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Optical Properties of Lithium Tantalate (LiTaO3) by Doping With Different Material Performance

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Abstract— Organic electronics and specifically organic light-emitting diode (OLED) devices based on organic semiconductor materials economically viable large-area flexible application. Opto-electronic properties of pristine lithium tantalate (LiTa$O3$) and metal doped lithium tantalate (LiTa$O3$) are calculated using DFT computations. The results suggest that the absorption coefficient edges for metal doped structures move towards the visible range or from higher energy to lower energy (red-region) of the spectrum as compared with pristine lithium tantalite (LiTa$O3$). For pristine lithium tantalate (LiTa$O3$), higher absorption is observed in ultraviolet (UV) region (~ 380 nm) whereas, for metal doped structures like Cu (3.33 %) and Ag (3.33 %) the absorption is majorly observed in visible region (~ 380 nm-780 nm) and for other metal doped structures like Cu (6.67 %), Ag (6.67 %), and Al (6.67 %), absorption slightly increases in visible range of the spectrum. The reduction in energy bandgap is also observed for all metal doped structures, which is favourable for photovoltaic applications. Refractive index and dielectric constant calculations show that absorption is in trend with dielectric constant. Metal doped structures show enhanced absorption in visible range which makes LiTaO3 a promising material for solar cells and other photovoltaic applications..

Keywords— *Visual Light Communication (VLC), Density Function Theory (DFT), Ultraviolet (UV), Lithium Niobate (LN), Stoichiometric Lithium Tantalate (SLT), Atomistic Toolkit (ATK), Generalized Gradient Approximation GGA)*

I. INTRODUCTION

Lithium Tantalate (LITaO3) is similar to Lithium Niobate (LiNbO3). Both are grown by the Czochralski method which yields large, high quality single crystal. Lithium Tantalate possesses unique electro-optical, acoustic, piezoelectric, and pyroelectric properties, which makes it attractive for numerous applications including opto-electric modulators, pyroelectric detectors, piezoelectric transducer and sensors.The mineral CaTi$O3$ (calcium titanate) was discovered by geologist Gustav Rose in 1963 and later the mineral was given the name perovskite. Perovskite is a term given to any chemical of form AB$C3$, in which the C ions surround the B ion. The perovskite materials are capable of a wide range of electrical characteristics and solid-state behaviours, such as insulating, semiconducting, metallic, and super conducting.

As a result, these compounds are used in a wide range of applications and are particularly intriguing for research. A range of optical, magnetic, and electrical properties are also present in these materials.

Due to their remarkable photorefractive qualities, doped lithium tantalum (LiTa$O3$, LT) crystals are interesting for use in piezoelectric, electro-optic, surface acoustic wave, waveguide, and nonlinear optical systems.Transition metal or rare earth ions are used for doping crystals for changing the efficiency, sensitivity, speed, and spectral response of the photo refractive effect. Numerous researches on LiTa$O3$ crystals doped with different elements, including Fe, Ce, Zn, Cr, Tm, Ho, and others have been performed. For industrial operations, holographic storage media has been chosen.

1.1 Density Function Theory (DFT)

First-principal calculations by using density functional theory (DFT) can efficiently calculate the ground state properties of any material. DFT calculations are used in the present study to optimize the geometry and calculate the properties of pristine LiTa$O3$ and all metal-doped structures. All the calculations were performed on atomistic toolkit (ATK) [30]. To approximate the exchange-correlation energy of any system, generalized gradient approximation (GGA) with Perdew-Burke-

Ernzerhofer (PBE) is used in DFT calculations [31] [32]. For geometry relaxation of pristine LiTa$O3$ and all metal doped LiTa$O3$ structures, LBFGS algorithm is used with force tolerance 0.04 eV/Å.A 9x9x1 k-point sampling is used in x-y-z direction with mesh cut-off density 150 Hartree by utilizing Monkhorst-Packk scheme [33]. Broadening is set to 0.05eV for consideration of thermal effects on optical properties. GGA was used to capture many body interactions in the calculation of electronic properties [34-36]. To calculate optical properties of all the structures, DFT with meta-GGA is used with 9 x 9x 1 k-point Brillouin zone sampling.It is proposed that the efficiencies of perovskite solar cells have advanced from single digits to a certified 23.3% in less than a decade of concerted worldwide effort. The soft nature of the hybrid perovskite materials, their stability against moisture, heat, oxygen and electric field will continue to be an area of intense activity. Recent advances on this front are encouraging, including operating stability of 1,000 hours under 1 sun illumination. Integrated encapsulation strategies have increased stability against external humidity and heat. Compared with solar cells, though, LEDs still rely on charge injection rather than extraction; and also see higher fields in light of the > 3 V often used to drive devices. This indicates promise for perovskite lasers with reduced heat generation under the required high-power continuous-wave optical pumping.

