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A Literature Survey- Optical Properties of Lithium Tantalate (LiTaO3) by Doping With Different Materials

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***Abstract*— This survey discusses about the 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 (LiTaO3) and metal doped lithium tantalate (LiTaO3) 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 (LiTaO3). For pristine lithium tantalate (LiTaO3), 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 CaTiO3 (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 ABC3, 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 (LiTaO3, 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 LiTaO3 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 chose.

II. LITERATURE SURVEY

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.

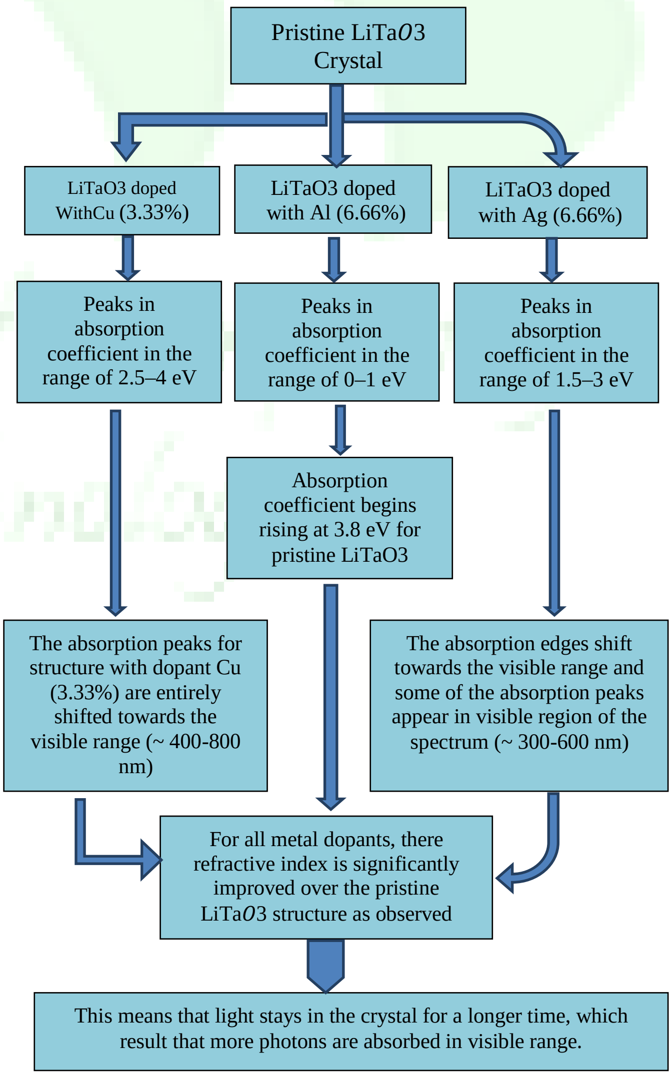
Al-Amri, Amal M., Bin Cheng,et al[4] In this work we proposed Lead free based halide perovskite material plays a crucial role due to its nontoxicity and excellent performance. Crucial parameters for champion device require the appropriate band gap, low background charge carrier density, low carrier effective 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. PROPOSED WORK

It is therefore of interest to study doped LiTaO3 structures. In the present study, electronic and optical properties of pristine lithium tantalate (LiTaO3) and substitutionally doped LiTaO3 with metal is like Al, Ag, and Cu are investigated. LiTaO3 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. EXPECTED OUTCOMES

Here we are using doped metals are Cu, Al and Ag. First, we will discuss about the structure of LiTaO3. The Lithium Tan talate 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 Tan talate. 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 band gap (Ev).

Table 1. Lattice constant (a, b,c) and energy band gap E(eV) of metal doped Lithium Tan talate (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

Here we can see the lattice constant of Pristine LiTaO3 and metal doped LiTaO3 are found same. For pristine and metal doped LiTaO3 the lattice constant are relaxed and optimized.

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.

IV.CONCLUSIONS AND FUTURE WORK

This means that light stays in the crystal for a longer time, which result that more photons are absorbed in visible range. used to determine the optical and electrical characteristics of pristine and metal (Al, Ag, Cu) doped LiTaO3 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 band gap for pristine LiTaO3is 3.81 eV, band gap 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 do pants (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 LiTaO3 can be used as an important material in photovoltaic applications.

