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Fundamental Optical Characterization of $CH_3NH_3PbBr_3$ Perovskite Synthesized via Furnace Method

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Abstract: Lean films of $CH_3NH_3PbBr_3$ perovskite were prepared by using a simple one-step deposition method, followed by a controllable thermal treatment process for the study of their optical properties and stability under ambient conditions. Two thermal annealing processes were studied: One at a fixed temperature of 80 °C and one at a slow temperature slope from 80 °C to 120 °C. The UV-Vis absorbance measurements showed a strong absorbance in the visible wavelength range. A distinct peak was observed at 555 nm for the 80 °C annealed sample indicating a direct bandgap transition. In this sample, a distinct physical decay was observed over a two day timeframe, indicated by new peaks and loss of an absorption of greater than an order of magnitude. In contrast, the slowly heated sample had stronger absorption and fewer remnants of $PbBr_2$, showing a red shift of the maximum absorption peak to about 545 nm. Properties of the as-cast films suggest that the film's quality and crystallinity were very elevated. Stability tests of the film showed that the film could retain complete optical and fundamental quality for three days; quality loss could be noted on the fourth day. An analysis of the Tauc plot showed that both films showed adjustable properties, however, the continuously processed film had a slightly larger optical bandgap, indicating improved thermal stability and greater resistance to light induced degradation. Coincidently, photoluminescence (PL) measurements confirmed these observations: A large shift within the emission wavelength from 557 nm to 645 nm wavelength from 557 nm to 645 nm- was observed over time, particularly in the less stable film verifying ongoing degradation. These results suggest that processing conditions will significantly influence the optoelectronic properties and overall stability of $CH_3NH_3PbBr_3$ perovskite solar films, providing helpful information for developing better devices.

Keywords: *Perovskite, optical properties, physical properties, photoluminescence, band gap.*

1. Introduction

Halide perovskites are a very attractive family of materials for optoelectronic applications due to their outstanding optical and electrical properties like high photoluminescence quantum yield, high carrier diffusion lengths, and tunable absorption spectra[1]. These qualities certainly make them enticing for potential uses in solar cells, light-emitting diodes (LEDs), photodetectors, and lasers [2-4]. In addition to this, the performance of perovskites is strongly reliant on the morphology and crystallinity of the material, as well as the dimensionality of the material, where lower-dimensional structures have been shown to improve properties for device fabrication [5]. Solution-based methods, including spin coating and furnace annealing, are the most common synthesis techniques for perovskite thin films and single crystals[6, 7] . Although solution depositing techniques result in high-quality films, the actual synthesis conditions, including temperature, solvent, etc. greatly impact the films properties [8] . Garcia et al.[8] . points out that by thermal treating materials in a furnace as opposed to conventional room-temperature methods significantly improves the crystallinity and optical properties of the material[9]. More specifically $CH_3NH_3PbBr_3$ ($MAPbBr_3$) is well recognized for its optoelectronic properties, such as its direct bandgap and strong light absorption[10]. Previous investigations established that the annealing of perovskites via the furnace method enhances crystallinity and minimizes defect density (which, together, are key to realize a device performance gain)[11] . Still, the role of temperature on the growth mechanisms and morphologies of $CH_3NH_3PbBr_3$ remains largely unexplored, warranting further extensive study[12].The objective of this investigation is tostudy the synthesis of $CH_3NH_3PbBr_3$ microstructures through one-step self-assembly from a solution followed by furnace annealing. The morphology and crystallinity of the microstructures are characterized using X-ray diffraction (XRD). The focus will be on the impact of the annealing process on the optical properties of the material (measured via photoluminescence (PL), sharing information on the development conditions and the impact on materials performance.

2. Experimental Procedure

2.1. Materials

All chemical reagents employed in this study were of analytical quality and utilized without further purification. Methylamine hydrobromide (CH_3NH_3Br) was prepared in house by reacting equal molar amounts of methylamine and hydrobromic acid in a two-neck round-bottom flask by placing a 150 mL capacity flask in an ice-water bath while continuously stirring to control the exothermic nature of the reaction. The white crystalline salt was collected and dried in a desiccator before use. The Lead (II) bromide ($PbBr_2$, 99% purity; Sigma-Aldrich) anhydrous dimethylformamide (DMF, 99.8% purity; Sigma-Aldrich) was acquiredand used as received.

