

## NE201B Project Report

### *Photoluminescence Quantum Yield (PLQY) of solid and liquid samples using the FLS1000*



Centre for Nanoscience and Engineering (CeNSE)

Indian Institute of Science, Bengaluru, Karnataka

Submitted By:

J Laxmipriya - 25149

PVS Nikhil – 24240

Aasheik Saran.S - 24478

Guided By :

Prof. Akshay Naik

Prof. Aditya Sadhanala

## ACKNOWLEDGEMENTS

We would like to express our sincere gratitude to all those who supported us in completing this project. First and foremost, we extend our heartfelt thanks to our guides, Prof. Akshay Naik, CENSE, IISc for giving the opportunity to get experience in the lab and Prof. Aditya Sadhanala, CENSE, IISc whose expertise, mentorship, and encouragement were crucial throughout this journey.

We are also deeply grateful to the faculty technologists of the MNCf, CENSE, for their exceptional technical expertise, assistance, and support.

We would like to thank Dr. Suresha sir and Chetan sir for their constant support in helping with the process and guiding us. We are also thankful to the Faculty Technologists of the Optical Bay in guiding us and helping us. Their dedication to ensuring a seamless research environment and their willingness to share their knowledge was vital for performing the experimental work effectively. Their guidance in handling advanced tools and processes played a significant role in the progress and success of this project.

Thank you all for making this journey a profoundly enriching and rewarding experience.

J Laxmipriya

PVS Nikhil

Aasheik Saran. S

3rd May 2025

## **ABSTRACT**

Photoluminescence (PL) is a process where materials absorb photons, exciting electrons to higher energy states, and emit light upon returning to their ground state. This phenomenon, encompassing fluorescence and phosphorescence, is pivotal in applications like LEDs, quantum dot displays, and fluorescence microscopy. PL involves absorption, relaxation, and emission stages, with emitted light often differing in wavelength from the absorbed light. Materials such as quantum dots, organic dyes, and certain minerals exhibit PL, enabling advancements in lighting, imaging, and materials science.

## CONTENTS

CHAPTERS	PAGE NO.
<b>CHAPTER 1: INTRODUCTION</b>	5,6
1.1 Overview	5
1.2 Objectives	6
<b>CHAPTER 2: LITERATURE REVIEW AND EXPERIMENTATION</b>	7-16
Photoluminescence (PL) and Quantum Yield (PLQY)	7
MEH-PPV Sample	7
Challenges	8
Instruments used	9-16
<i>FLS1000 Photoluminescence Spectrometer</i>	9-13
<i>Alternate instruments used</i>	14-16
<b>CHAPTER 4: RESULTS</b>	17-20
<b>CHAPTER 5: CONCLUSION</b>	21
REFERENCES	22

# I. INTRODUCTION

## 1.1 Overview

Photoluminescence (PL) is the emission of light from a material after it absorbs photons and undergoes electronic excitation. When a material absorbs light, electrons are excited to higher energy states. As these electrons return to their ground state, they may release energy in the form of emitted photons, producing PL. The nature of this emission—its intensity, spectral profile, and energy—offers valuable insight into the electronic and optical properties of materials, such as their band structure, defect density, and radiative versus non-radiative decay pathways.

Photoluminescence Quantum Yield (PLQY) is a key metric that quantifies the efficiency of the PL process. It is defined as the ratio of the number of photons emitted to the number of photons absorbed:

$$PLQY = \frac{\text{Number of photons emitted}}{\text{Number of photons absorbed}}$$

A PLQY value of 1 (or 100%) represents perfect radiative efficiency, where every absorbed photon leads to the emission of a photon. In real materials, PLQY is typically reduced by non-radiative processes such as defect-mediated quenching, exciton–phonon coupling, or surface traps. Therefore, PLQY serves as a crucial indicator of material quality and performance, especially in applications such as organic light-emitting diodes (OLEDs), quantum dot displays, photovoltaic cells, fluorescent probes, and lasers. Together, PL and PLQY measurements provide a non-invasive, highly sensitive means to evaluate the optoelectronic properties of semiconductors, nanomaterials, organic polymers, and dyes. These measurements help identify optimal processing conditions (e.g., solvent choice, annealing temperature), monitor material degradation, and assess the effectiveness of surface passivation or doping strategies.

In this study, PL spectra and PLQY values are obtained using the FLS1000 photoluminescence spectrometer, which uses a 405 nm excitation source and a high-resolution spectrometer for emission detection. To ensure accurate PLQY measurements, an integrating sphere accessory is used. This sphere eliminates angular bias by diffusely scattering all emitted photons uniformly across the detection surface, making it ideal for samples with anisotropic emission profiles—such as thin films and nanostructured materials. By capturing both emitted and transmitted light, the system enables precise determination of photon absorption and emission, allowing reliable PLQY calculation.

## 1.2 Objective

The objective of this project is to evaluate and understand the photoluminescence quantum yield (PLQY) of solid and liquid luminescent materials, with a focus on MEH-PPV, using the FLS1000 photoluminescence spectrometer. The study aims to:

- Grasp the fundamental theory behind PL and PLQY, and their relevance in assessing material efficiency.
- Investigate the impact of thermal annealing at various temperatures and environments (air vs. glovebox) on PL and PLQY behaviour.
- Analyse the correlation between PLQY, radiative efficiency, and material degradation, and how these influence practical applications in optoelectronics.

