

# **Understanding the structure-optical property relationship in new organic materials: Design, synthesis and OLED applications**

A Thesis

submitted

by

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for the award of the degree of

**Doctor of Philosophy**



**School of Basic Sciences  
Indian Institute of Technology Mandi**

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*To the memories of Asha*

*&*

*To my beloved Parents*

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### Declaration by the Research Scholar

This is to certify that the thesis entitled “**Understanding the structure-optical property relationship in new organic materials: Design, Synthesis and OLED applications**”, submitted by me to the Indian Institute of Technology Mandi for the award of the degree of Doctor of Philosophy is a bonafide record of research work carried out by me under the supervision of Dr. Subrata Ghosh. The contents of this thesis, in full or in parts, have not been submitted to any other Institute or University for the award of any degree or diploma.

In keeping with the general practice of reporting scientific observation, due acknowledgements have been made wherever the work described is based on the findings of other investigators.

Mandi 175001  
Date:

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### Thesis Certificate

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Research Guide

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## Abbreviations

A.....	acceptor
ACQ.....	aggregation caused quenching
Ag.....	silver
AIE.....	aggregation induced emission
CE.....	current efficiency
CIE.....	commission internationale de l'eclairage
CT.....	charge transfer
CV.....	cyclic voltammetry
D.....	donor
DCM.....	dichloromethane
DMF.....	dimethylformamide
DMSO.....	dimethylsulfoxide
EA.....	electron acceptor
ED.....	electron donor
EL.....	electroluminescence
EM.....	electromagnetic
HTL.....	hole transport layer
EML.....	emission layer
EQE.....	external quantum efficiency
ESI.....	electrospray ionization
ETL.....	electron transport layer
eV.....	electron volt
Fc.....	ferrocene
HIL.....	hole injection layer
HOMO.....	highest occupied molecular orbital
HRMS.....	high resolution mass spectrometry

ICP-OES..... inductively-coupled plasma-optical emission spectroscopy

ITO.....indium tin oxide

J-V-L.....current density-voltage-luminescence

KBr.....Potassium bromide

LUMO.....lowest unoccupied molecular orbital

*m.p.*.....melting point

NMR.....nuclear magnetic resonance

OLED.....organic light emitting diode

ORTEP.....oak ridge thermal ellipsoid plot

PE.....power efficiency

PLQY..... photoluminescence quantum yield

QY..... quantum yield

SSL.....solid state lighting

TD-DFT.....time-dependent density functional theory

$T_g$ .....glass transition temperature

TGA.....thermo gravimetric analysis

UV.....ultraviolet

Vis.....visible

3-D.....three dimensional

$\lambda_{ex}$ .....excitation wavelength

$\lambda_{em}$ .....emission wavelength

## **Abstract**

Organic materials provide advantages such as design flexibility, cost effective synthesis and tuning of optical properties and thus the organic semiconducting materials have been the subject of active research and widely applied in the areas of organic light-emitting diodes, field-effect transistors, nonlinear optics, photovoltaic devices, biological fluorescent probes, and so on. The commercialization of high efficiency organic light-emitting diodes (OLED) has revolutionized solid state lighting and display technologies. The future of OLEDs depends on the availability of solid state emissive organic materials having efficient quantum yield and balanced charge carrier transport properties. Although many emissive organic materials have been developed and many useful display and lighting products based on OLED devices are available in the market there remains a wide scope to study structure based optical properties and their underlying emission mechanisms. Aggregation of luminophores affects luminescence efficiency of organic materials. Therefore, the research of luminescent solid state organic materials has been and continues to be one of the hot topics for research community. In this regard, our focus has been to develop efficient solid state emitters through chemical structure engineering. In order to make a useful contribution to the literature, new organic frameworks were synthesized and their photophysical properties were studied deeply.

This thesis seeks to understand the optical properties of OLED materials in solid state and provides a systematic study to tether the emission property in solid state to the coumarin derivatives which are known to lack emission in solid state despite of their tremendous emission property in solutions. This is accomplished through the manipulation of intermolecular interactions at molecular level and packing arrangement in the solid state. It was also found that through careful manipulation of the intermolecular interactions and packing arrangement, tuning of emission color

could be achieved through simple design strategies. The practical applications of acquired strategy are the white and green emitting diodes. The understandings at molecular level were further utilized to explore other material designs for other color emitters in visible region.

This thesis also seeks to introduce synthetic techniques towards the development of new dual state emitters and deep blue emitters. The understanding of intramolecular charge transfer process in consort with molecular geometry along with the molecular level understanding of intermolecular interactions and packing arrangement helped to develop organic materials with blue and green emission. The developed green emitters was found to have dual state emission characteristic. As a result of these design strategies, the green and deep blue emitters were obtained and corresponding green and blue emitting diodes were fabricated. The positive aspect of the present thesis is the theoretical simulation to study the designed architectures. The experimental findings were well supported by density functional theory (DFT) calculations and also, the DFT calculations were used to design materials in the present study. The support of theoretical calculations to the experimental results and vice versa proved the importance of theoretical studies in material designs.

Hence, a combination of synthetic development, molecular level understanding, theoretical studies and device applications led to understand of the key issues associated with the solid state emitters particularly those which are used as emitters in OLEDs.