Structural, Electronic and Optical Properties of $\text{Be}_2\text{X}(\text{X} = \text{C, Si, Ge, Sn})$: First Principle Study

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Abstract

We computed structural, electronic and optical properties of $\text{Be}_2\text{X}(\text{X} = \text{C, Si, Ge, Sn})$ family of antifluorite with ab initio DFT calculations using the generalized gradient approximation (GGA). The different parameters such as geometry optimization, band structure, density of states, elastic constants, dielectric functions have been studied. We also calculated bandgap using PBE0 and HSE hybrid functionals to compare experimental bandgap of $\text{Be}_2\text{C}$. Although three of the compounds are hypothetical in nature, their formation energy found to be negative. The calculated values of elastic constants indicates antifluorite $\text{Be}_2\text{X}$ are mechanically stable. The graph of real part of epsilon shows negative value giving promising result for blanket behaviour of $\text{Be}_2\text{X}$ from radiation damage.

INTRODUCTION

Antifluorite $\text{Be}_2\text{X}(\text{X} = \text{C, Si, Ge, Sn})$ structure form the simplest family of metal - semiconductor (Group II-IV elements) hybrid materials. Antifluorite structure has a similar structure to diamond. Group IV atoms occupy fcc sites with eightfold coordination and II atoms are at tetrahedral sites with fourfold coordination of resulting structure of cubic Fm-3m space group. The first member of the family Beryllium carbide is a transparent (colourless when pure) crystalline solid and very hard compound, like diamond, a pure carbon compound [1]. $\text{Be}_2\text{C}$ is refracting in nature and chemically instable in the presence of moisture. It has large elastic constants, hardness, sound velocities, a high melting point and a good thermal conductivity [2]. It is observed that $\text{Be}_2\text{C}$ is a bit harder than SiC [3]. $\text{Be}_2\text{C}$ is also resistance to radiation damage and may be used in fission reactor components and as a blanket material in fusion reactor [4]. The $\text{Be}_2\text{C}$ is among the few known alkaline earth methanides. The $\text{Be}_2\text{C}$ used in ceramic and nuclear technology, has attracted quite a few theoretical as well as experimental studies [5]. $\text{Be}_2\text{C}$ is highly poisonous and therefore only few experimental research has been done. The three compounds $\text{Be}_2\text{X}(\text{X} = \text{Si, Ge, Sn})$ are hypothetical materials and are not known to exit in bulk at present. But some experiments strongly suggests existence of clusters ($\text{Be}_2\text{Si}_n$) on the surface of Silicon [6, 7]. So, there are very few study on these materials yet. The goal of this paper is to obtain the basic structure, electronic and optical properties of $\text{Be}_2\text{X}$ by DFT [8].
Computational Methods

Calculations were carried out through DFT package Quantum Espresso (version 6.7) using pseudopotential plane-wave method [9]. The PBE-PAW pseudopotentials were used with an energy cutoff of 50 Ry and k-point mesh 6 x 6 x 6 is employed and further increased to 14 x 14 x 14 in calculating electronic and optical properties. The lattice vectors were optimized with total energy converging within $10^{-4}$ a.u. Non-conserving pseudopotentials are used for calculations of optical properties and Projector Augmented Waves pseudopotentials are used for all other calculations. PBE exchange-correlation functional of GGA [10] is used in all calculations. In the calculations, the $Be(2s^2)$, $C(2s^22p^2)$, $Si(3s^23p^2)$, $Ge(4s^24p^2)$ and $Sn(5s^25p^2)$ states are treated as valence electrons. Hybrid functionals PBE0 [11] and HSE [12] are also used for calculating Bandgap of the four structure to incorporate a portion of exact exchange from Hatree-Fock theory with rest of exchange-correlation energy from ab initio calculations.

The elastic constants were calculated out through ElaStic code [13] using Energy-strain method and the maximum strain value was 0.03%. The optical properties were determined using many-body effects solving Bethe-Salpeter Equations for accurate theoretical description and compared with Independent Particle Approximation [14] using YAMBO code [15] from the complex dielectric function, $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$.

The crystal structure is shown in figure 1. It has cubic space group number 225 where Be atom occupy 8c and X atom occupy 4a Wyckoff positions [16].

![Figure 1: Primitive cell (a) and Cubic crystal structure (b) model of Be₂X](image)

Table 1: Atomic Positions of Be₂X

| Site | Location | Co-ordinates |
|------|----------|--------------|
| Be   | 8c       | (0.25, 0.25, 0.25), (0.75, 0.75, 0.75) |
| X    | 4a       | (0, 0, 0)    |
RESULTS

Structural Properties

The antifluorite has cubic structure and its space group is Fm-3m with space group number 225. It has 4 molecules per unit cell. The atomic positions are given in Table 1. In order to analyze structural properties of $Be_2X$, cut-off energy and k-points optimizations were performed followed by geometry optimization. The Total energy vs. Volume (Annex 1) graphs have been plotted coupled with Murnaghan equation of state [17] for the four structures. The minimum total energy corresponds to the stable point of the crystal. The lattice constant parameter at this point and the Bulk modulus for the four structures is listed in Table 2 and Table 3 with available previous similar work and experimental data.

