# SYNTHESIS AND OPTICAL CHARACTERIZATION OF $Yb^{3+}$ DOPED $LiY(MoO_4)_2$

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## ABSTRACT

**The lithium yttrium molybdate $LiY_{1-x}(MoO_4)_2$: x $Yb^{3+}$ (x= 0.01, 0.03, 0.05 and 0.07) phosphors were prepared by combustion synthesis method at $750^0$ C. Combustion synthesis is a method that provides some advantages as low synthesis temperatures and uniform rapid heating. The phases of prepared phosphors were confirmed by X-ray diffraction pattern. Morphology, crystal structure, and luminescent properties of phosphor materials were systematically studied.$LiY(MoO_4)_2$ is isostructural and crystallize in the scheelite ($CaWO_4$) structure type (space group $I4_1/a$). Photoluminescence spectra were measured which helps to understand the efficient energy transfer from host to $Yb^{3+}$ ions. The Photoluminescence characteristics of the sample are studied using excitation light of 340 nm, phosphor material shows emission spectra with two peaks at 980 nm and 996 nm in the range of 900 – 1100 nm. All results suggested that prepared phosphor material could be used to enhance the efficiency and stability of modern solar cells i.e. DSSCs and solar panels.**

**Keywords: Luminescence, Double, molybdate, Phosphor, DSSCs, Upconversion, Solar cell**

## 1. Introduction

Rare earth doped double molybdate square measure of sensible interest as economical, high color rendering phosphors. Such molybdate square measure used as a fabric for light lamps, gain media, light show panels, dye and clear light films[1, 2]. In recent years, the dye-sensitize solar cells (DSSCs) have become one of the most promising solar cells due to its potential relatively low fabrication cost in contrast with crystal silicon solar cell [3]. The practical use of DSSCs shows stability issue and relatively low conversion efficiency [4]. The stability of DSSCs is controlled by their physical and chemical stabilities. Physical stabilities mainly focus on the liquid electrolyte while chemical stability associated with inevitable electrochemical and thermal changes in the dye or electrolyte components during exposure ofultraviolet radiation [5-9]. The dye by selection responds to color spectrum thus to avoid actinic ray radiation a further actinic ray filter is employed. Such actinic ray filters cause loss of solar power in addition the absorption vary is restricted to 700 nm solely [10]. To beat this upconversion material will be used that add up the energies of near-infrared quanta to emit a quantum of upper energy. [11-16].

The trivalent lanthanide ions with abundant energy levels arising from the 4 $f^n$ inner shell configuration offer the ability of photon management and thus well suited for spectral conversion in solar cells [17].A famous trivalent lanthanide $Yb^{3+}$ is considered due to its interesting features in comparison to other $RE^{3+}$. $Yb^{3+}$ion in its $4f^{13}$ electronic configuration has only two manifolds i.e. $^2F_{7/2}$ (ground state) and $^2F_{5/2}$ (excited state) well suited for upconversion sensitizer. The selected host material $LiY(MoO_4)_2$is isostructural and crystallize in the scheelite ($CaWO_4$) structure type (space group $I4_1/a$). $LiY(MoO_4)_2$has great potential applications in various fields such as phosphors, optical fibers, scintillators, magnets, and catalysts. The distorted structure of $LiY(MoO_4)_2$, in which $Li^+$ and $Y^{3+}$ occupy the same lattice site with a random distribution, will induce inhomogeneous broadening of $Yb^{3+}$ absorption band. Given that the incident solar spectrum is continues, broad NIR band harvesting of sunlight can be expected [18]. This paper expounded the synthesis, upconversion of $Yb^{3+}$ in $LiY(MoO_4)_2$ to improve the efficiency and stability of modern solar cells.

## 2. Experimental Section

### 2.1 Materials and Methods

The lithium yttrium molybdate $LiY_{1-x}$ $(MoO_4)_8$ : $x$ $Yb^{3+}$ ($x$= 0.01, 0.03, 0.05 and 0.07) phosphors were prepared by combustion synthesis method at $750^0$ C. Stoichiometric amount of $LiNO_3$ (99.9%)and Ammonium Molybdate $(NH_4)_2Mo_7O_{24}$ $.4H_2O$ (99.99%) taken in a mortar pestle. Then various amount equi-molar mixture of Urea ($NH_2CONH_2$) was added to it. Weighing was done on highly precise meter pan balance having accuracy up to four digits. Then Ytterbium Oxide $Yb_2O_3$ (99.99%) and Yttrium oxide $Y_2O_3$(99.99%), according to molar concentration dissolved in Con.$HNO_3$ was added and heated on magnetic stirrer to prepare Ytterbium nitrate and Yttrium nitrate.This completeconstituent was crushed about 1 hour until pasty mass was formed, as most nitrate and urea are hygroscopic and absorb moisture during mixing. The absorption of moisture is not undesirable, on contrary, it helps to form a homogeneous mixture. These mixtures were transferred to china crucible and placed in a furnace maintained at temperature 750ºC. The mixture is formed in the form of foam with the evolution of gases tremendously. The flame was observed. At the completion of the reaction, the china crucible was removed from the furnace and this sample was crushed in mortar pestle to obtain $Yb^{3+}$ activated $LiY(MoO_4)_2$ phosphor of which PL, XRD and SEM characterization were taken at room temperature.

