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Opto-Electronic Properties of Li_2C_2 Polymorphs

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Article Info

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Abstract

The electronic and optical properties of Li_2C_2 in different structural phases are studied in the frame work of density functional theory. Full potential linearized augmented plane waves plus local orbitals (FP-LAPW+lo) method is applied within the Engel-Voskogeneralized gradient approximation. The compound is metallic in *Bmmb* phase, while insulating in *Immm* and $I2_1$ 3 phases. The calculated bandgaps are in close agreement with the previous predictions. The two phases *Immm* $I2_1$ 3 and show a high dielectric function and optical conductivity in the UV range and are therefore suitable to be used in the fabrication of optoelectronic devices.

Keywords: Optical Conductivity; Fabrication; Optoelectronic devices; Bandgaps.

Introduction

Metal-intercalated graphite Li_2C_2 owing to its unique physical and chemical properties have been of scientific [1-3] and technological interest in the recent years. In a recent experimental study, the *Immm* phase has been reported to be the thermodynamically stable phase of Li_2C_2under ambient conditions [1]. A previous density functional theory (DFT) based study of lithium carbide (Li_2C_2) predicted a pressure induced structural phase transition from orthorhombic (*Immm*) at 0 GPa → hexagonal (*Bmmb*) at 5GPa → cubic ($I2_1$ 3)at 215GPa [4]. It was also reported that insulating ground state phase of Li_2C_2 with the band gap of 3.7eV turns metallic in the *Bmmb* phase, while $I2_1$ 3 phase is again insulating with a band gap of 2.7eV. This interesting shift in the band gap and electronic properties of Li_2C_2 in three phases perused us to investigate the optical properties of the same in the three phases which are not yet reported. Furthermore being high band gap insulator Li_2C_2 is predicted to have useful optical properties for potential applications in optoelectronic devices.

The present work is intended to investigate in detail the electronic and optical properties of Li_2C_2 in *Immm*, *Bmmb* and $I2_1$ 3 phases using full potential linearized augmented plane wave method plus local orbitals (FP-LAPW+lo) method

Computational Details

In order to investigate the structural, electronic and optical properties, the accurate FP-LAPW+lo method is used to solve Kohn–Sham equation within DFT [5] formulation as employed in the WIEN2k computer code [6]. The Engel-Voskogeneralized gradient approximation (EV GGA) [7] scheme is adopted to calculate the exchange-correlation energies. The charge density and potential were all expanded into two different basis sets. Inside the non-overlapping spheres surrounding the atomic sites (muffin-tin (MT) spheres), the potential was expanded into spherical harmonics with l_{max} = 10, while in the remaining (interstitial) regions the potential was expanded as plane waves. A plane wave cut off of $K_{max} = 7/R_{MT}$ was used for the expansion of the wave function inside the interstitial regions;

where R_{MT} is the average radius of the MT spheres and K_{max} is the maximum value of the wave vector K = k+G.

Results and Discussion

The band structure (BS) and density of states (DOS) of Li_2C_2 are calculated and shown in figures 1 and 2, respectively. It is clear from the DOS profile that the top of the valence band and the bottom of the conduction band for '*Immm*' phase have a major contribution from hybridizations of 'p' and 'd' states of both 'Li' and 'C' atoms. Clearly, an indirect band gap of 4eV along 'N' to 'Γ' direction can be seen from the band structure profile shown in Fig. 2(a) for *Immm* phase.