1.2Lithium Niobate (LN)

Lithium niobate (LiNb$O3 - LN$) are well-known materials that can be used in ferroelectric, piezoelectric, acoustic-optical, electro-optical, and nonlinear optical applications. However, it is challenging to build many millimetre-thick devices due to the strong coercive field (21 kV/mm) for polarisation reversal in ordinary congruent LiTa$O3$ crystal.Stoichiometric Lithium tantalate crystals (SLT) that are nearly stoichiometric have recently become commercially available. By shifting the crystal composition towards stoichiometry, coercive field can be reduced. This is necessary in order to build thick quasi-phase matched (QPM) devices for high-power applications. Additionally, SLT outperforms stoichiometric LiNb$O3$ (SLN) in several other ways, a bigger damage threshold, a broader transmission range, less green-induced infrared absorption, a better thermal conductivity, and a lower thermal-optical coefficient.

1.3 Atomistic Toolkit(ATK)

All the calculations were performed on atomistic toolkit (ATK). To approximate the exchange-correlation energy of any system, generalized gradient approximation (GGA) with Perdew-Burke-Ernzerhofer (PBE) is used in DFT calculations. For geometry relaxation of pristine LiTa$O3$ and all metal doped LiTa$O3$ structures, LBFGS algorithm is used with force tolerance 0.04 eV/Å.A 9x9x1 k-point sampling is used in x-y-z direction with mesh cut-off density 150 Hartree by utilizing Monkhorst-Packk scheme. Broadening is set to 0.05eV for consideration of thermal effects on optical properties. GGA was used to capture many body interactions in the calculation of electronic properties. To calculate optical properties of all the structures, DFT with meta-GGA is used with 9 x 9x 1 k-point Brillouin zone sampling.

The soft nature of the hybrid perovskite materials, their stability against moisture, heat, oxygen and electric field will continue to be an area of intense activity. Recent advances on this front are encouraging, including operating stability of 1,000 hours under 1 sun illumination. It has been shown that the optical properties of LiNbO3 are enhanced significantly by doping of metal dopants (M = Au, Ag, Al, Cu, Fe, Mn, Mo and Ni). Hence, it is envisaged that the metal doped LiNbO3 may find vital usage in photonic- and optoelectronics-based applications. Because of its enhanced absorption in visible region, it is envisaged that LiTa$O3$ can be used as an important material in photovoltaic applications

II. LITERATURE REVIEW

Raturi, A., Mittal, P. and Choudhary [1] It is found that the electronic and optical properties of pristine and M-doped LiNbO3 (M = Au, Ag, Al, Cu, Fe, Mn, Mo and Ni) are computed by using DFT-based simulations. And the calculated bandgap of the M-LiNbO3 that the metal doping is helpful to improve the optoelectronic performance of LiNbO3 owing to the narrowing of bandgap. In this study, the pristine LiNbO3 is doped with the metals (M = Fe, Mn, Mo and Ni) along with a superior class of metal, i.e., plasmonic metal (M = Au, Ag, Al and Cu). In the M-LiNbO3 (M = Au, Ag, Al and Cu), due to surface plasmonic resonance, the optical absorption is extraordinarily enhanced in the visible region. Among the plasmonic dopants, the enhancement is very much significant for the dopants Au and Ag, due to their extraordinary plasmonic properties. The other plasmonic dopants Cu and Al also showed an enhanced absorption in the visible region. However, for the other metal-dopants like Ni, Fe, Mn and Mo, a slightly increased absorption in the visible region along with red-shift is observed. It has been shown that the optical properties of LiNbO3 are enhanced significantly by doping of metal dopants (M = Au, Ag, Al, Cu, Fe, Mn, Mo and Ni). Hence, it is envisaged that the metal doped LiNbO3 may find vital usage in photonic- and optoelectronics-based applications.