2.2. Synthesis of $CH_3NH_3PbBr_3$ Perovskite Thin Films

Perovskite precursor solutions were prepared by dissolving CH_3NH_3Br and $PbBr_2$ in a 1:1 molar ratio in anhydrous DMF to form a 0.1 M solution. The mixture was stirred at 60 °C for 1 hour to ensure all solidresolubilized, and homogeneity in the resulting mixture. The solution was then filtered into a clean glass vial and utilized immediately for deposition. The substrates were glass microscope slides (1 × 1 cm^2, ~1 mm thick), which were cleaned by ultrasonic agitation in ethanol and then deionized water for 15 minutes for each cleaning. After drying the substrates at 80 °C for a suitable amount of time, ~100 μL of precursor solution was applied by drop-casting to each glass slide to form uniform thin films with a thickness of approximately 0.1 mm. To study the effect of temperature on the optical properties

of $CH_3NH_3PbBr_3$ films we utilized two thermal treatment conditions. The first condition was a constant 80 °C for 24 hours, where the films were placed in a convection oven. The second treatment was a ramp from 80 °C to 120 °C at a rate of 0.028 °C per minute, also 24 hours in length. The thermal treatment allowed for controlled crystallization of the perovskite phase and evaporated all solvent.

3. Results and Discussion

3.1 Optical Properties Analysis Using UV-Vis and PL Spectroscopy

The optical properties of $CH_3NH_3PbBr_3$ perovskite thin films prepared from the furnace-assisted method were studied using ultraviolet-visible (UV-Vis) absorption spectroscopy and photoluminescence (PL), which provide valuable information about the electronic structure and energy transitions in this material. The Tauc method (Ganose et al., 2022) was used to determine the optical band gap of the material since it is widely used to describe semiconductor materials. In the Tauc method, the relationship between absorption coefficient (α) and photon energy ($h\nu$) are linked by the Tauc Relation.

3.2 Tauc Relation

To determine the optical bandgap from the UV-Vis absorption spectrum, the Tauc relation is commonly employed. The Tauc equation is expressed as follows:

$(\alpha h\nu) = B\,(h\nu - E_g)^{\frac{n}{2}}$ Eq 1

Where α is the absorption coefficient, hν is the photon energy, Eg is the optical bandgap energy, B is a constant related to the material, n is a parameter that depends on the type of electronic transition. For organic-inorganic hybrid perovskites, such as $CH_3NH_3PbBr_3$, the value of n is typically taken as 1, corresponding to a direct allowed transition.

The absorption coefficient α\alphaα can be calculated using the following equation:

$\alpha = 2.0303\times10^3 \left(\frac{A\rho}{LC}\right)$ Eq. 2

Where A is the absorbance obtained from the UV-Vis spectrum, ρ is the density of the material (g/cm³), L is the optical path length (1 cm), C is the molar concentration of the sample (mol/L).

This relation enables the estimation of the optical bandgap Eg by plotting $(\alpha h\nu)^n$ versus hν and extrapolating the linear region of the curve to intercept the energy axis.

3.3 Optical Properties of the Synthesized Perovskite:

3.3.1 Absorption Spectrum:

The UV or Ultraviolet Spectrum is a part of the electromagnetic spectrum that lies between visible light and X-rays. This spectrum has higher energy and shorter wavelengths than visible light and plays a very important role in optical analysis, physics, chemistry, and biology[13]. One of the most important aspects in evaluating the optical properties of the synthesized perovskite is its absorption spectrum. Through this analysis, it is possible to determine the energy band gap, structural defects, type of optical transition, light absorption capability, and photostability. These aspects are discussed below. According to Figure 1, related to the perovskite synthesized at 80 °C, the main absorption peak appears around 555 nm, indicating strong absorption in the visible region and confirming the successful formation of

the desired perovskite phase. Additional peaks are observed in the 440–480 nm region, attributed to the presence of a small amount of residual $PbBr_2$, suggesting minor impurities in the final product. The shape and intensity of the absorption spectrum also indicate that the optical transition is direct. Figure 2 presents the absorption spectrum of the same sample after being stored for two days to evaluate its photostability. A comparison of the spectra reveals that although the main peak remains identifiable, several additional peaks have emerged, indicating the onset of structural degradation and reduced optical efficiency. Figure 3 corresponds to the perovskite synthesized at temperatures between 80–120 °C. The main absorption peak is slightly shifted to 545 nm, and the overall absorption intensity is higher, suggesting improved light-harvesting efficiency and confirming a direct band gap. Moreover, the reduction in the intensity of the impurity-related peaks in the 440–480 nm region implies that the residual $PbBr_2$ content is lower, indicating higher material purity.