Ultimately, this project aims to identify optimal conditions under which MEH-PPV and similar materials exhibit high PLQY, thereby enhancing their potential for use in devices like LEDs, photodetectors, and solar energy system

## II. LITERATURE REVIEW AND EXPERIMENTATION

### PHOTOLUMINESCENCE (PL) AND QUANTUM YIELD (PLQY)

Photoluminescence (PL) refers to the emission of light from a material following the absorption of photons. It serves as a sensitive probe into the electronic structure of materials, enabling analysis of energy band gaps, defect levels, and recombination pathways.

Photoluminescence Quantum Yield (PLQY) is defined as the ratio of emitted photons to absorbed photons:

$$PLQY = \frac{\text{Number of photons emitted}}{\text{Number of photons absorbed}}$$

It is a critical parameter in assessing the radiative efficiency of materials, particularly relevant for optoelectronic applications such as LEDs, lasers, and solar concentrators. High PLQY indicates that most of the absorbed energy is re-emitted as light, while low PLQY suggests losses through non-radiative pathways.

### MEH-PPV SAMPLE

**MEH-PPV** (poly[2-methoxy-5-(2-ethylhexyloxy)-1,4-phenylenevinylene]) is a widely studied conjugated polymer known for its strong photoluminescence in the orange-red region and high photoluminescence quantum yield (PLQY). Its side chains improve solubility in organic solvents, enabling smooth film formation.

Smaller MEH-PPV chains or those blended with electron-accepting moieties (e.g., benzothiadiazole) can reach PLQY values up to 45%, while longer chains tend to suffer from conformational defects and interchain quenching, reducing efficiency. The polymer's emission is also influenced by film thickness, solvent polarity, and thermal treatment. For instance, annealing or blending with inert matrices like polystyrene (PS) has been shown to significantly suppress aggregation and enhance PL intensity—sometimes by as much as sixfold.

In this study, MEH-PPV was deposited as a thin film on a quartz substrate using the spin coating technique. Quartz was chosen due to its excellent optical transparency in the UV-visible range and its inert, smooth surface, which supports uniform film formation.

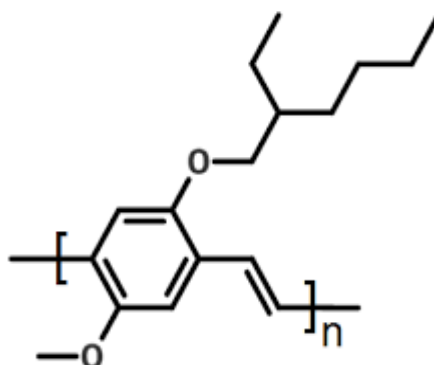


Fig 1. MEH-PPV molecular structure

## **CHALLENGES**

Accurate measurement of photoluminescence (PL) and photoluminescence quantum yield (PLQY) in solid-state and thin-film samples presents several challenges due to the complex optical behaviors of materials. Below are the primary issues and their solutions:

### **1. Anisotropic Emission**

- In thin films, molecules (e.g., polymer chains) are often aligned, causing directional emission. This violates the assumption of isotropic emission, which is valid for solutions but not for solids. Detectors that measure emission in only one direction may miss a significant portion of the total emitted light.

Hence, an integrating sphere randomizes light by scattering it uniformly over the internal surface, allowing for angle-independent collection of all emitted photons.

### **2. Waveguiding Effects**

- In thin films on substrates (like glass), light emitted at shallow angles is internally reflected and guided within the sample or substrate. Much of this light is trapped and never reaches the detector if only free-space emission is measured.

Hence, integrating sphere captures both direct and waveguided emission, including photons that would normally be lost in conventional setups.

### **3. Reabsorption of Emission**

- If the emission spectrum overlaps with the absorption spectrum, some emitted photons are reabsorbed by the sample. This reduces the apparent PL signal and causes underestimation of PLQY.

Reabsorption is corrected by:

- Using thin samples to minimize path length,
- Comparing spectra measured inside and outside the sphere,
- Scaling the true emission spectrum using longer wavelengths (which are unaffected by reabsorption).

### **4. Overlap Between Emission and Laser Scattering**

- The excitation laser wavelength may partially overlap with the emission spectrum, especially in short-wavelength emitters. The detector may record laser scatter as part of the emission, inflating PL values incorrectly.
- Use optical filters to selectively block the laser line while transmitting the emission.

Apply spectral correction factors to mathematically subtract the laser contribution from the raw spectrum. The FLS1000 software enables this correction by isolating the laser contribution through a reference measurement.



## **INSTRUMENTS USED**

### ***FLS1000 Photoluminescence Spectrometer***

The FLS1000 is a high-resolution, modular photoluminescence (PL) and photoluminescence quantum yield (PLQY) measurement system developed by Edinburgh Instruments. It is capable of recording steady-state and time-resolved PL spectra with high sensitivity, making it ideal for characterizing the optical properties of both liquid and solid samples such as MEH-PPV thin films.

