [14]. Mercury dibarium copper oxide has been considered one of the most attractive to scientists due to the relationship intervening atomic structure and physical properties. The HgO_δ and CuO_2 layers are flatted while the Ba and O atoms in the BaO layers act as they are shown ~ 0.9 Å from one another along the c axis between atoms with side by layers. It is generally noticed that the layer mentioned HgO_δ layers are used as a charge reservoir for the CuO_2 planes. The relationship between Tc and δ is controversial and contradicts to parabolic dependence [15]. Recently it has been found that the fermi liquid behavior over doped CuO. YBCO is the first superconductor Ba214 synthesized at high pressure up to (18GPa) and high temperature of 1000^{oc}.

2. COMPUTATIONAL APPROACH

The structure of cuprite Cu_2O forms the space group of hmm/p4/mmm. The calculation of the compound is done by using Density Functional Theory, pseudopotential. Quantum ESPRESSO is used for the calculation of Ba_2HgCuO_4. The ewf are SCC threshold for the total energy 10-12 Ry. BFGS algorithm [16] is used to optimize the structure under pressure up to 22GPa. All these electronic structure calculations are implemented through Quantum ESPRESSO codes viz pwx and thermopower [17-19]. Ba_2HgCu0_4 is a tetragonal crystal has space group p4/mm. The structure of mercury dibarium copper oxide and the total energy of Ba_2HgCuO_4 and the similarity oxides have been calculated by Medea VASP projected augmented plane wave basis set and (GGA-PBE). Enthalpy formation has been calculated by using the first value of the DFT. Final energy has been calculated using ab in-to the calculation. Quantum Expresso generally known as QE with Projector Augmented wave (PAW) [20] method has been used to calculate all the studies present here. The plane wave e cutoff was set to the value of 529 eV, and GGA is a generalized gradient approximation with semi-local Perdew Burke Ernzerhof (PBE) [21] function had been expected to explain the exchange-correlation relation. Γ explained the Brillouin zone centered K Mesha with the spacing of 0.027Å for the crystal optimization and 0.013 Å for the electronic structure calculation. The tetrahedron method with the Bloch correction was used to express the accurate DOS i.e. the criteria of convergence of energy and the force were expressed to 10^{-5} eV and 0.005eV/Å.

3. RESULTS AND DISCUSSION

3.1 Crystal Structure

The cuprate superconductors have built a layered crystal structure which is constituting of CuO planes and also has the intervening charge reservoir layers' plane has been concluded as a square lattice where sites have a hole of $d_{x^2-y^2}$. The mercury-containing superconductor having a single layer of HgO and varying layers of CuO_2. $HgBa_2CaCuO_8$ compound was first to be prepared as mercury-based superconductors and the method was used for solid-state reaction in an evacuated silica tube. In the tetragonal P4/mmm space group, $HgBa_2CuO_4$. Ba^{2+} is having square faced bicapped trigonal prism bonded with 8-coordinate geometry related to 8 O^{2-} atoms.

There has been four shorter (2.75 Å) and four longer (2.95Å).Cu^{2+} is bonded in shape of square planar geometry to four O^{2-} atoms. All Cu-O bonds have a length of 1.97Å. Hg^{2+} has bonded in a linear geometry to the two equivalent O^{2-} atoms. Both HgO bonds have a length of (2.01Å).There are two different O^{2-} sites, In the 1st O^{2-} is bonded in a 5-coordinate geometry to four equivalent Ba^{2+} and one Hg^{2+} atom. In the second O^{2-} site O^{2-} is bonded with four equivalent Ba^{2+} and Cu^{2+} atoms forming a mixture of distorted face, corner, and edge-sharing OBa_4Cu_2 octahedra. The crystalline structure containing of 3 lattices such as a=b=3.93 Å, c=9.43Å. As we know tetragonal structures have angles 90 degrees. Hence we used an approximate and studied the fundamental characteristics of cuprate. From the VESTA we have calculated that the unit volume is 1026.2396Å. The following tables will be able to display the atomic cell.