Quan, Li Na, P. Rand, Richard, et al[2] It is proposed that the efficiencies of perovskite solar cells have advanced from single digits to a certified 23.3% in less than a decade of concerted worldwide effort. The soft nature of the hybrid perovskite materials, their stability against moisture, heat, oxygen and electric field will continue to be an area of intense activity. Recent advances on this front are encouraging, including operating stability of 1,000 hours under 1 sun illumination. Integrated encapsulation strategies have increased stability against external humidity and heat. Compared with solar cells, though, LEDs still rely on charge injection rather than extraction; and also see higher fields in light of the > 3 V often used to drive

devices. This indicates promise for perovskite lasers with reduced heat generation under the required high-power continuous-wave optical pumping.

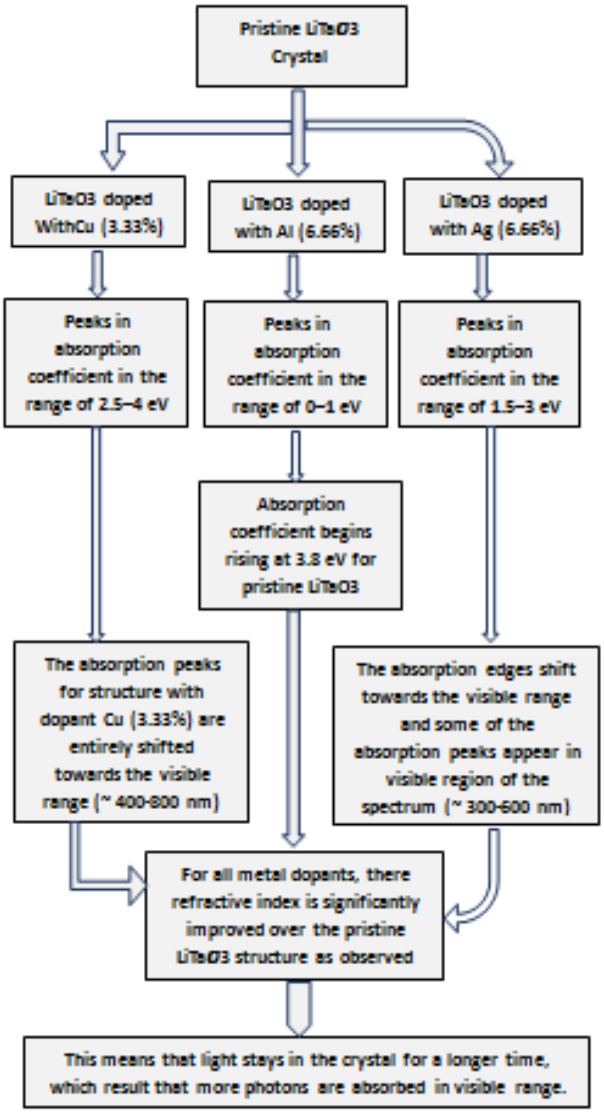
Thiele, Frederik, Felix Bruchet al [3] In this work we have presented an electro-optic polarisation converter at 0.8K in titanium in-diffused Lithium Niobate waveguides. We have demonstrated mutual compatibility between active electro-optic components for quantum photonics circuits and the operating conditions required for superconducting detectors. Under these conditions, we have shown a fibre-to-fibre coupling efficiency of 43% and a modulation depth of 23.6±3.3dB. Furthermore, we observed an increase in the modulation voltage from 12.7±0.1V to 19.2±2.1V, which suggests temperature dependence of the electro-optic coefficient in Lithium Niobate. This functionality shows that polarisation conversion is compatible with other low-temperature technologies required for integrated quantum photonics.

Al-Amri, Amal M., Bin Cheng,et al[4] In this work we proposed Lead free based halide perovskite material plays a crucial role due to its nontoxicity and excellent performance. Crucial parameters for champion device require the appropriate band gap, low background charge carrier density, low carrier effective mass, high absorption co-efficient and stronger stability at ambient atmosphere. Tin based halide perovskites have exhibited high power conversion efficiency up to date of 13% in single junction. Pb-based perovskite solar cells have outstanding optoelectronic properties, mass production of PSCs has been hindered due to their toxicity and poor stability.