#### **Main Components of the FLS1000 System**

<b>Component</b>	<b>Function</b>
<b>Excitation Source</b>	Typically a tunable xenon lamp or diode laser (e.g., 405 nm), used to excite the sample.
<b>Excitation Monochromator</b>	Selects a specific wavelength of light for sample excitation.
<b>Sample Chamber</b>	Holds cuvettes (for solutions) or mounts for thin films or powders. Can include an integrating sphere.
<b>Emission Monochromator</b>	Disperses emitted light from the sample into individual wavelengths.
<b>Detector</b>	Usually a photomultiplier tube (PMT) or CCD that measures emission intensity across wavelengths.
<b>Integrating Sphere</b>	Collects all emitted and scattered light from the sample for accurate PLQY measurements.
<b>Control Software</b>	Manages scan parameters, records data, and performs PLQY calculations.

#### **Photoluminescence (PL) Measurement in FLS1000**

To measure PL:

1. The excitation source illuminates the sample at a chosen wavelength (e.g., 405 nm).
2. The sample emits light due to radiative recombination of excited electrons.
3. The emitted light is collected at 90° to the excitation beam (to avoid direct laser scatter).
4. The emission monochromator separates the light into wavelengths, and the detector records the PL spectrum.
5. The output is a plot of emission intensity vs. wavelength, which helps identify emission peaks, spectral shifts, and intensity changes.

## Photoluminescence Quantum Yield measurement in FLS1000

There are two different methods for measurement of absolute fluorescence quantum yield. Direct Excitation measurements and Direct & Indirect Excitation measurements.

In Direct Excitation measurements one records the scatter and emission of the sample being directly excited by the radiation from the excitation monochromator only, whereas with Direct & Indirect Excitation one also records the emission of the sample while it is in a position where it is only indirectly excited by radiation bouncing with the sphere.

### Direct Excitation measurement

In this method the emission measurement contains information of both direct and indirect excitation, as photons that pass the sample in the direct excitation beam may still be absorbed after scattering in the sphere.



Fig 2: Two different measurements required. A-reference sample and B-test sample in position 1(position 2 is empty for both measurements)

For example, let us consider an example where some sample has been used and the readings were noted. The absolute fluorescence quantum yield can be calculated as follows in this method:

$$\eta_D = \frac{E_B - E_A}{S_A - S_B}$$

$E_A(\lambda)$  and  $S_A(\lambda)$  as well as  $E_B(\lambda)$  and  $S_B(\lambda)$  are measured in individual scans. It can be measured in two scans only. The final calculation of  $\eta_D$  uses the quantum yield wizard which is supplied by the FLUORACLE software. If the sphere background is sufficiently low the measurement of this region can be neglected.

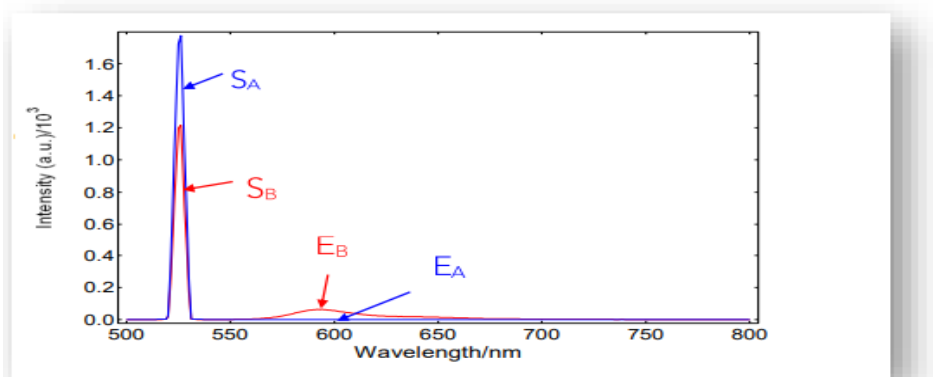


Fig 3: Spectral scans of the excitation scatter region or S-region and the emission region E-region of the sample. The indices A and B refer to experimental setup

## Direct & Indirect Excitation Method

This method includes a third setup in addition to the two above: measurements of the emission of the sample in a position where it is not directly excited by the excitation beam, instead the sample is excited indirectly, i.e., by photons that are scattered at the sphere surface before entering the sample.

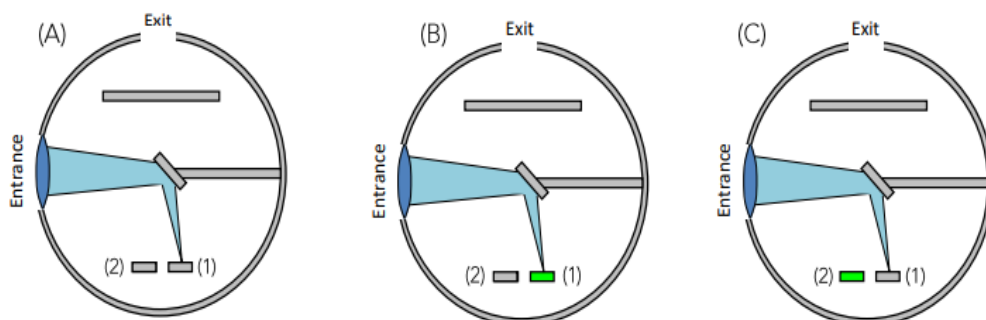


Fig 4: Three different measurement configurations: A- reference sample in both sample positions 1 & 2, B- test sample in position 1 reference sample in position 2, C- reference sample in position 1 and test sample in position 2.

