Research Article

Electronic and optical properties of $ZnCl_4H_2Me_2biim$ Polymeric Complexes (DFT study)

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The composition of zinc chloride and Me_2biim (Me_2biim = N, N′-dimethyl-2,2-′-biimidazole) gave the noncoordinated $ZnCl_4H_2Me_2biim$ polymeric complexes. In this article, the electronic and optical properties of $ZnCl_4H_2Me_2biim$ using density functional theory (DFT) and the Quantum espresso code have been investigated. The electronic band structure results showed that this material is a semiconductor with a direct band gap. The optical results showed that the highest static refractive index corresponds to the case where the light was applied to the material along the x-axis. According to the imaginary part of the dielectric function, the optical gap along the y-axis has the highest value. These results are in agreement with the electronic band structure results. The absorption graph showed that the highest absorption is in the UV region, and the lowest is in the IR region.

Keywords: DFT, $ZnCl_4H_2Me_2biim$, Optical properties, Electrical properties

Introduction

Today, cancerous tumors kill many people and cause many problems for many families. Millions of cells in our body go through a life cycle. They reproduce and replenish themselves by dying or becoming disabled, usually without problems. But sometimes, things don't go well. Instead of getting rid of old cells or cells that have been damaged, they begin to divide rapidly and make abnormal copies of themselves over and over again [1-3].

Finally, they form a mass or tumor, which can be benign or malignant. A tumor is a mass or group of abnormal cells that form in the body and are not necessarily cancerous. Many are benign (non-cancerous) and can occur throughout the body. They can affect bone, skin, tissues, glands, and organs [4-6].

Tumors vary in size depending on their type, from a small nodule to a large mass, appearing almost anywhere in the body. Benign tumors are not cancerous. They either fail to expand or grow, or they grow very slowly. If the doctor removes them, they generally do not come back. Most of them are not harmful and are unlikely to affect other body parts. However, if they press on nerves or blood vessels or cause an overproduction of hormones, such as in the endocrine system, they can cause pain or other problems. Malignant tumors are cancerous. They develop when cells grow uncontrollably. If the cells grow and spread, the disease can be life-threatening. Malignant tumors can grow rapidly and spread to other parts of the body through metastasis. Cancer cells that move to other parts of the body are the same as primary cells, but they can invade other organs. For example, if lung cancer spreads to the liver, the liver cancer cells are the same as the lung cancer cells [7-12]. Chemotherapy is often used to treat cancer; in some cases, drugs are used as chemotherapy drugs. Preparing cancer medicine is sometimes challenging and has obstacles. In the case of cancer, there is no need to use cancer drugs, and the patient can return to health only with surgery and other drugs [13, 14]. Using polymer materials is very effective in treating and eliminating them [15-17]. One of the polymer materials used in this field is bimidazole ($C_6H_6N_4$). By adding zinc chloride ($ZnCl_2$) to this material, a crys-

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talline polymer composite is formed that has unique properties. In this work, according to the first principles calculation, the electronic and optical properties are studied for $ZnCl_4H_2Me_2$biim polymeric complexes.

Computational details

QE (Quantum Espresso) computing code has been used to simulate $ZnCl_4H_2Me_2$biim polymeric complexes and obtain their physical properties [18]. To consider the interactions in the electron-many body system, the generalized gradient approximation (GGA) of Perdew–Burke–Ernzerhof (PBE) has been used for the exchange-correlation energy functional [19]. An energy cut-off of 350 eV and 12 times higher charge density energy cut-offs were used to simulate structural, electronic, and phonon properties. To stop the calculations and place the boundary, the energy selfconsistency limit for convergence was considered to be of order 10- 7 eV.
The limits of the integral were performed in the first Brillouin zone, and the variable of integration was performed in the k space. For k-point amounts, Monkhorst–Pack meshes and a matrix of 8×8×8 were used
[20].

Results and discussion

Structural optimization

To achieve the equilibrium lattice constant of $ZnCl_4H_2Me_2$biim material at different volumes, the energy of the system was calculated, and this calculation was continued until the most stable structure was obtained. The QE code and BFGS approximation have been used to optimize the geometry evaluation of Figure 1 shows the 2D and 3D views of this structure. The Bravais lattice of this material is monoclinic. The constants of the equilibrium lattice were obtained after optimizing the structure of values a=15.81, b=8.98, and c=11.47 Å.

Electronic properties

To investigate the electronic properties of the $ZnCl_4H_2Me_2$biim structure, the electronic band structure was calculated. The electronic band structure of these compounds with high symmetry points in the Brillouin zone (ΓYDX) is displayed in Figure 2. According to this figure, the upper part of the valence band and the end of the conduction band move upwards with a pseudo band gap of 0.13 eV. The results for the energy band structure of $ZnCl_4H_2Me_2$biim indicated that this compound is semiconducting with a direct energy band gap. In Figure 2, the Fermi level is located at 0 eV, and sulfur p orbitals contribute most to the valence level between -0.25 eV to -0.1 eV. As well, both Cl (p orbitals) and Zn (d orbitals) relatively dominate the conduction level. Also, the lowest and higher valence bands of electronic conductor structures are related to C-p and M-d, respectively. As shown in this figure, the $ZnCl_4H_2Me_2$biim structure is a direct band gap semiconductor with the valence band maximum (VBM) and the conduction band minimum (CBM) at the Γ point.