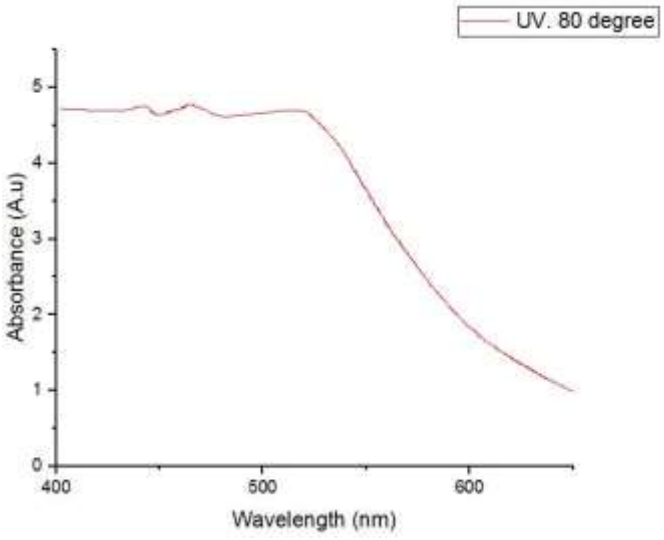


Figure 1: *UV-Vis Analysis of Perovskite Film Synthesized at 80 °C.*

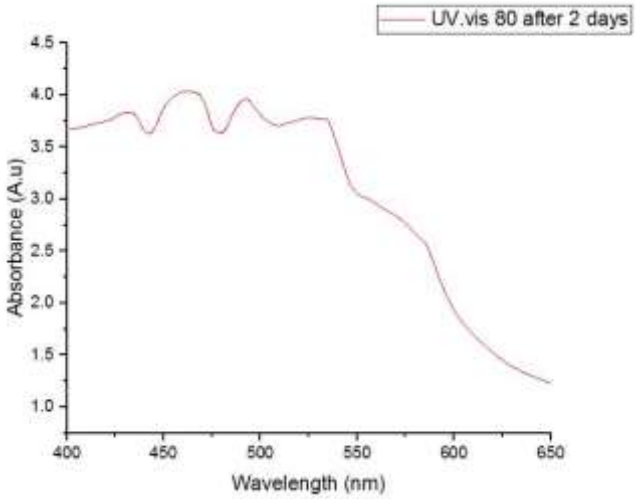
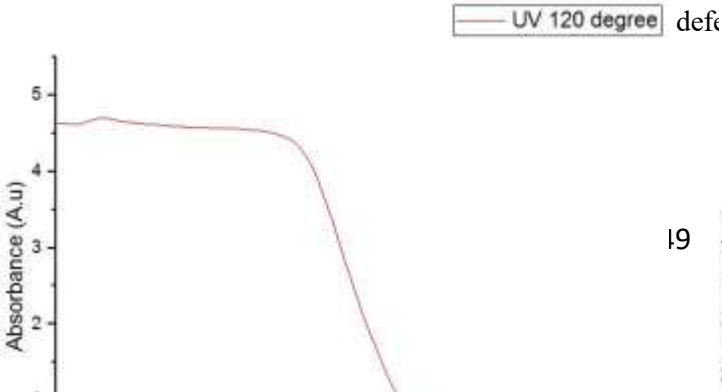


Figure 2: *UV-Vis Analysis of Perovskite Film Synthesized at 80 °C after 2 days.*

In order to evaluate the photostability of the sample synthesized at 80 - 120 °C, the film was then stored in a room temperature environment and absorption readings were taken daily. The results produced over the first 2 days are depicted in Figure 4. The main absorption peak was at 568 nm and the spectrum indicates that the perovskite structure remained mostly intact with only minor decrease in intensity. After the fourth day there was a minor reduction in absorption after which the lowering of absorption became significant after the fifth day. By the sixth day the absorber had degraded almost entirely. This trend is shown in Figure 5 which corresponds to the sample after 5 days of storage. The main broad and shifted peak was at approximately 640 nm indicating significant decomposition as well as high levels of impurity having clearly increased from 4day. In summary the perovskite synthesized at 80-120 °C demonstrated significantly enhanced photostability compared to the sample synthesized purely at 80 °C. This is most likely due to improved ion mobility and better crystal lattice arrangement due to the increased temperature. In addition the lower level of $PbBr_2$ in the resultant material suggests defe



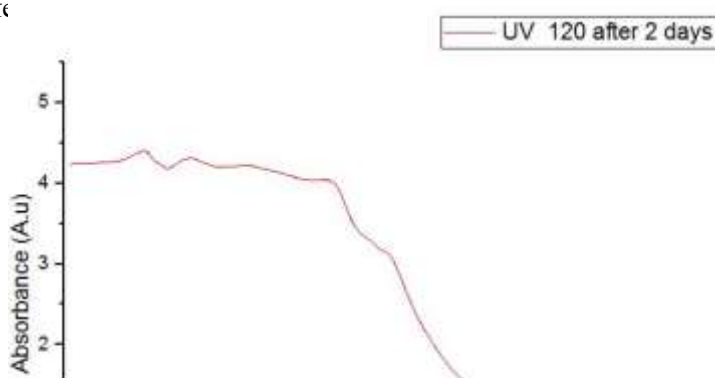


Figure 6:

Figure 3: *UV-Vis Analysis of Perovskite Film Synthesized at 120°C*

Figure 4: *UV-Vis Analysis of Perovskite Film Synthesized at 120 °C after 2 days.*

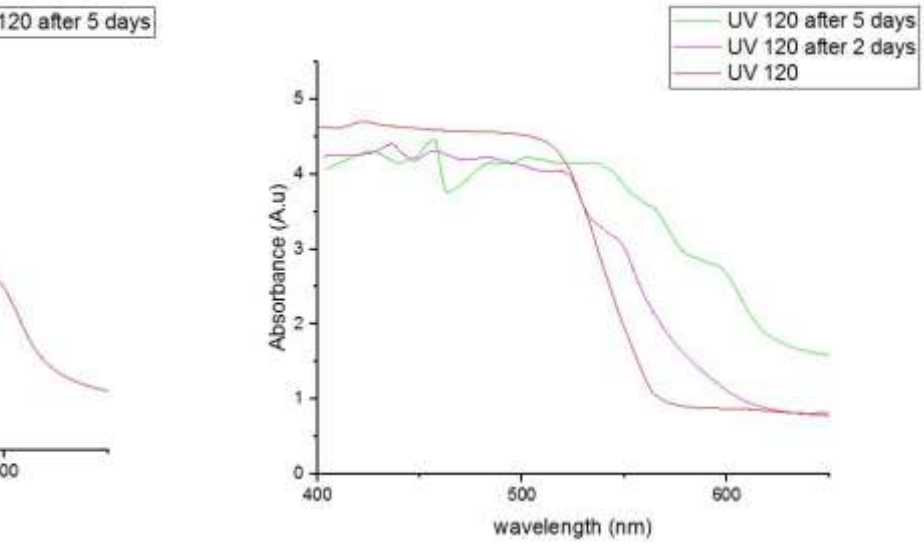


Figure 5: *UV-Vis Analysis of Perovskite Film Synthesized at 120 °C after 5 days.*

Figure 6: *UV-Vis Analysis of Perovskite Film Synthesized at 120 °C, 120 °C after 2 days, 120 °C after 5 days*

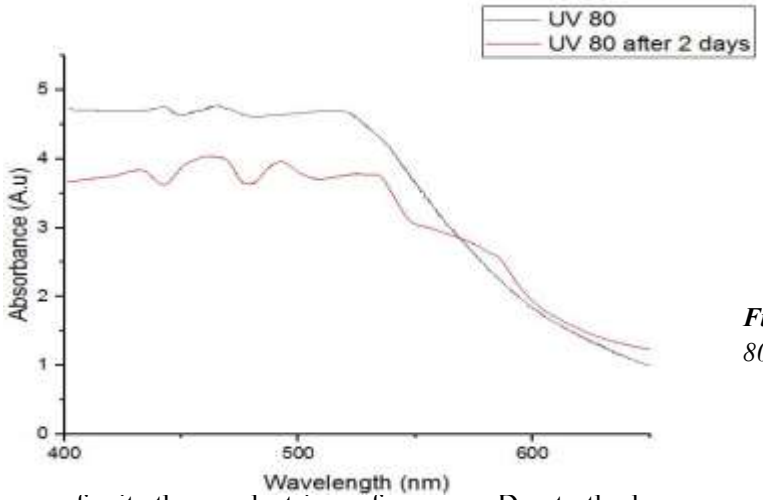


Figure 7: *UV-Vis Analysis of Perovskite Film Synthesized at 80 °C,80 °C after 2 days.*

for its thermoelectric performance. Due to the large amount of data (features) related to bandgap that are now available, it is possible to use a machine learning (ML) approach to predict the bandgap of the

material[14]. One important characteristic of the absorption spectrum is the energy gap, which can be determined using the Tauc relation (Eq 1).
Table 1 presents the energy gap values of the synthesized samples under different conditions.

***Table 1**: Energy Bandgap of Perovskite Samples Synthesized at Various Temperatures*

Synthesis temperature (˚c)	Storage time at room temperature (days)	E_g
80	-	**1.89**
80	2	**1.63**
80-120	-	**2.14**
80-120	2	**1.9**
80-120	5	**1.49**

Looking at the energy gap of synthesized samples we will also see that the sample synthesized at 80-120 °C has better efficiency, photo and thermal stability, because the perovskite has a larger energy gap, therefore the photo and thermal stability is greater due to the pre-requisite energy to excite an electron being greater. Lastly, as the energy gap increases, the formation of synthesized perovskite nanocrystals decreases.