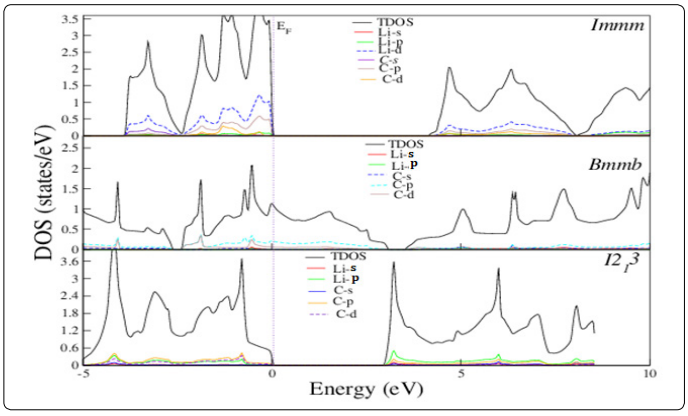

Figure 1. Total and partial DOS for Li_2C_2 for the three phases

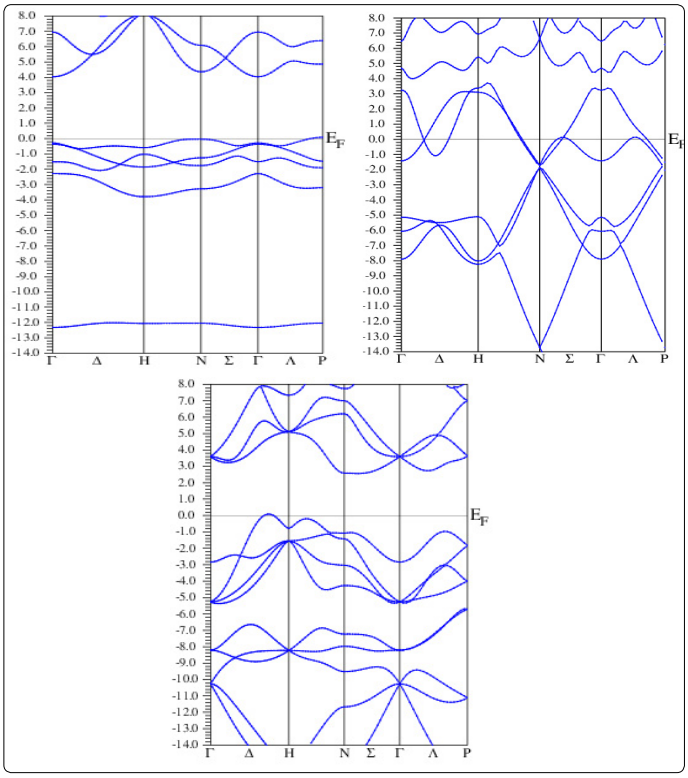

Figure 2. Bandstructure of Li_2C_2in (a) *Immm*, (b) *Bmmb* and (c) phases

For *Bmmb* phase's' and 'p'orbitals of carbon forms three σ and one π band lying in the energy range from '-14eV to -2.5eV'. Furthermore, anti-bonding π band of carbon hybridizes with's' and 'p' states of 'Li' and is dispersed from '-1eV' (below the Fermi-level) to 2eV (above the Fermi-level)is responsible for the metallic character of Li_2C_2 in *Immm* phase. The metallic character is due to sp^2 like hybrids in *Immm* phase. The cubic $I2_1$ 3 againacquires an insulating nature with a band gap of 2.9eV due to diamond like sp^3hybridization. Our calculated bandgap values for Li_2C_2 for *Immm* and $I2_1$ 3 are in close agreement with earlier studies [4].

Optical properties are calculated in terms of dielectric function, reflectivity and optical conductivity. Dielectric functions of the ternary alloys are calculated using the following equations [8, 9].

$$\varepsilon_2(\omega) = \frac{8}{2\pi\omega^2}\sum_{n\acute{n}}\int |P_{n\acute{n}}(k)|^2 \frac{dS_k}{\nabla\omega_{n\acute{n}}(k)}, \quad (1)$$

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi}P\int_0^{\infty}\frac{\acute{\omega}\varepsilon_2(\acute{\omega})}{\acute{\omega}^2-\omega^2}d\acute{\omega} \quad . \quad (2)$$

where $P_{n\acute{n}}(k)$ is the dipole matrix elements between initial and final states, S_k is an energy surface with constant value, $w_{n\acute{n}}(k)$ is the energy difference between two states and p in Eq. 2, denotes the principal part of the integral.

The optical conductivity $\sigma(\omega)$ and normal incident reflectivity $R(\omega)$, are calculated using the following equations

$$\sigma(\omega) = \frac{2W_{ev}\hbar\omega}{\vec{E}_0}, \quad (3)$$

$$R(\omega) = \left|\frac{\tilde{n}-1}{\tilde{n}+1}\right| = \frac{(n-1)^2+k^2}{(n+1)^2+k^2}, \quad (4)$$

Where, W_{ev} is transition probability per unit time.

Frequency dependent real and imaginary parts of the dielectric functions–($\varepsilon_1(\omega)$& $\varepsilon_2(\omega)$) of Li_2C_2 with electric field polarization along different crystallographic axis is shown in Fig.3. A considerable anisotropy in spectra of $\varepsilon_1(\omega)$ & $\varepsilon_2(\omega)$ for *Immm* and *Bmmb* is observed while $I2_1$ 3 being cubic phase show no anisotropy. For *Immm* phase real part of the dielectric function for all electric field polarizations starts with a value between 2 to 4 at zero frequency and remains smooth up to energy below 5eV and then shows abrupt peaks at around 5eV which is linked with the fundamental band gap. Furthermore, it can be seen that the relative optical anisotropy (i.e. the difference between values of $\varepsilon_1(\omega)$ for $\vec{E}//x$, $\vec{E}//y$ and $\vec{E}//z$ axis) increases with increase in energy. The dielectric function for $I2_1$ 3 remains high in the energy range 4 to 9eV. On the basis of a high dielectric coefficient in the high UV range this material is highly suitable for use in opto-electronic devices.