Optical properties

To find the dielectric constant of a material, the real and imaginary parts of the dielectric function must be calculated. Figure 3 shows the real part of the dielectric function (RPDF) for $ZnCl_4H_2Me_2$biim polymeric

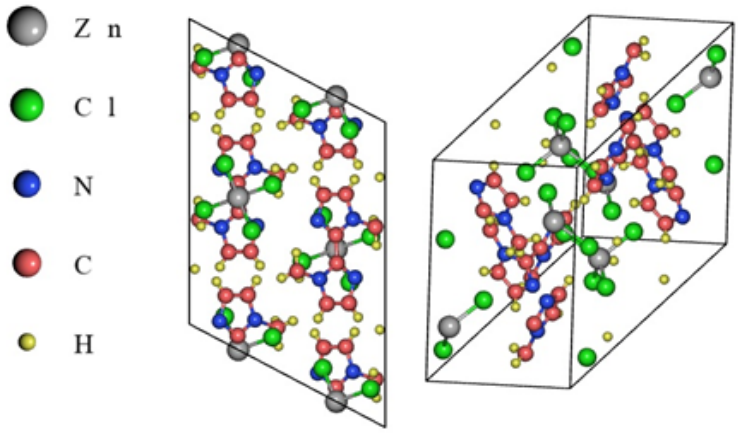

Figure. 1. 2D and 3D view of $ZnCl_4H_2Me_2$biim structure.

complexes from energy 0 to 10 eV. Considering that the light is applied in three directions (x, y, and z) the dielectric constant is calculated in these three directions. In the RPDF diagram, where the energy is zero, it represents the static dielectric constant ε(0). For three directions of light radiation (x, y, and z), the dielectric constant is 2.83, 2.23, and 2.53, respectively.

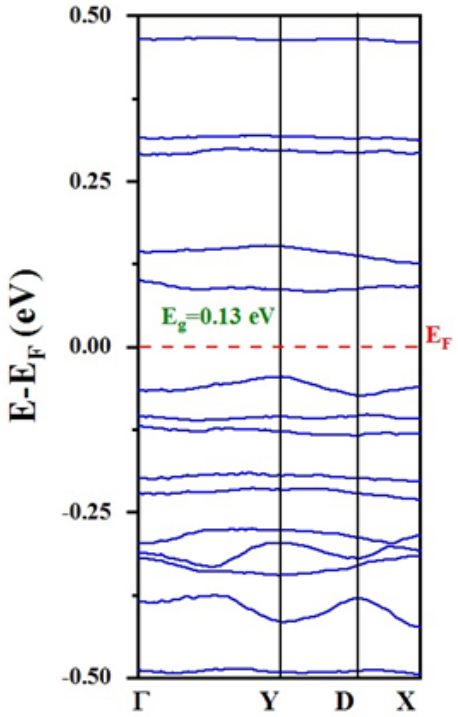

Figure.2. Calculated band structure of $ZnCl_4H_2Me_2$biim Polymeric Complexes.

The graphs of the imaginary part of the dielectric function (IPDF) for $ZnCl_4H_2Me_2$biim polymeric complexes are shown in Figure 4. The highest amount of IPDF occurs along the x, y, and z directions at energies of
4.76, 6.04, and 6.05 eV respectively. By the way, ε2x has the largest amount. The ε_2 values of the three directions have different behavior because of the different optical gaps. The amount of optical gap in $ZnCl_4H_2Me_2$biim in the x, y, and z directions is 0.07, 0.41, and
0.17 eV, respectively.

To investigate the optical properties of $ZnCl_4H_2Me_2$biim polymeric complexes more precisely, absorption A(ω) and reflectivity R(ω) spectra were calculated using the real ε1 and imaginary ε2 parts of the dielectric function. These quantities in the energy Figs. 5 and 6.

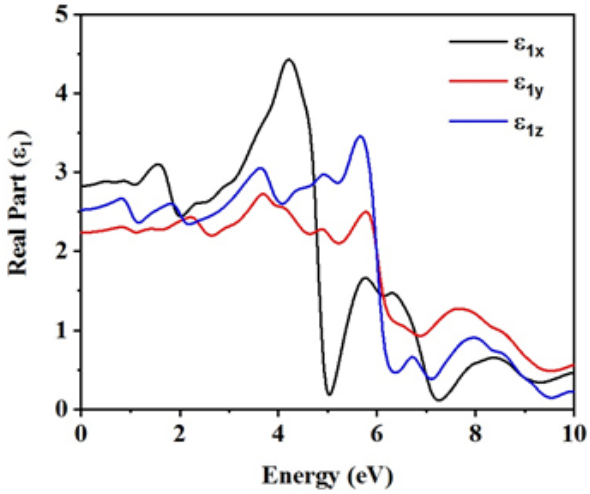

Figure. 3.The real part of the dielectric function of $ZnCl_4H_2Me_2$biim Polymeric Complexes.