FUTURE WORK

- 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.

REFERENCES

[1] Al-Amri, Amal M., Bin Cheng, and Jr-Hau He. "Perovskite methylammonium lead trihalide heterostructures: progress and challenges." IEEE Transactions on Nanotechnology 18 (2018): 1-12.

[2] Negi, Shubham, Poornima Mittal, and Brijesh Kumar. "Impact of different layers on performance of OLED." Microsystem Technologies 24, no. 12 (2018): 4981-4989.

[3] Raturi, A., Mittal, P. and Choudhary, S., Effect of metal doping on visible light absorption and optical properties of lithium niobate (LiNbO3) crystal: a first-principles calculation, Bulletin of Materials Science, vol. 44(3), pp.1-10, 2022.

[4] Thiele, Frederik, Felix Vom Bruch, Victor Quiring, Raimund Ricken, Harald Herrmann, Christof Eigner, Christine Silberhorn, and Tim J. Bartley. "Cryogenic electro-optic 20 polarisation conversion in titanium in-diffused lithium niobate waveguides." Optics Express 28, no. 20 (2020): 28961-28968.

[5] Negi, S., Mittal, P. and Kumar, B In-depth analysis of structures, materials, models, parameters, and applications of organic light-emitting diodes. Journal of Electronic Materials, 49(8), pp.4610-4636. (2015).

[6] Quan, Li Na, Barry P. Rand, Richard H. Friend, Subodh Gautam Mhaisalkar, Tae-Woo Lee, and Edward H. Sargent. "Perovskites for next-generation optical sources." Chemical reviews 119, no. 12 (2019): 7444-7477.

[7] Huang, He, Lakshminarayana Polavarapu, Jasmina A. Sichert, Andrei S. Susha, Alexander S. Urban, and Andrey L. Rogach. "Colloidal lead halide perovskite nanocrystals: synthesis, optical properties and applications." NPG Asia Materials 8, no. 11 (2016): e328-e328.

[8] Holm, Q. Sturzer, Y. Xu, and R. Weigel, Investigation of surface acoustic waves on LiNbO3, quartz, and LiTaO3 by laser probing, Microelectron Eng 31 (1996), 123–127.

[9] D.Ma,B.Wang,S.Fang,T.Zhang,R.Wang,andY. Wei, “Growth and studies of optical properties of double-doped in: Fe: Litao3 crystal,” Microwave and Optical Technology Letters, vol. 48, no. 11, pp. 2227–2230,2006.

[10] M.K. Kuneva, S.H. Tonchev, and P.A. Atanasov, Infrared spectra of proton-exchanged waveguides in LiNbO3 and LiTaO3, Mater Sci Eng B 118 (2005), 301–305. [27] Y.N. Korkishko, V.A. Fedorov, S.M. Kostritskii, A.N. Alkaev, E.I.Maslennikov, E.

[11] Huang,He, LakshminarayanaPolavarapu, Jasmina A. Sichert, Andrei S. Susha, Alexander S. Urban, and Andrey L. Rogach. "Colloidal lead halide perovskite nanocrystals: synthesis, optical properties and applications." NPG Asia Materials 8, no. 11 (2016): e328-e328.

[12] **Presa’s** P R and García M P F 2016 in Applications of molecular spectroscopy to current research in the chemical and biological sciences, Intech, 2016 32 https://doi.org/10. 5772/61896.

[13] Klein, R. S., G. E. Kugel, A. Maillard, K. Polgár, and A. Péter. "Absolute non-linear optical coefficients of LiNbO3 for near stoichiometric crystal compositions." Optical Materials 22, no. 2 (2003): 171-174.

[14] Abdi, F., M. D. Fontana, Michel Aillerie, and Patrice Bourson. "Coexistence of Li and Nb vacancies in the defect structure of pure LiNbO3 and its relationship to optical properties." Applied Physics A 83, no. 3 (2006): 427-434.

[15] Imbrock, J., S. Wavering, K. Buse, and E. Krätzig. "Non-volatile holographic storage in photorefractive lithium tantalate crystals with laser pulses." JOSA B 16, no. 9 (1999): 1392-1397.