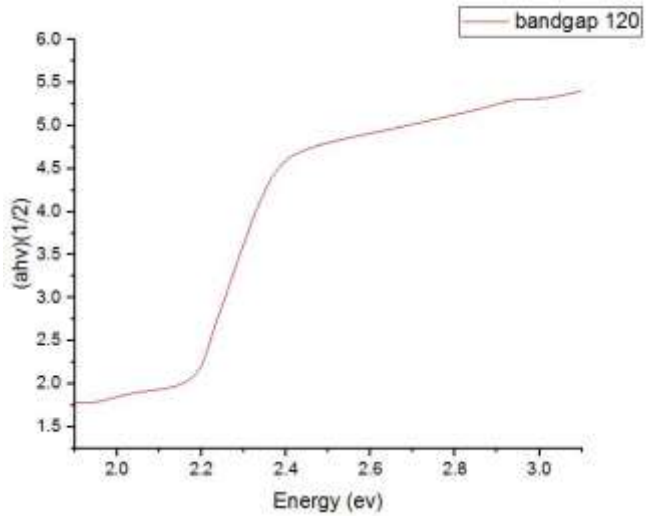


***Figure 8:** Optical Band Gap Estimation of $CH_3NH_3PbBr_3$ Thin Film Annealed at 120 °C.*

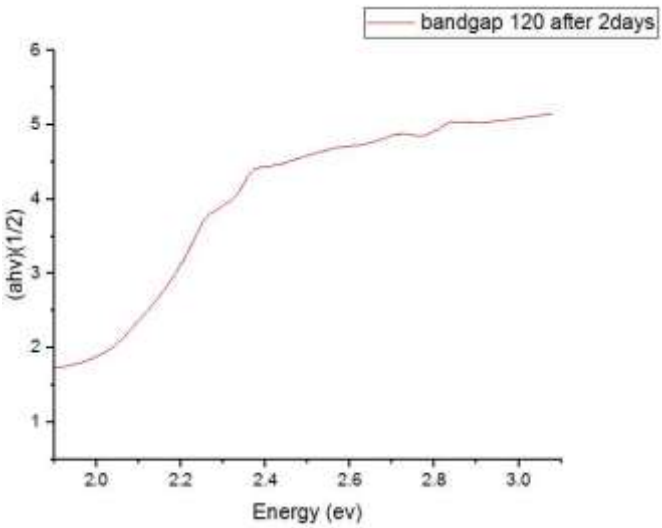
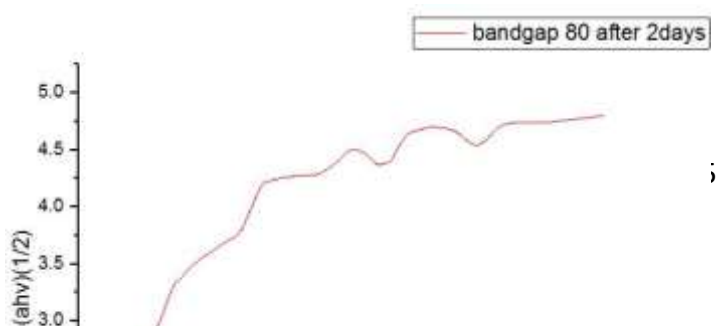


***Figure 9:** Optical Band Gap Estimation of $CH_3NH_3PbBr_3$ Thin Film Annealed at 120 °C after 2days.*



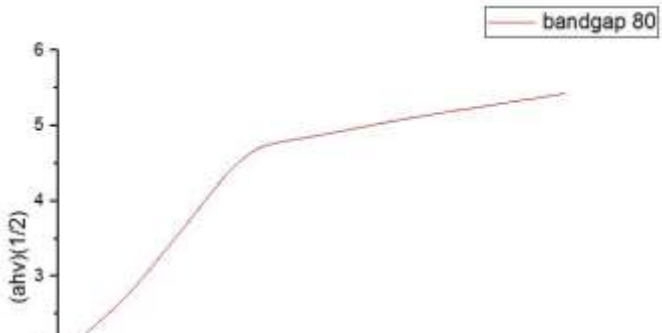


Figure 10: *Optical Band Gap Estimation of $CH_3NH_3PbBr_3$ Thin Film Annealed at 80 °C*

