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Study of Electronic and Dielectric Properties of Magnesium Phosphide

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Abstract **- First-principles calculations based on Density Functional Theory have been done on Magnesium phosphide. Its cubic unit cell has been simulated. Band gap in case of this material comes out to be 0.5eV. This value is in the range exhibited by semiconducting materials. Dielectric constant and Polarizability of the material have been computed. The value of dielectric constant comes out to be 51.9 along all the three axes. The polarizability values are found to be 46.7 (Å)^3 along all the three axes. Phonon modes at gamma point in the material range from 0 cm^{-1} to 452 cm^{-1}.**
Keywords: **Magnesium phosphide, Dielectric constant, Electronic Density of States, First-principles calculations, Polarizability, Phonon modes**

I. INTRODUCTION

Magnesium phosphide is a fumigant used to control insects and rodents. It is primarily used for indoor fumigation of raw agricultural commodities, animal feeds, processed food commodities and non-food commodities in sealed containers or structures, and for outdoor fumigation of burrows to control rodents and moles in non-domestic areas, non-crop land, and agricultural areas. Magnesium phosphide is formulated as tablet, pellet, impregnated material and dust. The simplest method of production of a metal phosphide is direct combination of the elements at an elevated temperature. Here white, red, or gaseous phosphorus can be used. Some phosphides can be prepared by reaction of phosphine with metals or their salts. Metallic phosphides can also be prepared by the electrothermal reduction of metal oxides in the presence of carbon [1]. Magnesium phosphide is a white or yellow crystalline solid. It reacts violently with water and may ignite upon contact with air. It is toxic by ingestion. It is also used to prepare other chemicals [2]. When heated to decomposition it emits toxic fumes of phosphorus oxides and phosphine [3,4].

It has been found that any little modification in the structure and composition of a material will bring in sufficient changes in the properties of the material [5, 6]. Thus it is important to study the structure of the materials and look at the parameters which can be altered to get a better material for technological applications. First-principles calculation based on Density Functional Theory[7] has been proved to be an effective tool in the study of structural, electronic and dielectric properties of organic materials [8, 9]. Magnesium phosphidecrystals have attracted the scientific community in various aspects [10 – 12]. With this in view, structure of a Magnesium phosphide crystal [Mg_3P_2] has been simulated using First-principles calculations based on Density Functional Theory and computation of Electronic density of states, Dielectric constant and Polarizability have been done and the results have been reported in the present paper.

II. COMPUTATIONAL DETAILS

Several codes are available for the theoretical structure simulation [13]. The density functional theory approach has emerged as a well established computational method. It has been widely employed to arrive at the conformations of a large number of molecular systems. The practical applicability and sophistication of DFT is strongly sensitive to the good choice of exchange–correlation function along with the appropriate basis set.

Quantum espresso is an integrated suite of Open-Source computer codes for electronic-structure calculations and materials modelling. It is based on density-functional theory, plane waves, and pseudopotentials. Authors have used plane wave self consistent field (PWSCF) [14] implementation of density functional theory (DFT), with a Local density approximation (LDA) [15] to exchange correlation energy of electrons and ultra-softpseudopotentials [16] to represent interaction between ionic cores and valence electrons. Kohn-Sham wave functions were represented with a plane wave basis with an energy cutoff of 30 Ry and charge density cutoff of 180 Ry. Integration over Brillouin zone was sampled with a Monkhorst-Pack scheme [17] with appropriate k point mesh and occupation numbers were smeared using Methfessel-Paxton scheme [18] with broadening of 0.03 Ry. The structure was relaxed to minimize energy.

III. RESULTS AND DISCUSSION

In the present study, the cubic unit cell of Magnesium phosphide was first simulated using “Avogadro” [19] taking the X-ray diffraction data published by Passerini, L.[20]. Later, atomic positions of the simulated structure have been used in the plane wave self consistent field calculations.

The structure was relaxed and the values of the unit cell parameters are; a=b=c=5.92Å, α=β= γ=90^o. “scf” calculation was done using the program 'pw.x' of Quantum espresso. Completely relaxed structure of the unit cell was visualized using the program “XcrysDen”[21] and the structure of unit cell of Magnesium phosphide as seen along Z-axis has been shown in Figure 1.

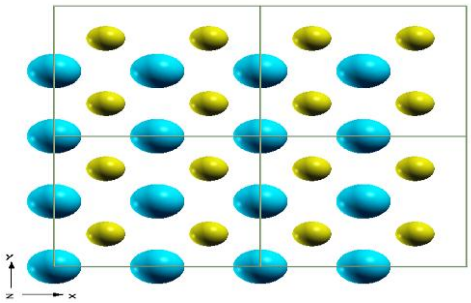

Fig. 1 Structure of four unit cells of Magnesium phosphide crystal as seen along Z-axis

A. Edos Calculation

Electron Density of States (EDOS) has been computed in Magnesium phosphideusing Electronic structure calculation code of Quantum espresso. EDOS in Magnesium phosphide has been shown in Figure 2. As it can be seen from the figure 2, the material shows semiconducting nature with a band gap of 0.5 eV.

Band gap in case of Azobenzene has been found to be 0.67eV [22]. A Band gap of 0.74eV has been observed in case of 4-Chloro-Phenyl-Benzamide [23]. Gallium arsenide shows a band gap of 1.43eV and Germanium shows a band gap of 0.67eV. Indium nitride, Gallium antimonide and Gallium arsenide antimonide show the band gap of 0.7eV, 0.726 and 0.7 respectively [24,25].

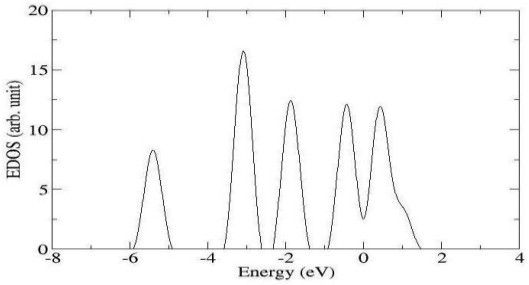

Fig. 2 Electron Density of States in Magnesium phosphide crystal

B. Dielectric Constant, Polarizabilityand Phonon Modes

Dielectric constant has been computed in case of Magnesium phosphide. The value of dielectric constant in Magnesium phosphide comes out to be 51.9 along all the three axes. Polarizability of Magnesium phosphide has also been estimated and it comes out to be 46.7 $(Å)^3$ along all the three axes. Phonon modes at gamma point have also been calculated in the material and they range from 0 cm^{-1} to 452 cm^{-1}.

IV. CONCLUSION

The EDOS calculation shows that the Magnesium phosphide shows semiconducting nature with a band gap of 0.5 eV. The material shows dielectric constant value of 51.9 along all the three axes. The polarizability values are found to be 46.7 $(Å)^3$ along all the three axes. Phonon modes at gamma point in the material range isfrom 0 cm^{-1} to 452 cm^{-1}.

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