Table 1

Elements /atoms	Position a	Position b	Position c
Hg	**0**	**0**	**0**
Cu	**0**	**0**	**1/2**
O	**0**	½	**1/2**
O	**0**	**0**	**0.794971**
Ba	½	½	**0.695597**

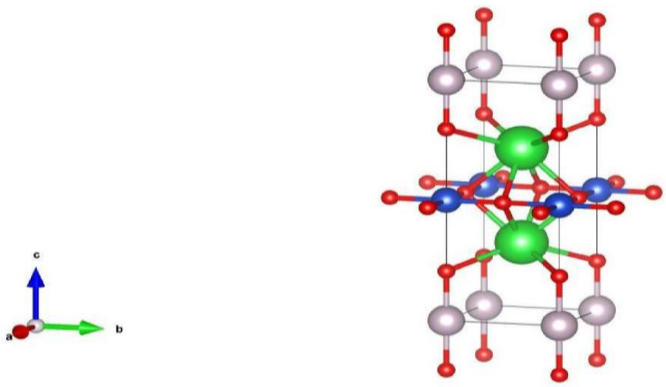

Fig. 1. Crystal Structure of Ba_2HgCuO_4 having lattice constant a=b=3.93 Å, c=9.43Å

The crystal structure has been optimized using VESTA's lattice parameter. Crystal has been optimized successfully and provided information regarding the properties of the cuprate material. The figure shows the ecut off values in x axis and the total energy in Y axis. The total energy is decaying with respect to ecut energy as shown in the Fig. 2 and convergence happen on 12 Ry. So, we can say that it ensures that the total energy reaches to 12Ry stable values

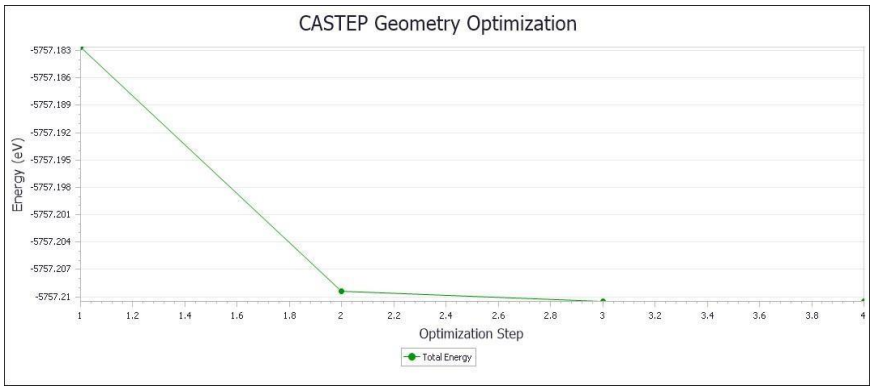

Fig. 2. Energy vs Optimization

as Ecut decaying. Form this information we can conclude about the Ba_2HgCuO_4 is having perovskite structure.