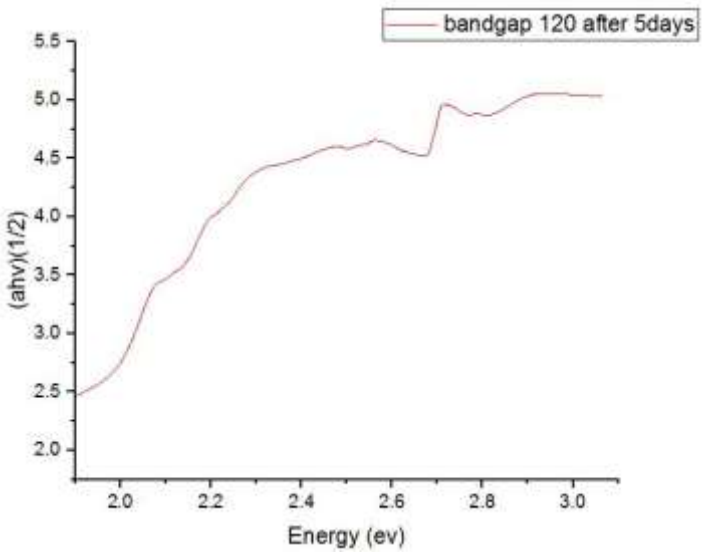


Figure 12: *Optical Band Gap Estimation of $CH_3NH_3PbBr_3$ Thin Film Annealed at 120 °C after 5 days.*

Figure 11: Optical Band Gap Estimation of $CH_3NH_3PbBr_3$ Thin Film Annealed at 80 °C after 2 days.

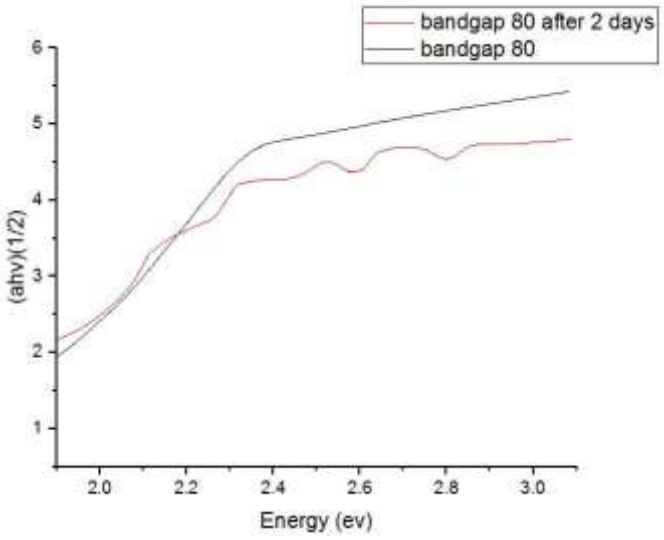


Figure 13: *Optical Band Gap Estimation of $CH_3NH_3PbBr_3$ Thin Film Annealed at 80 °C after 2 days.*

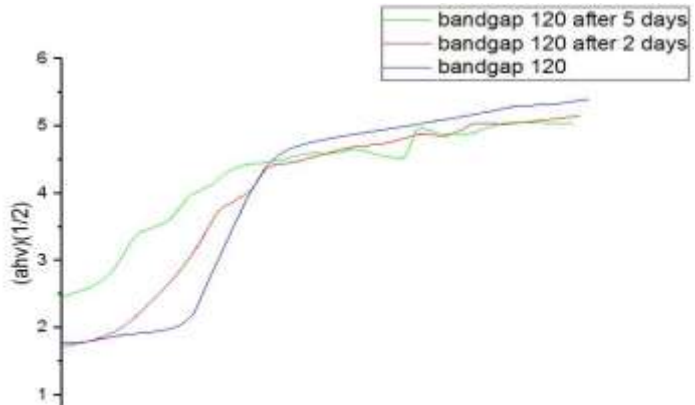


Figure14: *Optical Band Gap Estimation of $CH_3NH_3PbBr_3$ Thin Film Annealed at 120 °C, 120 after 2 days, 120 after5 days.*

3.3.3 Photoluminescence (PL):

Photoluminescence (PL) is when a material absorbs energy in the form of photons, or light, and re-emits light radiation (photons). This phenomenon can be observed in many semiconductor materials, molecules, nanostructures, and crystals, and is a powerful technique used to explore and characterize the electronic and optical properties of materials (Kim et al., 2016). Photoluminescence (PL) spectra can also be used to measure the emission wavelength and thereby draw tentative comparisons of the particle sizes formed. Figures number 15 and 16 show the PL spectra of perovskite made at 80°C and the perovskite made 2 days later, respectively. They demonstrate that the materials have emission wavelengths of 557 nm and 571 nm, respectively. The sights decrease in the peak intensity after two days shows that the perovskite is degrading. Figures number 17, 18, and 19 are the PL spectra of the perovskite material synthesized at 80 - 120°C, the same perovskite material after 2 days, and the same perovskite material after 5 days, respectively. The emission peaks are at 545 nm, 569 nm, and 645 nm respectively. The substantial decrease in the photoluminescence intensity in these samples, further supports the physical degradation of the synthesized perovskite material to occur over the timeframe of the experiment.