For example, let us consider some sample and the spectra for emission and excitation are similar to what shown in the figure below. The absolute fluorescence quantum yield is calculated in the Direct & Indirect Measurement method as follows:

$$\eta_{DI} = \frac{S_B(E_C - E_A) - S_C(E_B - E_A)}{(S_B - S_C)S_A}$$

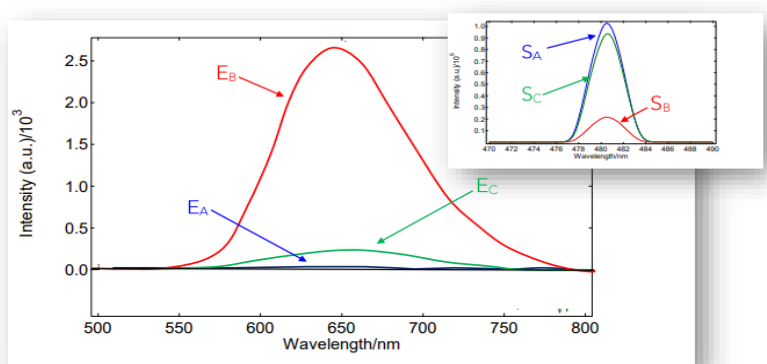


Fig 5: Spectral scans of the excitation region (peaks in the inset) and of the emission region of the sample and reference. A, B, C refer to experimental setup.  $S_A$ ,  $S_B$ ,  $S_C$ ,  $E_A$ ,  $E_B$  and  $E_C$  refer to integrals of the scans.

$E_A(\lambda)$  and  $S_A(\lambda)$  as well as  $E_B(\lambda)$  and  $S_B(\lambda)$  and  $E_C(\lambda)$  and  $S_C(\lambda)$  are measured in individual scans. It can be measured in three scans only. The final calculation of  $\eta_{DI}$  uses the quantum yield wizard which is supplied by the FLUORACLE software. If the sphere background is sufficiently low the measurement of this region can be neglected to save measurement time.

## PROCEDURE:

### Direct Excitation method

#### 1. Mount the Sample in the Sphere

Place the sample (solid or liquid) inside the integrating sphere so that the excitation beam directly hits the sample. Ensure that the sample is positioned perpendicular to the beam and securely held to avoid movement.

## 2. Set Excitation Parameters

Choose an appropriate excitation wavelength which was taken in the PL measurement. Set appropriate slit widths and acquisition settings in the software for both excitation and emission.

## 3. Record the Excitation Reference (Laser Spectrum)

First, measure the **laser spectrum** with no sample or with a blank in place to record the baseline intensity of the excitation beam.

## 4. Measure the Emission Spectrum

With the sample in place, record the **emitted photoluminescence spectrum** across the desired wavelength range. This includes all **emitted and scattered photons** within the sphere.

## 5. Measure Scattered Excitation Light

Simultaneously or in a separate channel, measure the **scattered excitation light** that is not absorbed by the sample. This helps determine how much light was actually **absorbed**.

## 6. Calculate Absorbed and Emitted Light

From the intensity data:

$A = L_0 - L$  = absorbed photons (difference between reference and sample scattering),

$E = P$  = emitted photons (integrated PL emission).

These are corrected using the sphere's known geometry and detection response.

## 7. Determine PLQY

Use the formula:

$$PLQY = \frac{\text{Number of photons emitted}}{\text{Number of photons absorbed}} = \frac{P}{L_0 - L}$$

The result is output directly by the FLS1000 software or calculated manually from the integrated areas.

## Direct & Indirect Excitation method

### 1. Measure Reference (Laser Only, No Sample)

Place the integrating sphere **without any sample** (or use a blank quartz substrate). Direct the excitation beam into the sphere (hitting the wall). Record the **laser intensity spectrum** → this gives the **reference laser signal**  $L_{ref}$ .

### 2. Indirect Excitation (Sample in Sphere, Laser on Wall)

Insert the sample (e.g., MEH-PPV thin film on quartz) into the sphere. Direct the **laser at the sphere wall, not at the sample**. Record:

Scattered laser light  $L_{\text{indirect}}$

Emission from the sample  $P_{\text{indirect}}$

### 3. Direct Excitation (Laser on Sample)

Without moving the sample, redirect the laser **directly onto the sample** surface. Record:

Scattered laser light  $L_{\text{direct}}$

Emitted PL spectrum  $P_{\text{direct}}$

### 4. Calculate Absorbed Light (A)

Determine the amount of absorbed photons:

$$A = L_{\text{indirect}} - L_{\text{direct}}$$

This gives the **difference in scattered excitation light**, indicating how much was absorbed by the sample.

### 5. Calculate Emitted Light (E)

Determine the amount of emitted photons by subtracting background:

$$E = P_{\text{direct}} - P_{\text{indirect}}$$

This isolates emission due only to direct excitation, corrected for background fluorescence and stray signals.