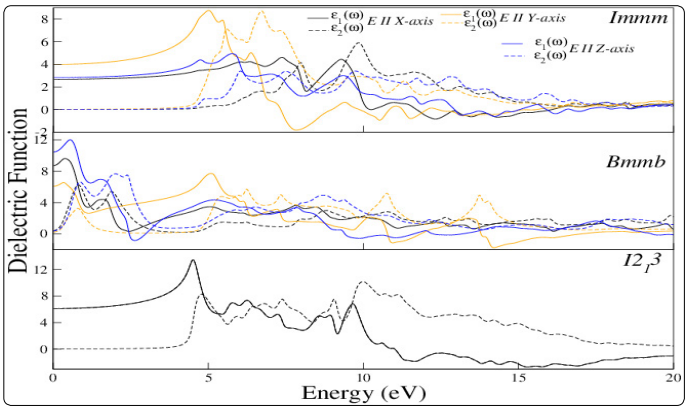

Figure 3. Real and imaginary ($\varepsilon_1(\omega)$& $\varepsilon_2(\omega)$) parts of the dielectric function for Li_2C_2 as a function of energy.

Reflectivity and optical conductivity of the compound in different phases is also studied. The reflectivity spectra are shown in Fig. 4. Reflectivity spectra of Li_2C_2 show different behaviour for *Immm* and $I2_1$ 3 phases i.e. the reflectivity is maximum at about 5eV for *Immm* phase and keeps on decreasing with increase in energy on the other hand reflectivity for $I2_1$ 3 phase is small at low energy, keep increasing and attains maximum value at 23eV energy. The optical conductivity spectra are shown in Fig. 5. Optical conductivity of Li_2C_2 for *Immm* and $I2_1$ 3 phases remain high in the energy range '5 to 15 eV'. It may further be noted that the relative anisotropy for reflectivity and optical conductivity spectra increase with energy.

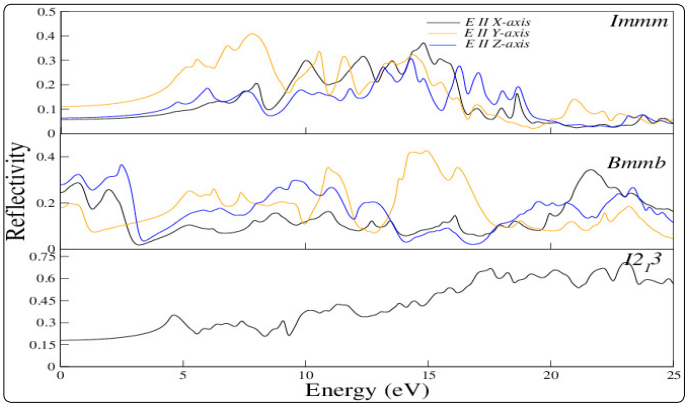

Figure 4. Spectra of Reflectivity of Li_2C_2as a function of energy

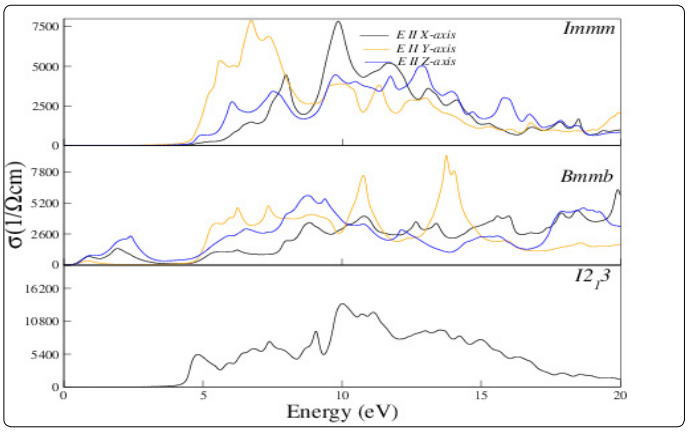

Figure 5. Spectra of Optical conductivity for Li_2C_2

Conclusions

In summary, electronic and optical properties of Li_2C_2 are calculated using FPLAPW within DFT. *Immm* and $I2_1$ 3 phases show insulating behaviour and *Bmmb* phase have metallic characteristics. The two phases *Immm* and $I2_1$ 3 show high dielectric function and optical conductivity in the high UV range and are therefore suitable to be used in the fabrication of optoelectronic devices.

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