Figs. 3 and 5 show that the main peaks in ε1 and R charts almost match each other. Also, the reflectivity percentage increases at energies higher than 4 eV. The value of the reflectivity percentage in the x direction is

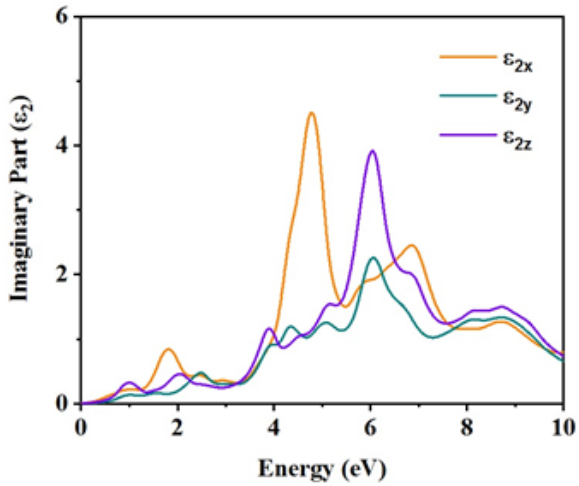

Figure.4. The imaginary part of the dielectric function of $ZnCl_4H_2Me_2$biim Polymeric Complexes

higher than in the y and z directions, as seen in Figure 5. The amount of light reflection for these materials in the x, y, and z directions is about 6, 3, and 5%, respectively. By applying light to the system, inter-band transitions occur for occupied and empty electronic states. Inter-band transitions occur due to the application of light at these energies. Figure 6 shows the absorption spectrum A(ω) of monolayers. Considering that the absorption according to the relation A(ω)=2k(ω)E/ħc is obtained from the extinction coefficient k(ω) (the

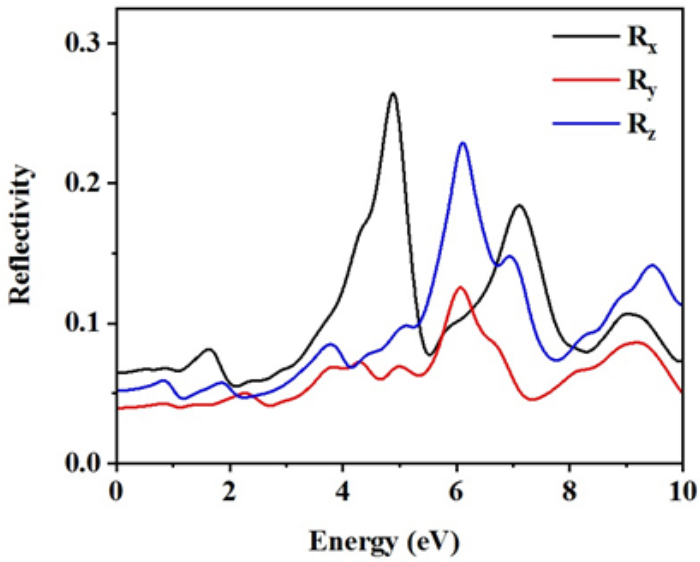

Figure. 5. The reflectivity diagram of $ZnCl_4H_2Me_2$biim Polymeric Complexes

imaginary part of the refractive index), the graphs of IPDF and A(ω) are similar [21]. According to Figure 6, the states with more occupied electrons have stronger and sharper peaks than the occupied states with fewer electrons. The energy degeneracy of the bands also has an effect in this case. In optical devices and solar cells, more materials are used that absorb light well.

According to Figure 6, the highest absorption of light in $ZnCl_4H_2Me_2$biim polymeric complexes is related to the ultraviolet region.

Conclusions

$ZnCl_4H_2Me_2$biim polymeric complexes were simulated using density functional theory and QE code. Electronic investigations showed that this compound is a semiconductor. The results of the optical properties showed that the x direction has the maximum refractive index and the smallest band gap. Also, the amount of light absorption and percentage of reflectance in the infrared, visible, and ultraviolet regions was calculated.

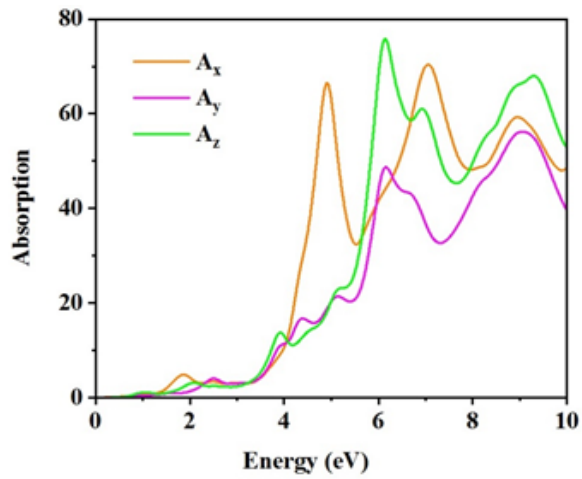

Figure. 6. The absorption diagram of $ZnCl_4H_2Me_2$biim Polymeric Complexes.

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