### 6. Calculate PLQY

Finally, compute PLQY using:

$$PLQY = \frac{E}{A} = \frac{P_{\text{direct}} - P_{\text{indirect}}}{L_{\text{indirect}} - L_{\text{direct}}}$$

The result reflects **absolute PL efficiency**, corrected for scattering, reabsorption, and sample geometry.

This method is preferred because it is more accurate than direct method especially for thin films.

## ALTERNATIVE METHOD FOR PL AND PLQY MEASUREMENT

The basic experimental set up is shown in Figure 1. An optical fibre leads from the wall of the sphere to a grating spectrometer with a CCD. Immediately in front of the optical fibre is a baffle coated with barium sulphate. to prevent direct illumination of the optical fibre. Laser illumination of appropriate wavelength is directed into the sphere through a small entrance hole. Three measurements are made using the sphere. For the first measurement, figure 1a, the sphere is empty, and laser light alone is detected by the spectrometer. For the second measurement, figure 1b, the sample is placed inside the sphere and the laser beam is directed on to the sphere wall. The third measurement, Figure 1c, is similar to the second, except that the collimated laser beam is now directed on to the sample (the sample is oriented such that laser light reflected from the surface of the sample is directed onto the sphere wall and not back through the entrance hole).

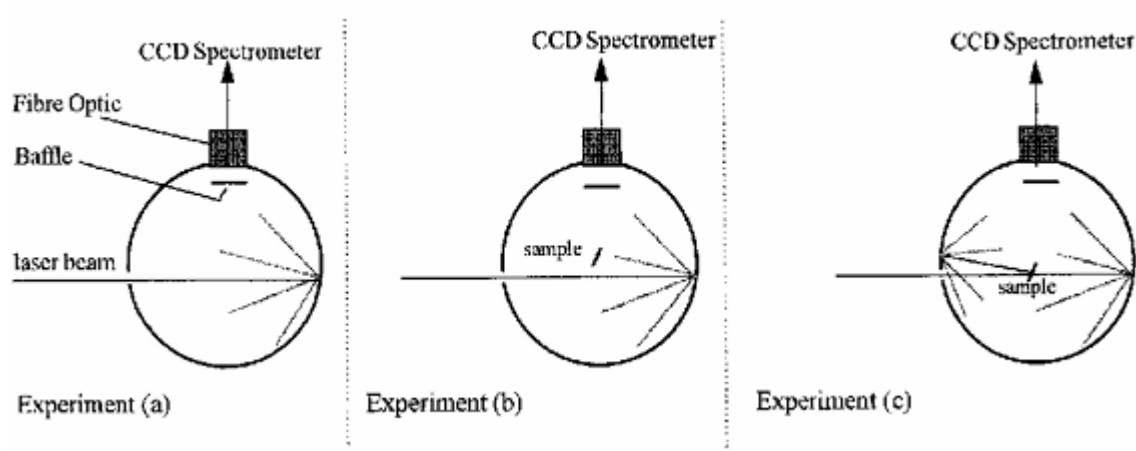


Fig 6: Diagram illustrating the three configurations of the sphere required for the efficiency measurement: a) the sphere is empty; b) the sample is in place and the laser beam is directed onto the sphere wall; c) the sample is in place and the laser beam is directed onto the sample.

### Components Used in PL Measurement

1. ICCD – Intensified Charge-Coupled Device: A high-sensitivity spectrometer used to detect and record emission spectra (both PL and laser scattering). Used in all three steps to record - Laser-only spectrum, Background spectrum, Emission + laser + PL spectrum.
2. Laser Source: Provides the excitation light, typically a 405 nm or 457.8 nm monochromatic laser. Aligned to enter the input port of the integrating sphere. The beam must be focused either:
  - Away from the sample (Step 2 – indirect),
  - Or directly on the sample (Step 3 – direct).
3. Integrating Sphere: A diffusely reflective hollow sphere that evenly redistributes all emitted and scattered light. Allows collection of total emission regardless of angular direction, including re-emitted and waveguided light. Ensures that both scattered laser light and PL emission are integrated over the whole sphere surface.

4. Sample Holder Holds either a blank quartz substrate (for background and laser-only steps) or the actual MEH-PPV-coated sample. Position must be adjusted so that:

- In Step 2, laser does not directly hit the sample,
- In Step 3, the sample is directly in the laser path.

5. Calibration Lamp (optional but recommended): Provides a known spectral reference for calibrating the ICCD response. Ensures intensity measurements are wavelength-corrected for reliable PLQY calculations.

6. Laser Beam Block / Shutter: Used to turn off or block the laser during background collection (before Step 1). Ensures no unwanted light is recorded when acquiring baseline or background signals.

#### **PROCEDURE:**

- In Step 1, the laser-only spectrum is collected using the ICCD with no sample, just laser light entering the sphere -  $L_a$
- In Step 2, the sample is placed in the sphere but off the laser path, and a small hump of PL with dominant laser scatter is recorded -  $L_b$
- In Step 3, the sample is aligned in the laser path, leading to decreased laser intensity and visible PL emission in the spectrum –  $L_c, P_c$

#### **Equation (5):**

$$A = 1 - \frac{L_c}{L_b}$$

- A: Fraction of the laser light absorbed by the sample.
- $L_c$  Scattered laser light detected in setup (c).
- $L_b$  Scattered laser light detected in setup (b).
- Interpretation: If less scattered light reaches the detector in (c) compared to (b), it means the sample absorbed more light.