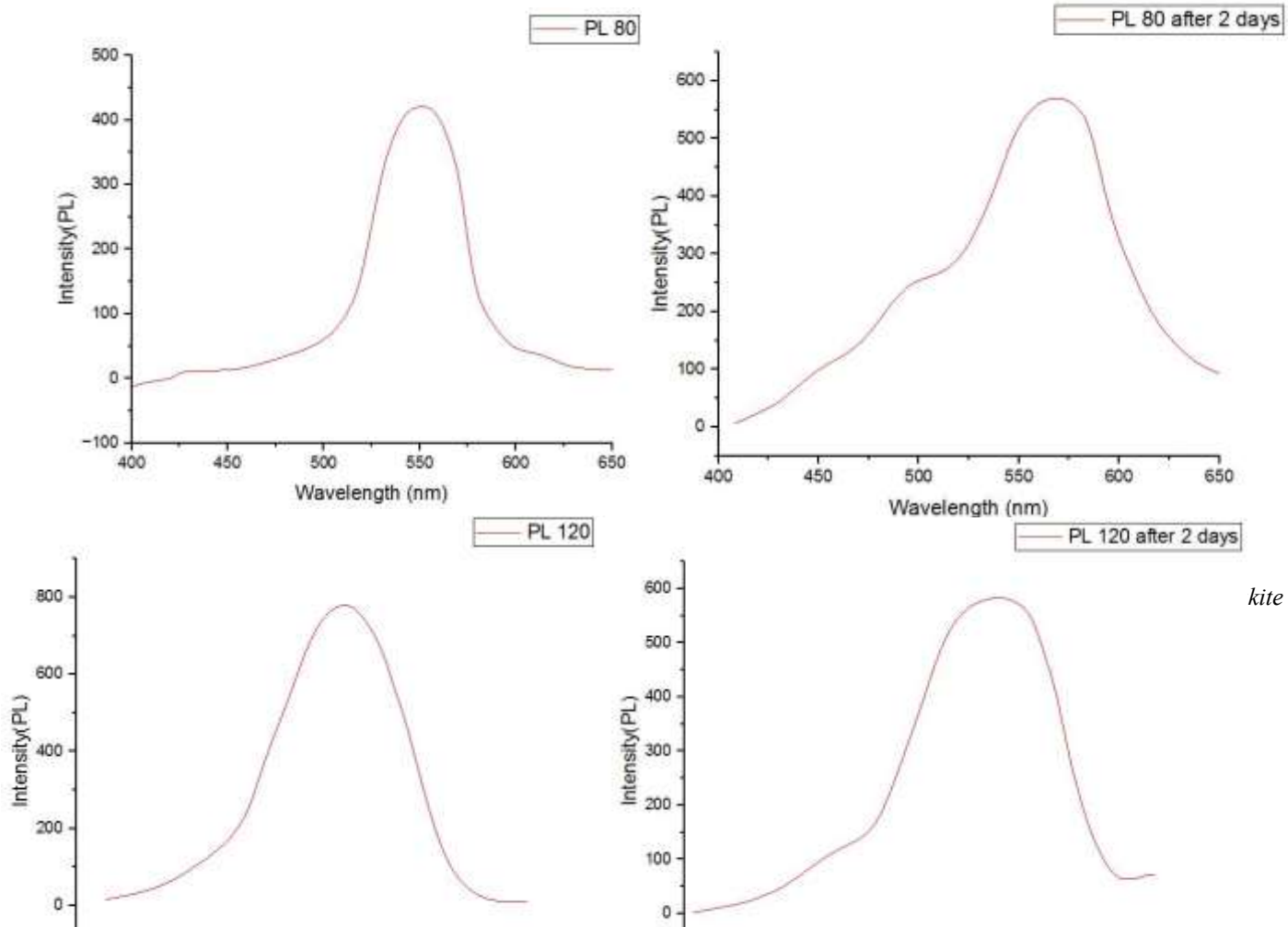


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Figure 17: *Photoluminescence Analysis of Perovskite Film Synthesized at 120 °C.*

Figure 18: *Photoluminescence Analysis of Perovskite Film Synthesized at 120 °C after 2days*