The calculated lattice constant for $Be_2C$ using GGA is in good agreement with the experimental data. No experimental data are available for other three structures. The calculated Bulk modulus value is in agreement with other GGA calculations [18, 19] but lower than the LDA results [20, 21]. This may be due to over binding tendency of Local density approximation (LDA).

Table 2: Lattice Constant $a$ of $Be_2X$ ($X = C, Si, Ge, Sn$)

| Work               | Method | $Be_2C$   | $Be_2Si$   | $Be_2Ge$   | $Be_2Sn$   |
|--------------------|--------|-----------|------------|------------|------------|
| This work          | GGA    | 4.327 Å   | 5.268 Å    | 5.366 Å    | 5.799 Å    |
| Paliwal et al.     | GGA    | 4.335 Å   |            |            |            |
| Yan et al.         | GGA    | 4.33 Å    | 5.28 Å     |            |            |
| Lee et al.         | LDA    | 4.27 Å    | 5.22 Å     |            |            |
| Corkill and Cohen  | LDA-CA | 4.23 Å    | 5.18 Å     |            |            |
| Experimental       | –      | 4.330 Å   |            |            |            |

Table 3: Bulk modulus $B_0$ of $Be_2X$ ($X = C, Si, Ge, Sn$)

| Work               | Method   | $Be_2C$  | $Be_2Si$  | $Be_2Ge$  | $Be_2Sn$  |
|--------------------|----------|----------|-----------|-----------|-----------|
| This work          | GGA      | 198.7 GPa| 97.4 GPa  | 91.5 GPa  | 72.1 GPa  |
| Paliwal et al.     | GGA      | 198.9 GPa|           |           |           |
| Yan et al.         | GGA      | 195.8 GPa| 94.5 GPa  |           |           |
| Lee et al.         | LDA      | 216.0 GPa| 102.5 GPa |           |           |
| Corkill and Cohen  | LDA-CA   | 216 GPa  | 103.2 GPa |           |           |
| Experimental       | –        |          |           |           |           |
Elastic Properties

The elastic properties of a crystal can be determined by computing its elastic stiffness constants \([C_{ij}]\), which is actually the response of material to external stress. The stiffness matrices \([C_{ij}]\) is calculated using PBE functionals and Energy-strain method. For a cubic system, there are three independent elastic constants \(C_{11}, C_{12}\) and \(C_{44}\). These elastic constants are used to calculate elastic properties using the Voigt-Reuss-Hill (VRH) averaging scheme for cubic system \([23, 24]\). The shear modulus \(G\) and the bulk modulus \(B\) are related to \([C_{ij}]\) as,

\[
G_v = \frac{C_{11} - C_{12} + 3C_{44}}{5} \\
G_R = \frac{5C_{44}(C_{11} - C_{12})}{4C_{44} + 3(C_{11} - C_{12})} \\
G = \frac{1}{2}(G_v + G_R) \\
B_v = B_R = \frac{C_{11} + 2C_{12}}{3} \\
B = \frac{1}{2}(B_v + B_R)
\]

We have also calculated Young’s modulus \(E\) and Poisson’s ratio \(\nu\) according to the relations,

\[
E = \frac{9BG}{(3B + G)} \\
\nu = \frac{3B - 2G}{2(3B + G)}
\]

Their calculated value is shown in Table 4. The calculated value of elastic constants satisfy the Born’s stability criteria for the cubic system \([25]\), i.e., \(C_{11} - C_{12} > 0, C_{11} + 2C_{12} > 0\) and \(C_{44} > 0\) for all four structures. This shows that \(Be_2X\) is mechanically stable. The calculated bulk modulus \(B_0\) by fitting the Murnaghan equation of states and the bulk modulus \(B\) derived with that from the above Voigt-Reuss-Hill approximation are well comparable, which indicates that our elastic calculations are consistent and reliable.

For \(Be_2C\), shear modulus is large and is expected to withstand shear strain to a large extent which makes it useful in technological applications as a hard material. The ratio of Bulk modulus to the Shear modulus is very low which indicated fragile nature of \(Be_2C\). The Poisson’s ratio is
calculated very less and shows high brittle nature of Be$_2$C. The calculated elastic constants for Be$_2$X (X = Si, Ge, Sn) are much smaller than Be$_2$C. This may be due to metallicity of these compounds.