#### **Equation (6):**

$$(1 - A)(L_b + P_b)$$

- This accounts for non-absorbed light and background emission, where:
  - $P_b$ : Background PL emission from scattered light (experiment b).
  - $L_b$ : Scattered laser component not absorbed.

**Equation (7):**

$$L_c + P_c = (1 - A)(L_b + P_b) + \eta L_a A$$

- $P_c$ : PL signal measured when laser hits the sample (experiment c).
- $L_a$ : Initial laser intensity (no sample).
- $\eta$ : PLQY ( $\eta$ ), the value we want to calculate.
- Rearranging this leads us to the final formula for PLQY:

**Final PLQY Formula**

$$\eta = \frac{P_c - (1 - A)P_b}{L_a A}$$

- $\eta$ : Photoluminescence Quantum Yield.
- Numerator: Actual emission from the sample corrected for background PL.
- Denominator: Total laser light that was absorbed by the sample.



### III. RESULTS

The five different samples were given for which we are calculating and analysing the PL and PLQY.

1

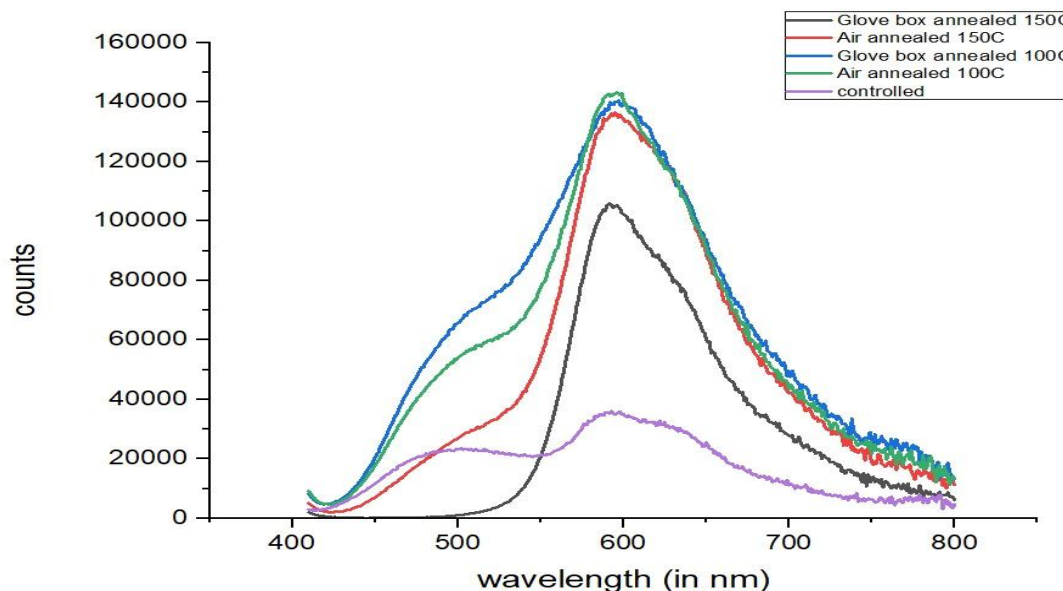


Fig 7: Intensity vs wavelength for the PL intensity observed for each sample

Sample Condition	Peak emission wavelength (nm)
Controlled	595
Air Annealed 100°C	608
Glovebox Annealed 100°C	612
Air Annealed 150°C	603
Glovebox Annealed 150°C	598

Table 1: Peak emission wavelength of each sample

Annealing Environment	Temperature (°C)	PL Intensity (a.u)
Controlled	None	72000
Air	608	145000
Glovebox (N <sub>2</sub> )	612	138000
Air	603	130000
Glovebox (N <sub>2</sub> )	598	102000

Table 2: PL intensity of each sample

#### PL Emission Peak Shifts and Interpretation

For the controlled sample, the emission peak wavelength is 599nm which is a baseline as there is no annealing the chains in the sample are disordered which limits conjugation

For the sample, which was annealed at 100C, the polymer chains gain energy to move and settle in a orderly manner. This increases the conjugation length (blue shift) therefore the material can absorb and emit more light

For the sample, which was annealed at 150C, oxygen reacts with the polymer chains, causing them to break. This creates defects and shortens the conjugation, reducing the material's ability to emit light efficiently.

For the sample, which was annealed in a glove box at 100C, glovebox annealing avoids oxidation, so while the chains become more ordered due to heat, they don't gain that extra rigidity, the conjugation length increases, but not as much as in mildly oxidized (air-annealed) films.

For the sample, which was annealed in a glove box at 150C, thermal energy alone can disturb the alignment of polymer chains. This leads to loss of order and a reduction in conjugation length, even without oxygen.

