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The effect of fluorine doping on the improvement of optical properties of lithium oxide

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Abstract – The field of optical properties encompasses a wide range of phenomena that offer insights into the interaction between light and matter. Understanding and manipulating these properties are essential for various technological applications, including optics, photonics, telecommunications, and advanced material design. In this research, the impact of fluorine doping on the optical properties of lithium oxide was explored using Density Functional Theory (DFT) calculations. DFT is a widely employed computational method in materials science, solid-state physics, and quantum chemistry for studying the electronic structure and properties of materials. It provides an efficient approach to calculate optical properties, facilitating predictions without extensive experimental measurements. The study involves analyzing the real and imaginary parts of the dielectric function, as well as absorption, transmission, and reflection behaviors of the novel fluorine-doped lithium oxide configuration. The optical properties of both pristine and doped Li2O were examined, leading to a comprehensive understanding of the material's characteristics. The resulting spectra exhibited distinctive peaks and valleys, providing valuable insights into the material's energy levels and electronic structure. Doping lithium oxide with fluorine enhanced the absorption power from 140 to 190 in the UV range, making it a promising candidate for applications in optics, photonics, and UV light protection.

Keywords – Lithium Oxide, Optical Properties, Absorption, Fluorine, DFT

I. INTRODUCTION

Light is an electromagnetic wave with oscillating electric and magnetic fields. When light interacts with a material, it experiences various phenomena like absorption, reflection, refraction, scattering, and transmission. Understanding the optical properties of materials is vital in multiple fields such as physics, chemistry, materials science, engineering, and optics. Experimental techniques, theoretical models, and computational methods are employed to investigate and understand the optical properties of materials. Spectroscopy, ellipsometry, and microscopy techniques enable the measurement and analysis of absorption, reflectance, and transmission properties. Theoretical and computational approaches, such as density functional theory (DFT) and time-dependent DFT, allow the prediction and interpretation of optical properties based on the electronic structure and quantum mechanical calculations. Li_2O, also known as lithium oxide, is an insulating material that possesses a wide bandgap [1]. This wide bandgap property enables Li_2O to transmit visible light without undergoing significant absorption. In the case of Li_2O, doping can have a significant impact on its properties. Doping refers to the intentional introduction of impurities into a material to modify the properties [2]. Rezaee et al [3] reported that Lithium oxide with fluorine doping is a novel material and studied its physical properties in detail and showed doping

does not decrease its mechanical stability. Therefore, in this study, optical properties of $Li_{(2-x)}O_{(1-x)}F_x$ as an important physical property were investigated using Density Function Theory (DFT). studying optical properties is crucial for material characterization, device design, energy applications, biomedical technologies, communication systems, and fundamental research. It enables the development of innovative technologies and advances our understanding of the physical world. This article aims to investigate and analysis optical properties of $Li_{(2-x)}O_{(1-x)}F_x$ including dielectric function, absorption, reflection, and transition.

II. MATERIALS AND METHOD

The Density Functional Theory (DFT) calculations [4] for geometrical and optical properties were conducted using the Quantum ESPRESSO Package [5]. The Perdew-Burke-Ernzerhof (PBE) type parameterization within the Generalized Gradient Approximation (GGA) [6] was employed to account for the interaction energy between electrons, considering both exchange and correlation effects. The electronic structure calculations and geometry optimizations, including lattice constant determination and atomic positions, were performed iteratively by solving the Kohn-Sham equation [7]. Ultrasoft pseudopotentials were utilized to minimize the total energy during the calculations.

Figure 1 illustrate $Li_{(2-x)}O_{(1-x)}F_x$ structure where $x = \frac{\text{number of doped- Fluorine}}{\text{number of Oxygen in undoped structure}}$ [8].

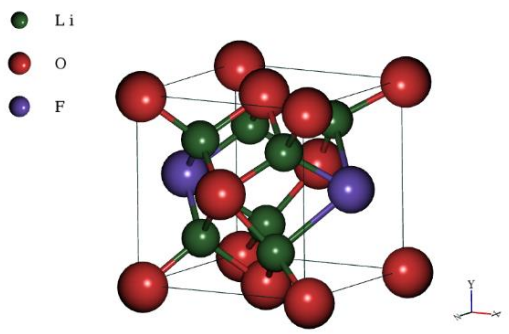

Fig1. configuration of $Li_{(2-x)}O_{(1-x)}F_x$ structure

Analysis The dielectric function is a complex quantity that characterizes how a material responds to an electric field at a specific frequency. It consists of a real part and an imaginary part. The real part describes a material's interaction with light without absorption, while the imaginary part relates to energy absorption due to electron transitions. using the formalism of Ehrenreich and Cohen, the dielectric function is determined as follows [9]:

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\,\varepsilon_2(\omega) \quad (1)$$

$$\varepsilon_2(\omega) = \frac{e^2 h}{\pi m^2 \omega^2} \sum_{v,c} \int_{BZ} |M_{cv}(K)|^2 \delta[\omega_{cv}(k) - \omega] d^3k \quad (2)$$

Where q, m, $M_{cv}(K)$ and $\omega_{cv}(k)$ are charge and mass of the electron, matrix elements for the transitions between the valence band and the conduction band and energy of excitement respectively.

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi} P \int_0^{\infty} \frac{\omega' \varepsilon_2(\omega')}{\omega'^2 - \omega^2} d\omega' \quad (3)$$

Where P represents the main value of the integral.

By analyzing the dielectric function across the electromagnetic spectrum, various optical properties such as absorption, conductivity, reflection, transmission, and refractive index can be theoretically understood, providing insights into light-matter interactions. All optical properties were done in 0-40 energy range.

