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GGA + U Study of the Optical Properties of α-BeH_2

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Abstract

The optical properties of α-BeH_2 in an Orthorhombic crystal structure with the space group (Ibam) are investigated. We have calculated the optical properties including dielelectric function, refractive index and extinction coefficient, using density functional approach. A theoretical explanation of the relationship between the dielectric function and other optical constants has been provided. Furthermore, the real and imaginary components of the dielectric function have been examined. The effects of the exchange-correlation potentials (GGA and GGA + U) applied on this compound's absorption peaks and edges have also been investigated. It was found that using the GGA + U approximation caused the conduction band to shift, which in turn caused the initial absorption peak to shift.

Keywords

Dielectric Function, Optical Properties, GGA and GGA + U Approximations

1. Introduction

α-BeH_2 is a promising material due to its unique properties for its light-weight nature and high hydrogen content. The electronic band structure and structural property (lattice constant) of α-BeH_2 in an orthorhombic crystal system with space group (Ibam) have been computed, using density functional theory. To solve the Kohn-Sham equations, the full-potential linearized augmented plane wave (FP-LAPW) approach was applied.

At ambient temperature or high pressure, BeH_2 is metastable so that the hydrogen can easily be released without excess heat [1]. The computing mechanism for the observables was thoroughly examined. The results of the work were consistent with those earlier experiments. We have calculated the optical properties of α-BeH_2 using a density functional approach [2].

The Generalized Gradient Approximation (GGA) and the GGA + U approximation were used as exchange-correlation potentials, both with WIEN-2k code [3], the computing mechanism for the observables was thoroughly looked into. The results of the work were consistent with those of earlier experiments. Previous work had been done on the optical properties of α-BeH_2, using a density functional approach [4], making use of the computationally costly all-electron GW approximation.

Recently, the density functional approach has also been used to study the optical characteristics of this compound. There have been two ways used: the plane wave pseudo potential and the Bryoden-Fletcher Goldfarb-Shanno approach. However, the convergence of the second approach is not certain unless the function has a quadratic Taylor expansion near an optimum.

This work aims at exploring the optical properties of α-BeH_2 using full-potential linearized augmented plane wave (FP-LAPW) using WIEN-2k codes and GGA and GGA + U approximations, all within the context of density functional theory (DFT).

2. Theoretical Consideration

2.1. Dielectric Function

The optical properties are obtained from the dielectric function $\varepsilon(w)$, which is calculated by the density functional theory (DFT) approach. A three-dimensional tensor dependent on the symmetry of the crystal is the dielectric function.

Only the diagonal components of this tensor are non-zero for an orthorhombic unit cell. Direct calculation of the dielectric function is based on the Kohn-Sham energy eigen values, ε_k.

In the Random Phase Approximation (RPA), [5]: the function, ε_{ij}, can be expressed as

$$\begin{aligned}\varepsilon_{ij}(w) = \delta_{ij} - \frac{4\pi}{Vw^2}\sum\left(-\frac{\partial F(\varepsilon)}{\partial \varepsilon_{\varepsilon_{n,k}}}\right)P_{i;n,m,k}P_{j;n,m,k} \\ -\frac{4\pi}{Vw^2}\sum_{k,c,v}\frac{P_{i,c,v,k}P_{j,c,v,k}}{\left(\varepsilon_{c,k}-\varepsilon_{v,k}-w\right)\left(\varepsilon_{c,k}-\varepsilon_{v,k}\right)^2}\end{aligned} \quad (1)$$

where $F(\varepsilon)$ is a Fermi-Dirac distribution function, V is the unit cell volume, and n, m, and k, are momentum matrix elements between the bands n and m for the crystal's point k.

$$F(\varepsilon) = \frac{1}{\exp\left(\frac{\varepsilon - F_K}{K_B}\right)+1} \quad (2)$$

where K_B is Boltzmann constant.

2.2. Optical Properties

2.2.1. Imaginary and Real Parts of the Dielectric Function

The optical characteristics of α-BeH_2 are determined by computing the imaginary part of the dielectric function.

With momentum matrix elements, the imaginary component, $\varepsilon_2(w)$, of the dielectric function can be computed [6].

The appropriate eigen-function of every occupied and unoccupied states contribute to these matrix components [7]. The real component $\varepsilon_1(w)$ can be obtained from the imaginary part $\varepsilon_2(w)$ of the dielectric function by applying the Kronig-Kramers connection, [7].