### Key Takeaways from Analysis:

- Red shift in emission is a sign of increased conjugation length or enhanced interchain interactions.
- Blue-shift indicates disruption in conjugation, caused either by oxidation (in air) or thermal disorder (in glovebox at high temp).
- The most intense and red-shifted PL emission occurs for air annealed at 100°C, where optimal chain packing occurs before oxidation starts.
- Glovebox 100°C has slightly less red-shift but avoids oxidative damage, making it structurally more stable despite marginally lower emission intensity.
- Air annealing at 150°C results in the most significant blue shift due to oxidation, breaking conjugation and lowering emission energy.

### PLQY Results Observed and Plotted on Origin software.

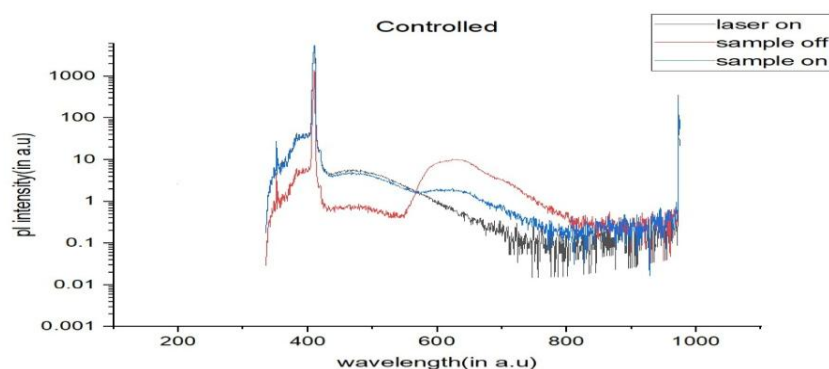


Figure 8: above represents the PL intensity vs Wavelength plots of controlled sample

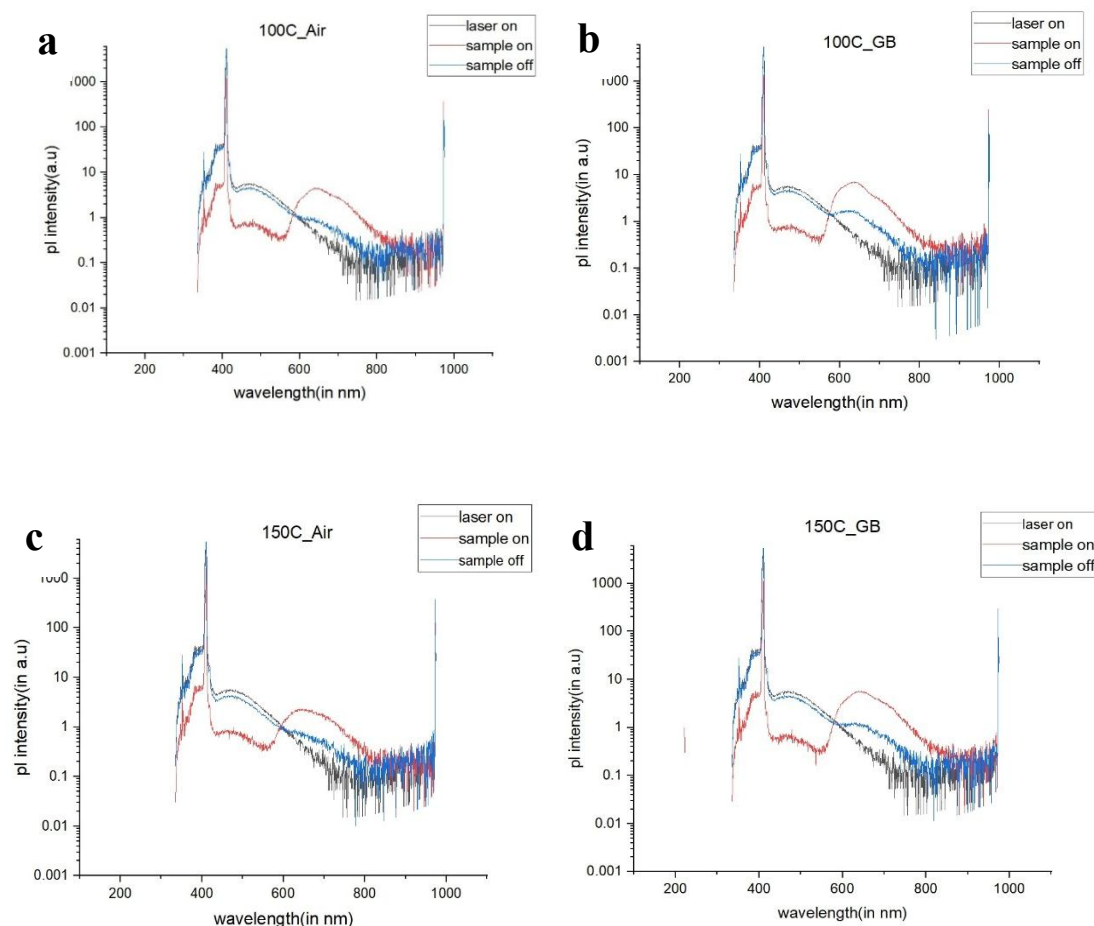


Figure 9: above represents the PL intensity vs Wavelength plots of each sample. The plot a, b, c, d are for control, 100\_C\_Air; 100\_C\_GB, 150\_C\_Air; 150\_C\_GB samples respectively. Each PL plot consists of Laser on (black), Sample off (blue) and sample on conditions (red).