[16] Hatanaka, Takaaki, Koichiro Nakamura, Tetsuo Taniuchi, Hiromasa Ito, Yasunori Furukawa, and Kenji Kitamura. "Quasi-phase-matched optical parametric oscillation with periodically poled stoichiometric LiTaO3." Optics Letters 25, no. 9 (2000): 651-653

[17] Yu, Nan Ei, SunaoKurimura, Yoshiyuki Nomura, Masaru Nakamura, Kenji Kitamura, Yasutoshi Takada, Jun Sakuma, and Tetsumi Sumiyoshi. "Efficient optical parametric oscillation based on periodically poled 1.0 mol% MgO-doped stoichiometric LiTaO3." Applied physics letters 85, no. 22 (2004): 5134-5136

[18] Kitamura, Kenji, Yasunori Furukawa, Kazuo Niwa, Venkatraman Gopalan, and Terence E. Mitchell. "Crystal growth and low coercive field 180 domain switching characteristics of stoichiometric LiTaO3." Applied physics letters 73, no. 21 (1998): 3073-3075.

[19] Hu, Pengchao, Lianhan Zhang, Jing Xiong, Jigang Yin, Chengchun Zhao, Xiaoming He, and Yin Hang. "Optical properties of MgO doped near-stoichiometric LiTaO3 single crystals." Optical Materials 33, no. 11 (2011): 1677-1680.

[20] J. P. Perdew, K. Burke and M. Ernzerhof, “generalized gradient approximation made simple,” Phys. Rev. Lett., 1996, 77, 3865.

[21] Monkhorst H J and Pack J D, 1976, “Special points for Brillouin-zone integrations”, 2002, Phys Rev. B 13 5188.

[22] Hu, Fengrui, Huichao Zhang, Chun Sun, Chunyang Yin, Bihu Lv, Chunfeng Zhang, William W. Yu, Xiaoyong Wang, Yu Zhang, and Min Xiao. "Superior optical properties of perovskite nanocrystals as single photon emitters." ACS nano 9, no. 12 (2015): 12410- 12416.

[23] Dogan, Fatih, Hong Lin, MarylineGuilloux-Viry, and Octavio Peña. "Focus on properties and applications of perovskites." Science and technology of advanced materials (2015).

[24] Negi, S., Mittal, P. and Kumar, B In-depth analysis of structures, materials, models, parameters, and applications of organic light-emitting diodes. Journal of Electronic Materials, 49(8), pp.4610-4636. (2015)

[25] Jaramillo-Quintero, Oscar A., Rafael S. Sanchez, Marina Rincon, and Ivan Mora-Sero. "Bright visible-infrared light emitting diodes based on hybrid halide perovskite with Spiro-OMeTAD as a hole-injecting layer." The journal of physical chemistry letters 6, no. 10 (2015): 1883-1890.

[26] Holm, Q. Sturzer, Y. Xu, and R. Weigel, Investigation of surface acoustic waves on LiNbO3, quartz, and LiTaO3 by laser probing, Microelectron Eng 31 (1996), 123–127.

[27] D. Ma, B. Wang, S. Fang, T. Zhang, R. Wang, and Y. Wei, “Growth and studies of optical properties of double-doped in: Fe: Litao3 crystal,” Microwave and Optical Technology Letters, vol. 48, no. 11, pp. 2227–2230,2006.

[28] M.K. Kuneva, S.H. Tonchev, and P.A. Atanasov, Infrared spectra of proton-exchanged waveguides in LiNbO3 and LiTaO3, Mater Sci Eng B 118 (2005), 301–305. [27] Y.N. Korkishko, V.A. Fedorov, S.M. Kostritskii, A.N. Alkaev, E.I.Maslennikov, E.

[29] Huang, He, LakshminarayanaPolavarapu, Jasmina A. Sichert, Andrei S. Susha, Alexander S. Urban, and Andrey L. Rogach. "Colloidal lead halide perovskite nanocrystals: synthesis, optical properties and applications." NPG Asia Materials 8, no. 11 (2016): e328-e328.

[30] Tan, Zhi-Kuang, Reza Saberi Moghaddam, May Ling Lai, Pablo Docampo, Ruben Higler, Felix Deschler, Michael Price et al. "Bright light-emitting diodes based on organometal halide perovskite." Nature nanotechnology 9, no. 9 (2014): 687-69.

