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FIRST PRINCIPLE STUDY OF BERYLLIUM CARBIDE

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Abstract: In present work, the electronic properties of Beryllium Carbide (Be_2C) are investigated using Density Functional theory (DFT) as implemented in Quantum Espresso package. Generalized gradient approximation (GGA) has been used for pseudo potential. First the structure has been optimized and using those values of lattice constants further calculations for density of states, band structure, and band gap have been done. The obtained results show it semiconducting with band gap 1.2078 eV. The calculated results are in good agreement with experimental data and other DFT calculations.

IndexTerms **– Beryllium Carbide, electronic structure, DFT, semiconductor**

I. INTRODUCTION

The study of solids formed from light elements has gained considerable attention due to their potential industrial and technological applications. Particularly, ceramic compounds composed of light elements—such as borides, carbides, and nitrides—are recognized for their exceptional mechanical strength, thermal stability, and unique electronic properties. Within this family, anti-fluorite type materials, including Be_2C, Mg_2Si, Mg_2Ge, Li2O, Na2O, K2O represent some of the simplest examples of metal–semiconductor hybrid materials [1-5]. Among these, beryllium carbide (Be_2C) is of particular interest [6-10]. Owing to the small atomic radii of beryllium and carbon, Be_2C exhibits exceptionally high elastic moduli and remarkable hardness, comparable in some respects to that of diamond [11]. Some of its properties are associated with strong chemical bonding and high melting point. This also makes it promising material for high temperature and pressure applications [12]. It has wide range of application from the diffusion barrier against copper [13] to ablation coatings in experimental fusion reactors [14]. In addition, Be2C may be used for shielding purpose in nuclear reactors as it is highly resistant to radiation damage [15].

Some other possible structures of beryllium carbide including quasi planar hexacoordinate carbon [16], stable monolayer [17] have also been identified and found that the monolayer has excellent stability as well as good mechanical properties, good thermal stability and maintained its structural integrity even at high-temperature. Yan et al. [18] reported that Be2C is mechanically stable. Bonding in such structures is complex mixture of covalent and ionic characters. The reported bulk modulus and shear modulus suggest that it is hard material. Recently some interesting studies are also there on its phonon properties such as phonon dispersion, phonon density of state, free energy, entropy, specific heat indicating that the Be2C structure is dynamically stable [19]. The optical and elastic properties study by Gupta etal [20] indicate fragile and brittle nature of beryllium carbide. Also, there is detail study on its thermoelectric and vibrational properties including power factor, Seeback coefficient, thermal conductivity, electrical conductivity, LO-TO splitting [21]. Current research is also focused on investigating its material compatibility with molten salts, radiation damage characteristics and properties like thermal stability for its use as promising high-temperature neutron moderator for salt reactors. One such comprehensive study of native and radiation-induced point defects in Be_2C is done by investigating the behavior of point defects under various charge states and chemical environments [22]. While toxicity and fabrication challenges limit widespread use, ongoing research continues to expand understanding and identify new opportunities for Be_2C in next-generation technologies.

Our aim in the present work is to explore electronic properties of this material in details. The paper is organized as: In first section, theoretical and computational approach is discussed. Thereafter, results for electronic properties are given. Finally, we conclude.

2. THEORETICAL AND COMPUTATIONAL FRAMEWORK

Be2C can be considered is face centered cubic (FCC) structure belonging to the space group Fm-3m (group no. 225). It belongs to the anti-fluorite structure family and has zinc blende like lattice. The present calculations are performed using density functional theory (DFT) [23] with Perdew-Burke-Ernzerhof (PBE) generalized gradient approximation (GGA) [24] using plane wave pseudo potential method as implemented in Quantum Espresso package [25]. Norm-conserving pseudo-potentials based on the Troullier–Martins scheme are used to model core electrons. The Brillion zone integration is performed over a Monkhorst–Pack [26] 8 × 8 × 8 meshes. The cutoff for the kinetic energy is set to 40 Ry. The Marzari- Vanderbilt smearing size is fixed at 0.003 Ry. The energy convergence set to 10-6 Ry. A very fine mesh of 24×24×24 points is used for calculations of density of states and other properties.