### 2.2 Characterization techniques

X-ray powder diffraction (XRD) analysis was performed with Bruker AXS D8 Advance diffractometer having Cu, Wavelength 1.5406 Å radiation in the 2θ range of 3° to 135° with Si(Li) PSD detector. The size and morphology investigations were performed by JEOL Model JSM 6390LV OXFORD XMX N with tungsten filament and specimen stage is 4 nm. The optical excitation and emission by samples are measured with Varian, Cary 5000, and spectral range 175-3300 nm UV-Vis-NIR spectrophotometer instrument.

## 3. Results and Discussion

### 3.1 Crystal structure and morphology of $LiY(MoO_4)_2$

$LiY(MoO_4)_2$is isostructural and crystallize in the scheelite ($CaWO_4$) structure type (space group $I4_1/a$). The structure contains three non-equivalent atom sites i.e. Mo site and O site and the site contains both $Y^{3+}$ and $Li^+$ in a 1:1 ratio and in complete disordered fashion. The Y and Li site has eight O ligands at distance of 24 nm and 24.7 nm respectively. The Mo atoms form the center of the fairly regular $MoO_4$ tetrahedron which is corner linked to adjacent $YO_8$polyhedra [19]. Fig.1 (a) shows crystal structure of $LiY(MoO_4)_2$[20]**.**Fig.1 (b) shows the SEM pictures of $LiY_{0.93}(MoO_4)_2$:0.07 $Yb^{3+}$ which investigate the structure and morphology of particles of prepared phosphor. It shows powder particles are of non-uniform shape and size of few micrometer scales.

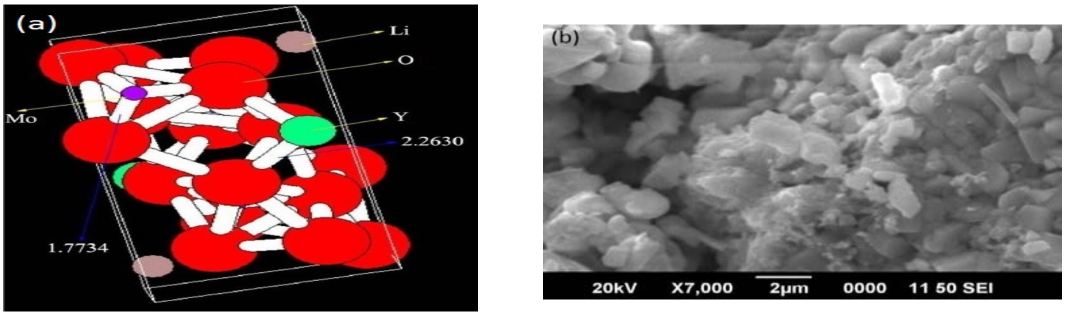

Fig.1. (a) Crystal structure of $LiY(MoO_4)_2$ (b) SEM of $LiY_{0.93}(MoO_4)_2$:0.07 $Yb^{3+}$

### 3.2 X-ray diffraction analysis

The phase characterization of $LiY_{1-x}(MoO_4)_2$: x $Yb^{3+}$ (x= 0.01 and 0.07) are demonstrated in fig.2. It is clear that the structure of prepared samples has no additional peaks and changes as increased $Yb^{3+}$ to host lattice where indexed to the pure phase of $LiY(MoO_4)_2$ according to the stand PDF card (JCPDS No. 17-773). This confirms that the structure of $LiY_{1-x}(MoO_4)_2$: x $Yb^{3+}$ (x= 0.01 and 0.07) samples have tetragonal scheelite structure with a space group of $I4_1/a$.

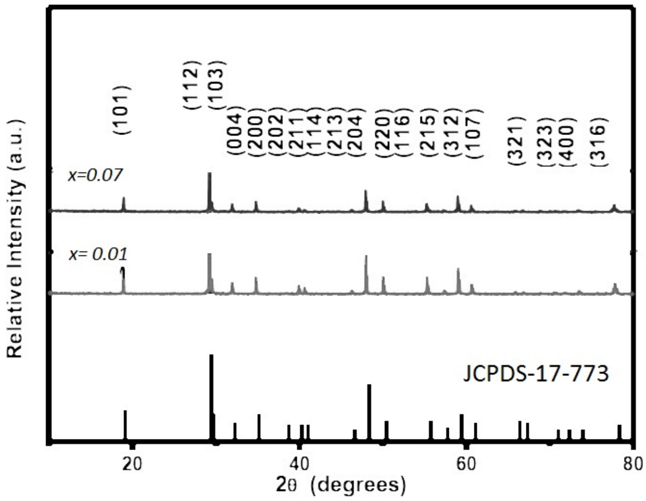

Fig.2. XRD pattern of $LiY_{1-x}(MoO_4)_2$ : x $Yb^{3+}$ (x= 0.01 and 0.07)