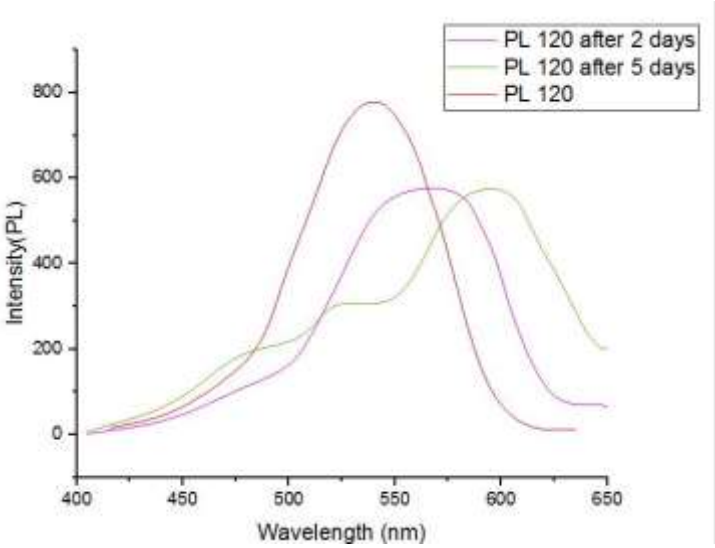

Figure 19: *Photoluminescence Analysis of Perovskite Film Synthesized at 120 °C after 5 days*

Figure 20: *Photoluminescence Analysis of Perovskite Film Synthesized at 120 °C, 120 after 2and5 days.*

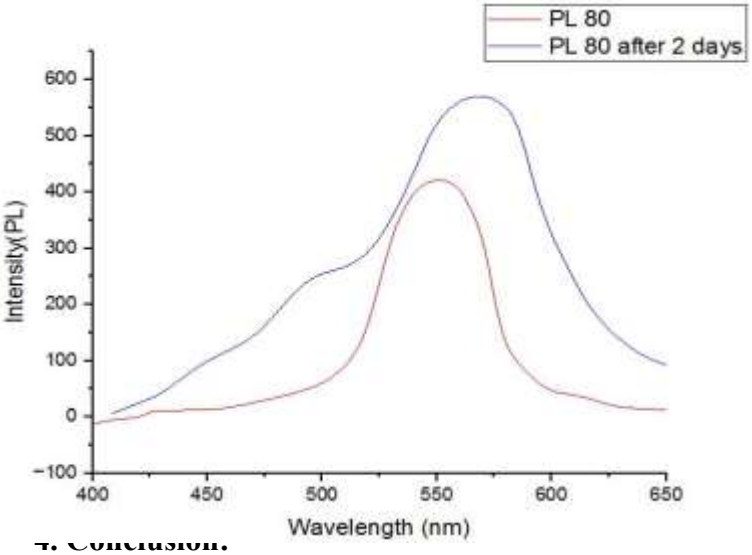

Figure 21: *Photoluminescence Analysis of Perovskite Film Synthesized at 80 °C, 80 after 2 days.*

4. Conclusion:

In this research study, $CH_3NH_3PbBr_3$ perovskite thin films were successfully prepared using a one step solution processing technique and subsequently thermally treated at either a constant temperature of 80 °C, or a ramp up of temperature (80 to 120 °C). Additionally, the films optical properties were

characterized utilizing UV-Vis absorption and photoluminescence (PL) spectroscopy. The UV-Vis spectra demonstrated significant visible absorption with all samples showing similar absorption bands/location; however the slight variation in energy was associated with the annealing condition, representative of changes in increase crystallinity and structure quality of the thin films. Under the lower temperature annealing condition (80 °C) impurity peaks associated with $PbBr_2$ decreased significantly, under annealing conditions with a temperature ramp (80-120 °C), indicating that the increased temperature provided enhanced film morphology and phase purity. Based on the information from the Tauc analysis, we estimated the optical band gap of the films was higher for the films treated at 80-120 °C and showed consistent stable absorption characteristics over time with decreased band gaps. The increase in band gap represents decreased particle sizes and fewer defects in the structure permitting better charge transport and improved optoelectronics performance. However, the photoluminescence indicated that the films treated at the higher temperatures actually exhibited improved stability and structural integrity as denoted by the decreased rates of degradation of the thin films over time. In conclusion, the results contained in this work have indicated that controlled thermal annealing of $CH_3NH_3PbBr_3$ perovskite thin films has a positive influence on optical quality, phase purity, and photostability. Most importantly, this work provides information that will aid in the optimization of perovskite processing conditions, for devices that require optical efficiency and durability, such as photovoltaic and optoelectronic devices.

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