Table 4: Elastic Constants ($C_{ij}$), bulk modulus (B), shear modulus (G), Young’s modulus (E) and Poisson’s Ratio ($\nu$) of Be$_2$X (X = C, Si, Ge, Sn)

| Parameter | Be$_2$C [GPa] | Be$_2$Ca [GPa] | Be$_2$Si [GPa] | Be$_2$Si$a$ [GPa] | Be$_2$Ge [GPa] | Be$_2$Sn [GPa] |
|-----------|---------------|----------------|----------------|-------------------|---------------|---------------|
| $C_{11}$  | 579.6         | 570.5          | 166.9          | 133.0             | 148.6         | 103.4         |
| $C_{12}$  | 13.3          | 16.0           | 73.5           | 82.5              | 69.2          | 59.8          |
| $C_{44}$  | 200.9         | 208.7          | 106.0          | 99                | 95.4          | 49.9          |
| B         | 202.05        | 200.8          | 104.63         | 99.3              | 95.65         | 74.37         |
| G         | 230.56        | 233.8          | 76.29          | 57.6              | 67.09         | 35.77         |
| E         | 501.08        | 505.4          | 184.11         | 154.8             | 163.13        | 92.49         |
| $\nu$     | 0.09          | 0.081          | 0.21           | 0.26              | 0.22          | 0.29          |

$a$ Using DFT with GGA. [Yan et al.]

Electronic Properties

The band structure, total and projected density of states (DOS) [26] were obtained using DFT with generalized gradient approximation. The energy band structure along principle symmetry points obtained is shown in Figure 2 with Fermi energy set to origin. The crystal has 4 valence bands and we demonstrated 6 conducting bands for Be$_2$C & Be$_2$Si and 5 conducting bands for Be$_2$Ge & Be$_2$Sn. The valence band can be classified into two group. The lower energy band is mainly due to Group IV atoms s states and Be atom p states. The remaining group of bands is mainly due to group IV atoms p states hybridized with the Be atom p states. The conduction bands are mixture of s and p states. This is shown in partial DOS Figure 3.

For Be$_2$C, the indirect band gap is obtained to be 1.170 eV and direct band gap is 4.132 eV. The result is close to experimental data [27]. This classify Be$_2$C as a semiconductor with a mid band gap. The calculated Total DOS shows the contribution of valence electrons from below 10 eV and conduction electron contributing to DOS above 10 eV. However, other three structures exhibit metallic behaviour in its crystalline state due to the finite density of states at the Fermi level. Thus, these structures are significantly different from Be$_2$C at the Fermi Energy level though they are assumed to have same crystal structure and similar electronic structure. This discrepancy may be due to overlap of other IV atom outer p orbitals with neighbour Be atoms than the C atom 2p orbitals.
Figure 2: Band Structure of $\text{Be}_2X(X = \text{C, Si, Ge, Sn})$ Crystal. Valence Band Maximum is set to 0 eV

The bandgap was also calculated using different functional with 8x8x8 k-grid and 8x8x8 q-grid shown in Table 5.

|          | GGA [eV] | PBE0 [eV] | HSE [eV] |
|----------|----------|-----------|----------|
| $\text{Be}_2\text{C}$ | 1.1701   | 2.5569    | 1.8885   |
| $\text{Be}_2\text{Si}$ | 0.8142*  | 0.1067*   | 0.5766*  |
| $\text{Be}_2\text{Ge}$ | 0.6218*  | 0.601     | 0.0352   |
| $\text{Be}_2\text{Sn}$ | 1.3015*  | 0.8821*   | 1.2888*  |

* Band Crossing
Figure 3: Density of states of Be$_2$X ($X = C, Si, Ge, Sn$) Crystal. Valence Band Maximum is set to 0 eV

Optical Properties

The dielectric function is the most general property of a material and can characterize how a material responds to the incident electromagnetic wave of light. We calculated the real $\varepsilon_1(\omega)$ and imaginary part $\varepsilon_2(\omega)$ of the dielectric function. The real part that shows the physical properties of a crystal and the imaginary part corresponds to the energy loss of photons in a material during electron transition between electronic bands are plotted in Fig 4.
In real dielectric function graphs the regions which decreases with the increasing of the photon energy gives the abnormal dispersion region. When ε value takes zero value at some phonon energies, these points give us plasmon frequencies [28]. Also, when ε values become negative in some regions which means that there is a reflection of the incident electromagnetic waves. Those points that correspond to plasmon frequencies and the negative regions of ε can be examined from Fig 4. The calculated static dielectric constant, $\varepsilon_1(0)$, for $Be_2X$ is shown in Table 6. The peaks in the imaginary ε shows the transitions of electron from valence to conduction bands [29].
Table 6: Static dielectric constants $\varepsilon_1(0)$ for $Be_2X (X = C, Si, Ge, Sn)$

|       | $\varepsilon_1(0)^p$ | $\varepsilon_1(0)^q$ |
|-------|-----------------------|-----------------------|
| $Be_2C$ | 4.65                  | 4.11                  |
| $Be_2Si$ | 10.04                 | 9.75                  |
| $Be_2Ge$ | 11.53                 | 10.70                 |
| $Be_2Sn$ | 10.68                 | 10.21                 |