### 3.3 Photoluminescence properties

The emission spectra of $LiY_{1-x}(MoO_4)_2$: $x$ $Yb^{3+}$ ($x$= 0.01, 0.03, 0.05 and 0.07) phosphors in range 900 nm – 1100 nm is excited by 340 nm is shown in fig.3 (a). It represents the transition characteristics of $^2F_{5/2} \rightarrow {}^2F_{7/2}$ of $Yb^{3+}$ [13, 21-25]. Emission broadband shows that strong influence of crystal lattice on electronic configuration of $Yb^{3+}$. The nature of emission spectra of all samples are similar containing two sharp peaks at 980 nm and 996 nm corresponds to the transition characteristics. The intensity increases with increase in the concentration of $Yb^{3+}$results into the up conversion of the phosphor. $Yb^{3+}$has single energy level excited state approximately 10000 $cm^{-1}$ above ground level corresponding to emission around 1000 nm. The absence of other energy level $Yb^{3+}$ exclusively pick up energy packages from 10000 $cm^{-1}$ from other lanthanides and emits a photon at 1000 nm[13]. Dieke diagram (not shown) reveals that $Yb^{3+}$ is couple potential for $Er^{3+}$, $Nd^{3+}$ and $Pr^{3+}$[26-27].

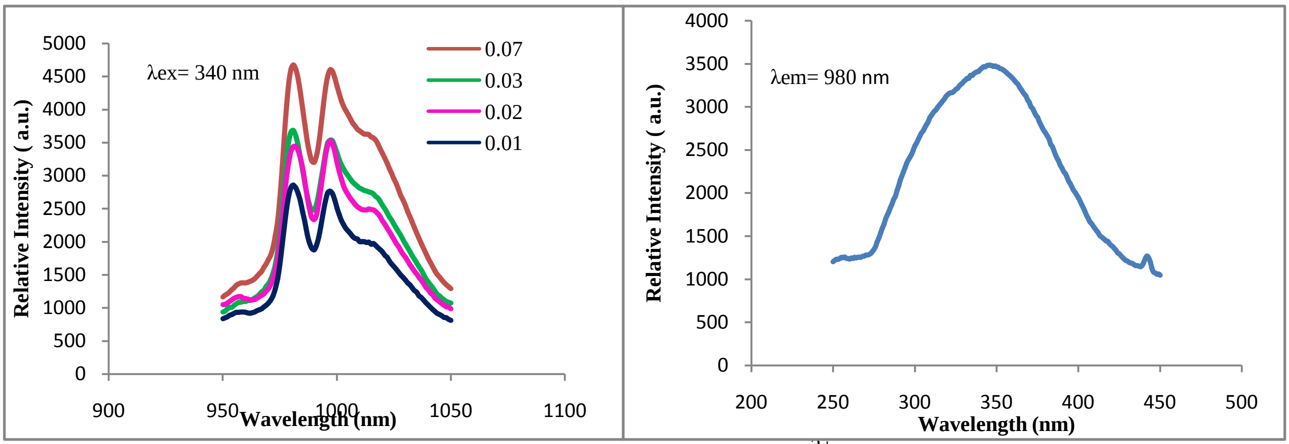

Fig.3 (b) shows the excitation spectra of $LiY_{0.99}(MoO_4)_2$:$0.01Yb^{3+}$ monitored by 980 nm. It can be seen as a broad excitation band which belongs to the Mo-O charge transfer absorption band (CTB).

Fig. 3(a) Emission spectra of $LiY_{1-x}(MoO_4)_2$: $x$ $Yb^{3+}$ ($x$= 0.01, 0.03, 0.05 and 0.07) phosphors (b) Excitation spectra of $LiY_{0.99}(MoO_4)_2$: $0.01Yb^{3+}$

## 4. Conclusions

In summary, the $LiY_{1-x}(MoO_4)_2$: $x$ $Yb^{3+}$ phosphors have successfully synthesized by using combustion synthesis method with concentration changes ($x$= 0.01, 0.03, 0.05 and 0.07). XRD reveals that the structure of the compound is tetragonal scheelite structure with space group $I4_1/a$ consistent with the standard PDF card available JCPDS-17-773. The morphology suggests powder particles are of non-uniform shape and size of few micrometre scales. The PL emission spectra of the phosphor materials show two peaks at 980 nm and 996 nm corresponds to the $^2F_{5/2} \rightarrow {}^2F_{7/2}$ of $Yb^{3+}$. The present results counsel these phosphors could have a possible application to boost the potency of DSSCs by upconversion by potential coupling.

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