Sample	L <sub>a</sub>	L <sub>b</sub>	L <sub>c</sub>	P <sub>a</sub>	P <sub>b</sub>	A	PLQY (%)
Controlled	19919	18736	3231	1050	262.094	0.82755	6.097
100C Air	19919	17473	3119	542.466	155.452	0.82149	3.146
100C GB	19854	16395	3684	301.097	138.82	0.77531	1.753
150C Air	19895	17787	3271	756.379	242.932	0.81606	4.384
150C GB	19853	17206	2817	676.262	168.547	0.83625	3.889

Table 3: Calculations of PLQY by using the formulae in the page no. 15 (Alternate instruments procedure)

- The highest PLQY was observed for the controlled (unannealed) sample because the unannealed sample keeps its long conjugation length because it hasn't been exposed to heat or oxygen. With fewer defects, most excited electrons emit light instead of being lost through non-radiative decay.
- For the 100C Air annealed sample, mild heating improves chain alignment and increases conjugation, but oxygen exposure causes some oxidation. This creates defects that reduce PLQY by increasing non-radiative energy loss.
- For the 150C Air annealed sample, oxidation breaks polymer chains, reducing conjugation length. This damage forms trap states, causing more non-radiative losses and the lowest PLQY.
- For the 100C Glove Box annealed sample, improves chain ordering and conjugation without oxidative damage. PLQY stays high, with only slight reduction due to mild thermal stress.
- For the 150C Glove Box annealed sample, heat disrupts chain alignment, reducing conjugation length. Though oxidation is avoided, thermal disorder lowers PLQY.

### **Takeaways from PLQY Trends**

1. Highest PLQY in the Control Sample indicates that no annealing is best for maintaining MEH-PPV's emissive efficiency if the device requires high photon output (e.g., OLEDs).
2. Annealing at 100 °C Improves Chain Packing especially in glovebox (inert) condition: enhanced order without oxidation → higher PLQY than 100°C air.
3. 150 °C Always Reduces PLQY: Regardless of atmosphere, higher temperature leads to oxidation in air environment and effective conjugation is reduced in glove box environment.

### **Correlations with Other Measurements**

- PL Peak Shifts: As noted in previous slides, higher annealing temperatures caused blue shifts, indicating reduced conjugation length.
- Bandgap Trends: Larger bandgaps in degraded samples (air-annealed at 150°C) show disrupted conjugation.
- TRPL Lifetimes: Shorter lifetimes correlate with lower PLQY, confirming higher non-radiative decay in degraded samples.

## IV. CONCLUSION

This study looked at how heating MEH-PPV films in different conditions (with and without oxygen) affects the material properties. When the film wasn't heated at all, it gave the best light output because the material stayed in its original, undamaged form. When heated gently at 100 °C in air, the chains in the material became more organized and glowed brighter, but the presence of oxygen caused some damage, slightly reducing efficiency. Heating in a glovebox (with no oxygen) at 100 °C gave both good organization and high efficiency, making it the best balance overall.

However, when the film was heated too much — especially at 150 °C in air — the material started to break down. The oxygen combined with the heat caused damage to the chains, making the glow weaker and shifting its color. Even without oxygen (in the glovebox), high heat alone caused the chains to twist and become disordered, reducing the efficiency. So, gentle heating helps the material glow better, but too much heat — especially with oxygen — breaks it down and makes it worse. Choosing the right heat treatment depends on how the material will be used in devices.

### Future applications

- Control Samples (Unannealed): Suitable for high-efficiency light-emitting devices like OLEDs and fluorescence sensors.
- 100 °C Glovebox Annealed: Ideal for stable, flexible devices such as organic lasers, bioimaging, and photodetectors.
- 100 °C Air Annealed: Useful in organic solar cells (OPVs) where strong light absorption is needed.
- 150 °C Glovebox Annealed: Can be used in thin-film transistors or charge transport layers.
- 150 °C Air Annealed: Applicable in quenching layers or degradation studies.

## REFERENCES

- [1]. Greenham, N. C., Samuel, I. D. W., Hayes, G. R., Phillips, R. T., Kessener, Y. A. R. R., Moratti, S. C., Holmes, A. B., & Friend, R. H. (1995). Electroluminescence in conjugated polymers. *Chemical Physics Letters*, 241(1), 89–96. [https://doi.org/10.1016/0009-2614\(95\)00576-Q](https://doi.org/10.1016/0009-2614(95)00576-Q)
- [2]. Palsson, L. O., Wang, C., Monkman, A. P., Bryce, M. R., Rumbles, G., & Samuel, I. D. W. (2002). Photophysics of MEH-PPV in solution. *Journal of Physical Chemistry B*, 106(38), 9842–9849. <https://doi.org/10.1021/jp020871u>
- [3]. Lin, L. C., Meng, H. F., Shiu, S. C., Chan, C. H., Tsao, C. H., & Horng, S. F. (2003). Excitation power dependence of photoluminescence in conjugated polymers. *Physical Review B*, 68(7), 075203. <https://doi.org/10.1103/PhysRevB.68.075203>