III. RESULS AND DISCUSSION

As mentioned earlier, the dielectric function provides insights into how a material's optical response depends on the wavelength or energy of incident light. Figure 2 illustrates the optical conductivity and dielectric function of pristine Li_2O, which aligns well with previous researches [9].

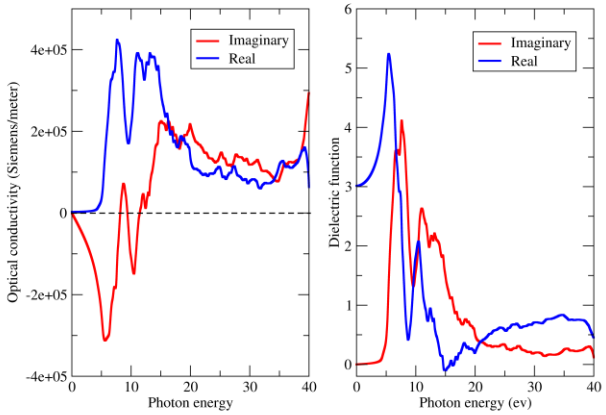

Fig1. a- Optical conductivity b- Dielectric function of Li_2O

In this study, the impact of fluorine doping on the optical properties of Li_2O was investigated. Figure 3 displays the calculated real and imaginary parts of the dielectric function. The real part, ε_1, describes the material's ability to interact with incident light without significant absorption. It characterizes the refractive index, which determines how light propagates through the material and governs phenomena like reflection, transmission, and refraction. The imaginary part, ε_2, of the dielectric function is related to the absorption of energy by the material. It arises from interband transitions of electrons between the valence band (VB) and the conduction band (CB). This part of the dielectric function signifies the energy loss or attenuation of light due to the absorption process [10].

A notable observation from Figures 2 and 3 is the absence of absorption peaks below 5 eV in Li_2O and $Li_{(2-x)}O_{(1-x)}F_x$. From figure3 the first sharp peak occurs at 7 eV, followed by peaks at 12 eV and 13 eV. Some negligible peaks are observed from 17 eV to 40 eV energies values.

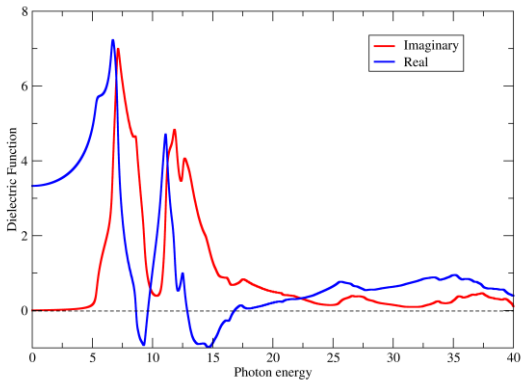

Fig3. Imaginary and real part of dielectric function for $Li_{(2-x)}O_{(1-x)}F_x$

Additional optical properties of $Li_{(2-x)}O_{(1-x)}F_x$ are demonstrated in Figures 4. Figure 4a illustrates the absorption within the energy range of 5 eV to 17 eV. Beyond this energy range, the absorption gradually decreases, as depicted in the absorption plot, which shows several small peaks. Figures 4b, 4c, and 4d display the reflectivity, transmission, and extinction spectra, respectively. The reflection spectrum provides insights into the smoothness of the surface, while the transmission spectrum clearly demonstrates higher transmission at minimal absorption [11]. It is evident from the figures that strong absorption appears in the ultraviolet range with amount of 190. These results indicate that fluorine doping in the Li_2O structure increased the absorption power in UV range. As a result, this new material shows promise for the advancement of optoelectronic devices used in energy conversion and protection against UV radiation.

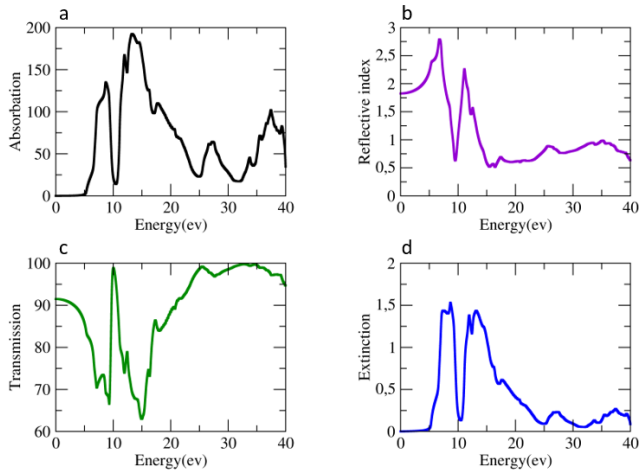

Fig4. optical properties for $Li_{(2-x)}O_{(1-x)}F_x$ with energy as a, absorption b, reflection, transmission and d, extinction.

IV. CONCLUSION

The exploration of optical properties offers numerous advantages in diverse fields. It provides fundamental insights into the interaction between light and matter, aids in the creation of advanced optical devices, contributes to scientific knowledge, enables the development of customized materials, and improves imaging and visualization capabilities. This research focused on studying the impact of fluorine doping on the optical properties of Li_2O. Doping refers to the deliberate introduction of impurities into a material to modify its properties. In this case, Fluorine doping can modify the optical behavior of materials, leading to changes in properties such as absorption coefficients or transmission characteristics. The findings revealed that fluorine doping can enhance the absorption coefficient which can increase from 140 to 190. This increase in the absorption coefficient is significant because it indicates that fluorine-doped Li_2O can efficiently absorb more light compared to undoped Li_2O. This property opens up potential applications for this material in the development of optoelectronic devices, particularly those involved in energy conversion and UV-light protection, especially in short-wavelength applications.

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