3.2 Band Structure

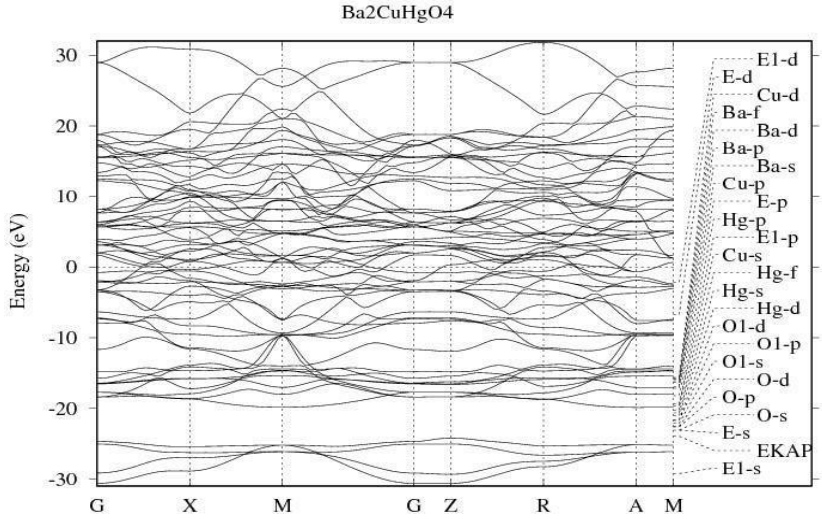

Fig. 3. The band structure diagram of Ba_2HgCuO_4 compound

The band closure to the fermi surface had a crucial role in providing information regarding understanding of the unconventional superconductor. The database that has shown the band structure under construction is calculated using Quantum Espresso within the general gradient approximation (GGA) of the DFT. We had used the projected augmented waves pseudopotential by PBE. With the help of Quantum ESPRESSO, the band structure has been published above graph encompasses a range of 30 to -30eV, and band structure has been constructed using the optimized values of lattice parameter and atomic position centered grid is chosen for faster convergence. The path that has been followed G-X-M- G-Z-R-A-M. Between the 30 to-30 the fermi energy lies, above fermi energy there is the conduction band and below the fermi energy, there is the valence band. M and X have high symmetry intersect in the Fermi Level. Ba_2HgCuO_4 has several fermi surfaces which indicates about multiple metallic bands. The E_f=0 this part contributes to the compound is insulator.

3.3 Density of State

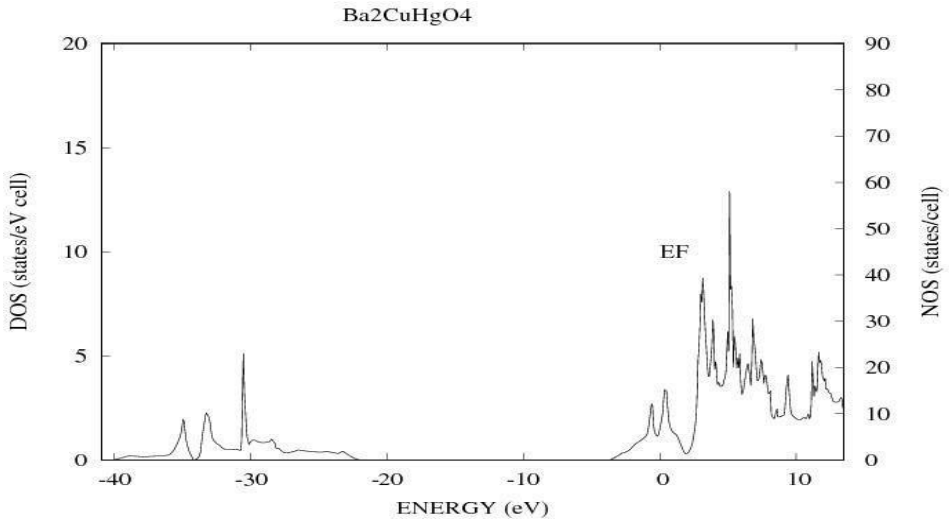

Fig. 4. The Density of State vs Energy of Ba_2CuHgO_4

DOS is termed as Density of state which can be defined as per unit volume per unit energy. Parent insulator compound Ba_2HgCuO_7 have found that the band gap is 0.00 eV. However, the theory has been that the mercury

dibarium copper oxides have semi-metallic features. This may be due to the smearing effect of $E_{f.}$ The TDOS values of $HgBa_2Ca_{n-1}Cu_nO_{2n+2}$ cuprate superconductor with minimal doping at the fermi surface are much higher than that of the stoichiometric $HgBa_2Ca_{n-1}$ CuO_{2n+2}, which indicates that doped O atom can make significant changes in the electronic structure and the benefits the superconductivity. DOS histogram for $HgBa_2CuO_4$ at various high-pressure ranges and EBS having symmetry points in IBZ have been presented. DOS is stated as the different states at a particular energy level that electrons are allowed to occupy i.e. the number of electrons states per unit volume per unit energy. DOS allows us to find out or to determine the general distribution of electrons state as the function of energy. Fig. 4 provides the information of different states are associated with different peaks number. From the graph we could identify that the horizontal X-axis in Fig. 4 represents the energy value in eV. Superconductivity point is at E_f=0. Peak near the range of -5eV to 0 eV has electronic properties of Ba_2HgCuO_4 and plays a significant role in the superconductivity.

4. CONCLUSION

Through investigation with the first principal theory, we conclude different type of electronic properties and structural properties of Ba_2HgCuO_4 is a cuprate based superconductor. Here we have used Quantum Espresso. We had done self -consistent field, Density of states and Band structure and came to conclude that we had a good agreement with theoretical data. Hence we came to the conformation about tetragonal structure of compound $Ba_2HgCuO4$ .This compound shows structure similar to K_2NiF_4.Band structure near M and X have electron pockets in the Brillouin zone. The electron pockets are responsible for interaction with other band and form superconductivity. The DOS plays a crucial role in coupling the copper pair which results on providing the superconductivity.

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