3. RESULTS AND DISCUSSION

To understand the electronic properties, we have calculated band structure, density of state (DOS), projected DOS. Firstly, the optimized value of lattice constant is found out and that is further used to study other properties. Electronic band structure of Be2C is shown in figure 1, from which it's clear that there is small forbidden gap and the minimum energy of the conduction band is not aligned vertically with the maximum energy of the valence band, making Be2C indirect gap semiconductor. The value of this band gap comes out to be 1.2078 eV. The valence bands are split into two sub-bands may be due to large electronegativity difference between the constituent atoms. The density of state is also shown in figure 2, again showing the small forbidden gap. Further to see the contribution of each orbital, the projected density of state is plotted in figure 3, from which is it is clear that p -states contribute significantly around the Fermi energy EF and extend to higher energies.

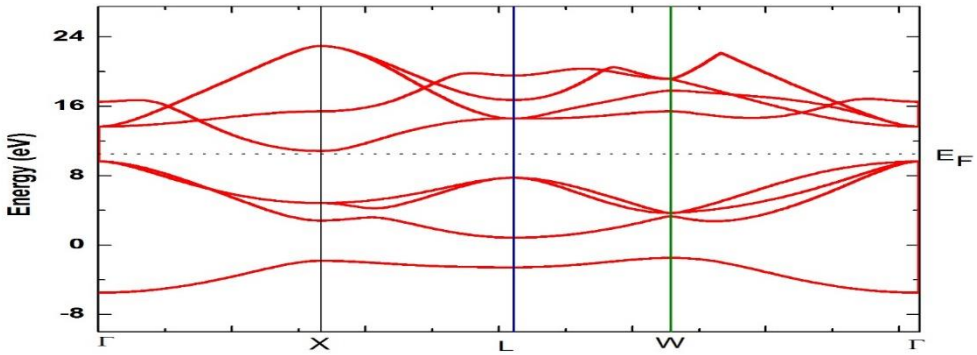

Fig 1: Electronic band structure of Be2C

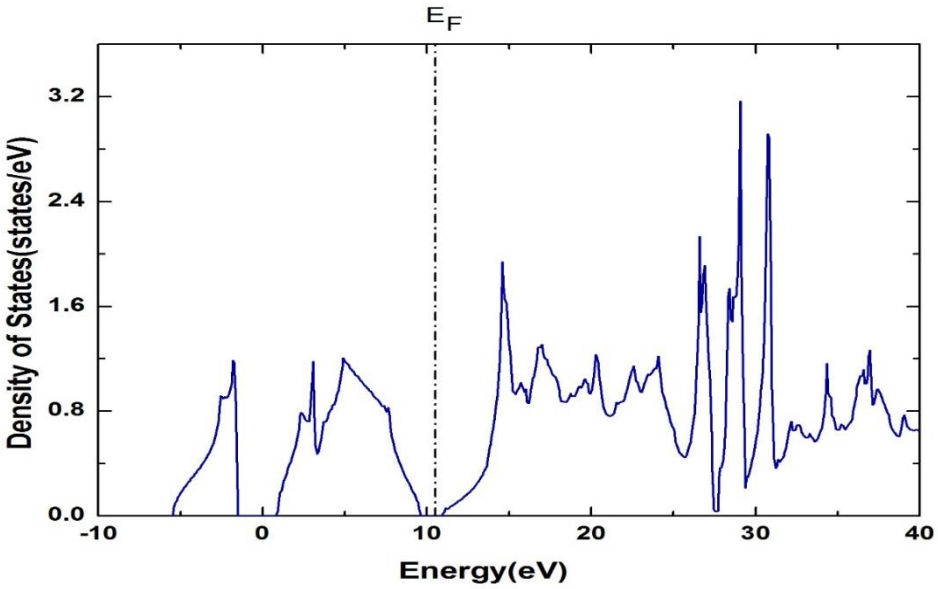

Fig 2: Density of state of Be_2C

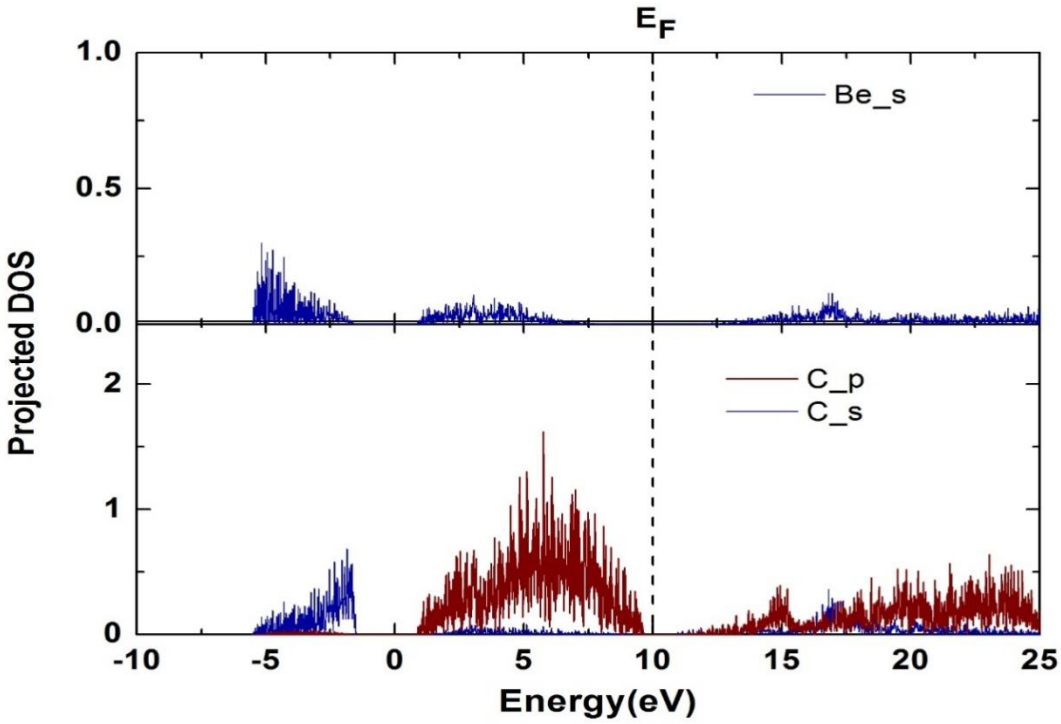

Fig 3: Projected Density of state of Be_2C

Also, the calculated values of lattice constant, bulk modulus, band gap are tabulated in table 1 along with comparison with other theoretical and experimental studies, showing a good agreement. Bulk modulus is calculated from fitting the 2nd order Birch equation of state.

Material Studied	Work	Method	Lattice Constant (A^0)	Bulk Modulus (GPa)	Band Gap (eV)
Be_2C	Present	GGA	4.315	224.6	1.2078
	Yan et al. [18]	GGA	4.33	195.8	1.25
	Gupta et al. [20]	GGA	4.327	198.7	1.170
	Osetskiy et al. [22]	GGA	4.302	------	1.169
	Corkill and Cohen [1]	LDA-CA	4.23	214.2	1.239
	Lee et al. [8]	LDA	4.27	216.0	1.2
	Ruschewitz et al. [4]	Experimental	4.33	-------	1.2

Table 1: Calculated lattice constant, bulk modulus and band gap

4. CONCLUSION

The electronic properties of Beryllium Carbide are studied using pseudo potential method with GGA approximation as in quantum espresso package. The calculated results are in good agreement with experimental data and other DFT calculations. Be_2C comes out to be semiconducting with band gap of about 1.2078 eV, which are in good agreement with early results.

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