The real part of the dielectric function accounts for refraction, but the imaginary part indicates actual transfers between the occupied and unoccupied states; thus, it controls attenuation. Put in another way, the real component in optical processes stands for loss and scattering.

2.2.2. Refractive Index and Extinction Coefficient

Owing to their shared physical origin, the refractive index and the extinction coefficient are closely associated.

Both the extinction coefficient and the refractive index, are tensors that are represented as [5]:

$$n_{ii}(w)=\sqrt{\frac{\left|\varepsilon_{ii}(w)\right|+\operatorname{Re}\varepsilon_{ii}(w)}{2}} \tag{3}$$

and

$$k_{ii}(w)=\sqrt{\frac{\left|\varepsilon_{ii}(w)\right|-\operatorname{Re}\varepsilon_{ii}(w)}{2}} \tag{4}$$

where $n_{ii}(w)$ is the refractive index and $k_{ii}(w)$ the extinction coefficient.

2.2.3. Reflectivity and Absorption Coefficient

Specifically, $n_{ii}(w)$ and $k_{ii}(w)$ cannot be measured in optical experiments. The quantitative quantities are the reflectance, $R_{ii}(w)$, and the absorption coefficient, $A_{ii}(w)$. It has been shown in the electromagnetic literature that these quantities can be expressed as

$$R_{ii}(w)=\frac{\left(n_{ii}(w)-1\right)^2+k_{ii}^2(w)}{\left(n_{ii}(w)+1\right)^2+k_{ii}^2(w)} \tag{5}$$

$$A_{ii}(w)=\frac{2wk_{ii}(w)}{c} \tag{6}$$

And we have estimated the dielectric function of α-BeH_2, which describes itsoptical characteristics and is the fundamental quantity associated with its electric structure. The predicted absorption edge of the compound was found to be 4 eV. When the GGA + U functional is applied, the conduction band moves, which causes the initial absorption peak to shift.

3. Computational Methods

The optical characteristics of α-BeH_2 were calculated within the context of density functional theory using a self-scheme that was created by applying the

FP-LAPW approach to solve the Kohn-Sham problem, [2]. In this method, computations were done, and, the details of these computations are presented in Electronic and Structural Properties of α-BeH_2, using GGA and GGA + U. GGA and GGA + U functional by WIEN-2k codes were also employed [3].

4. Results and Discussions

The calculated complex dielectric function for α-BeH_2 is illustrated in **Figure 1**.

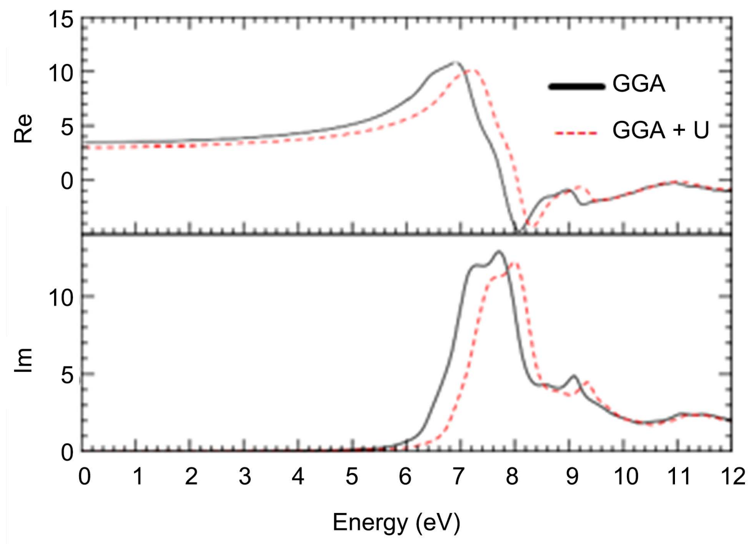

Figure 1. Real and imaginary parts of the dielectric function of α-BeH_2.

In **Figure 1**, the real and the imaginary parts of the dielectric function have been indicated.

The GGA calculation is shown by the solid lines, while the GGA + U computations are shown by the dotted lines.

The use of the GGA + U function was shown to result in a change in the conduction band, which shifted the initial absorption peak.

The absorption peak shifted as a result of the band gap correction, with an approximate absorption edge of 4 eV.

5. Conclusion

We have estimated the dielectric function of α-BeH_2, which describes its optical characteristics and is the fundamental quantity associated with its electric structure. The predicted absorption edge of the compound was found to be 4 eV. When the GGA + U functional is applied, the conduction band moves, which causes the initial absorption peak to shift.

Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

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