Negi, Shubham, Poornimaet al [5] It is found that the effect of applying different structures on OLED devices is an important area of research that can helpto optimize device performance and quality for specific applications. Limited to the specific materials and layer structures used in the study, and may not be generalizable to other OLED materials and structures. With ongoing research and development, it is likely that further improvements in OLED performance and quality will be achieved, leading to new and innovative applications for this exciting technology.

III. METHODOLOGY

It is therefore of interest to study doped LiTaO3 structures. In the present study, electronic and optical properties of pristine lithium tantalate (LiTa$O3$) and substitutionally doped LiTa$O3$ with metal is like Al, Ag, and Cu are investigated. LiTa$O3$ crystal belongs to the family of ferroelectric oxide in view of its excellence in piezoelectric, electronic, pyroelectric, optical, and electrical properties. It has been observed that metal doped structures give better absorption in visible region in comparison with pristine LiTaO3which suggests it is a promising candidate in optoelectronics applications.
We can observe it with flow chart given below.



IV. RESULT AND ANALYSIS

Here we are using doped metals areCu, Al and Ag. First, we will discuss about the structure of LiTaO3. The Lithium Tantalate crystal's which is hexagonal unit cell made up of 30 atoms, in which Lithium atom are 6, 6 tantalum and 18 Oxygen atoms. After doping we can see that some host atoms are replaced by impurity or doped metals, this optimized structure is showing doped Lithium Tantalate. The pristine or doped structure is consisting of either 66.7% or 3.33% of Impurity atoms. Optimized structure with doping Cu and Al is respectively 6.67% and 3.33%.
Now we will go for computational part. We will calculate the energy band gap of Pristine LiTaO3 and after that metal doped LiTaO3. The below table. 1 is shows that the calculated lattice constant and energy bandgap (Ev).

Table 1. Lattice constant (a, b,c) and energy bandgap E(eV) of metal doped Lithium Tantalate (LT).

Metal Doped	Doping (%)	a(A)	b(A)	c(A)	E(eV)
Pristine LiTaO3	-	5.20	5.20	13.93	3.81
Ag-LiTaO3	3.33	5.27	5.24	13.89	2.47
Al-LiTaO3	6.67	5.19	5.19	13.89	3.69
Cu-LiTaO3	6.67	5.26	5.27	13.87	0.056
Cu-LiTaO3	3.33	5.21	5.20	13.96	1.46

We can Calculate the wavelength of different Metal-LiTaO3 from below equation the approximate wavelengths of doped Lithium Tantalate (LiTaO3).

$$\lambda = \frac{1.24}{E\ (eV)}$$

With different values of wavelength (λ), the observation coefficient of different M-LiTaO3 is mostly in visible region.It has been observed from the results, that the highest peaks in absorption coefficient occurs entirely in the UV region (absorption edge at ~ 325 nm) of the spectrum.

V. CONCLUSION AND FUTURE SCOPE

In this review paper, a study of the thermal response of Lithium tantalate for DFT-based calculations were used to determine the optical and electrical characteristics of pristine and metal (Al, Ag, Cu) doped LiTa$O3$ structures. For pristineLiTaO3 structure, absorption is observed in UV region, whereas for metal doped structures like Cu and Ag (3.33 %) absorption is observed in visible region (~ 400-800 nm). However, absorption for Ag, Cu, and Al (6.67%) slightly enhances in visible range of the spectrum in comparison with pristine LiTaO3. Measured bandgap for pristine LiTaO3is 3.81 eV, bandgap reduction in all metal doped structures is observed which results in enhanced absorption in the visible region of the spectrum. It has been shown that the optical properties of LiNbO3 are enhanced significantly by doping of metal dopants (M = Au, Ag, Al, Cu, Fe, Mn, Mo and Ni). Hence, it is envisaged that the metal doped LiNbO3 may find vital usage in photonic- and optoelectronics-based applications. Because of its enhanced absorption in visible region, it is envisaged that LiTa$O3$ can be used as an important material in photovoltaic applications.

Future Scope

- Lithium Tantalate (LiTaO3) has the property to convert the solar energy into electric energy so we can widely use as piezoelectricsensors.
- We can make pyroelectric materials with Lithium Tantalate (LiTaO3), which is used to measure the temperature.
- With the help of Arduino UNO programming, we can make Lithium Tantalate as Light Sensors, which can be used to monitor the light status in energy saving prototype.
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