$^p$ solving BSE
$^q$ with IPA

Other optical properties such as refractive index $n(\omega)$, extinction coefficient $k(\omega)$, absorption coefficient $\alpha(\omega)$, reflectivity $R(\omega)$ and energy loss spectra $L(\omega)$ are calculated in terms of real and imaginary parts of the dielectric function obtained by solving Bethe-Salpeter Equations as:

$$n(\omega) = \frac{1}{\sqrt{2}} \left[ \sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega) + \varepsilon_1(\omega)} \right]^{1/2}$$

$$k(\omega) = \frac{1}{\sqrt{2}} \left[ \sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega) - \varepsilon_1(\omega)} \right]^{1/2}$$

$$\alpha(\omega) = \sqrt{2} \frac{\omega}{c} \left[ \sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega) - \varepsilon_1(\omega)} \right]^{1/2}$$

$$R(\omega) = \frac{(n(\omega) - 1)^2 + k^2(\omega)}{(n(\omega) + 1)^2 + k^2(\omega)}$$

$$L(\omega) = \frac{\varepsilon_2(\omega)}{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)}$$

They are shown in Annex. The refractive index of the four structures is shown in Table 6 which satisfies the relation $n(0) = \sqrt{\varepsilon_1(0)}$. The refractive index is greater than one because as photons enter a material they are slowed down by the interaction with electrons. The more photons are slowed down while travelling through a material, the greater the material’s refractive index.

The zero-frequency reflectivity $R(0)$ and maximum reflectivity $n(\omega)$ for the four structures are mentioned in the Table 7. The reflectivity shows high reflectivity in the UV region. The absorbance
Table 7: Calculated Optical parameters of $Be_2X$ ($X = C, Si, Ge, Sn$)

|          | $Be_2C$ | $Be_2Si$ | $Be_2Ge$ | $Be_2Sn$ |
|----------|---------|----------|----------|----------|
| $n(0)$   | 2.15    | 3.169    | 3.39     | 3.26     |
| $\varepsilon_1(0)$ | 4.65    | 10.04    | 11.53    | 10.68    |
| Maximum $n(\omega)$ | 5.93    | 6.37     | 6.97     | 6.91     |
| $R(0)$ % | 13.45   | 27.08    | 29.73    | 28.27    |
| Maximum $R(\omega)$ % | 82.09   | 86.31    | 92.78    | 94.19    |

spectra shows low absorbance in Visible region and high absorbance is found in the UV region for all four structures.

CONCLUSION

A first principle DFT method has been implemented to investigate Structure, Elastic, Electronic and Optical properties of $Be_2X$ ($X = C, Si, Ge, Sn$). The lattice parameter at equilibrium is in reasonable agreement with experiment and previously calculated for $Be_2C$ and $Be_2Si$. The study of elastic property indicates fragile and brittle nature of $Be_2C$. The band gap in cubic structure of $Be_2C$ is found to be 4.132 eV. The other three structures $Be_2X$ ($X = Si, Ge, Sn$) shows metallicity nature. The optical properties such as dielectric function, reflectivity, absorption coefficient, refractive index, extinction coefficient, and electron energy loss are studied in the energy range of 0-10 eV. The negative value of $\varepsilon$ shows that $Be_2C$ and other three structures can be used as blanket material for prevention from UV radiation damage. The low optical absorbance of $Be_2C$ against other three structures in the visible region restricts its use in Solar Cell and other optoelectronic applications. Due to less research work on $Be_2C$ and hypothetical compounds $Be_2X$ ($X = Si, Ge, Sn$), all results has not be compared. Thus, this study can be helpful for further research on this crystal.

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ANNEX 1 : Total Energy with respect to volume (au$^3$)
ANNEX 2: Calculated refractive index, extinction coefficient, absorption coefficient, reflectivity and Energy loss spectra of Be$_2$C.
ANNEX 3: Calculated refractive index, extinction coefficient, absorption coefficient, reflectivity and Energy loss spectra of Be$_2$Si.
ANNEX 4: Calculated refractive index, extinction coefficient, absorption coefficient, reflectivity and Energy loss spectra of $Be_2Ge$. 
ANNEX 5: Calculated refractive index, extinction coefficient, absorption coefficient, reflectivity and Energy loss spectra of $Be_2Sn$. 

![Graphs of refractive index, extinction coefficient, absorption coefficient, reflectivity and Energy loss spectra of $Be_2Sn$.]