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# Determining the Mobility of Charge Carriers in Organic Semiconductors

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MASTERS' THESIS

*Submitted in partial fulfillment of the requirements of  
BITS F421T Thesis*

*By*

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# Declaration of Authorship

I, Pranay VENKATESH, declare that this Masters' Thesis titled, 'Determining the Mobility of Charge Carriers in Organic Semiconductors' and the work presented in it are my own. I confirm that:

- This work was done wholly or mainly while in candidature for a research degree at this University.
- Where any part of this thesis has previously been submitted for a degree or any other qualification at this University or any other institution, this has been clearly stated.
- Where I have consulted the published work of others, this is always clearly attributed.
- Where I have quoted from the work of others, the source is always given. With the exception of such quotations, this thesis is entirely my own work.
- I have acknowledged all main sources of help.
- Where the thesis is based on work done by myself jointly with others, I have made clear exactly what was done by others and what I have contributed myself.

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# Certificate

This is to certify that the thesis entitled, “*Determining the Mobility of Charge Carriers in Organic Semiconductors*” and submitted by Pranay VENKATESH ID No. 2019B2A11004P in partial fulfillment of the requirements of BITS F421T Thesis embodies the work done by him under my supervision.

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# *Abstract*

Master of Science

## **Determining the Mobility of Charge Carriers in Organic Semiconductors**

by Pranay VENKATESH

The Thesis Abstract is written here (and usually kept to just this page). The page is kept centered vertically so can expand into the blank space above the title too...

# *Acknowledgements*

The acknowledgements and the people to thank go here, don't forget to include your project advisor. . .

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# Abbreviations

**LAH** List Abbreviations **Here**

# Physical Constants

$$\text{Speed of Light } c = 2.997\,924\,58 \times 10^8 \text{ ms}^{-\text{s}} \text{ (exact)}$$



*Dedicate this to someone, anyone.*

# Chapter 1

## Introduction

### 1.1 Semiconductor Materials

### 1.2 Electronic Structure

The electronic structure is the solution of the quantum states of electrons in a given chemical system. Typically, this involves determining the energies and wavefunctions of the various states. This can be done by solving the Schrödinger equation for molecules.

### 1.3 Phonons

## Chapter 2

# Organic Semiconductor Materials

### 2.1 Introduction

### 2.2 Rubrene

### 2.3 Y6



## Chapter 3

# Polarons

### 3.1 Introduction

### 3.2 Pekar's Polaron

### 3.3 Fröhlich Polaron

### 3.4 Holstein Polaron

### 3.5 Feynman Variational Approach to the polaron problem



## Chapter 4

# Path Integrals and Quantum Dynamics

### 4.1 Introduction

### 4.2 Dynamics of Open Quantum Systems

#### 4.2.1 Liouville-von Neumann Equation

#### 4.2.2 System-Bath Models and The Reduced Density Matrix

#### 4.2.3 Quantum Master Equations

#### 4.2.4 Adiabatic and Markov Approximations

### 4.3 Path Integral Formulation

### 4.4 Quasi-Adiabatic Propagator Path Integral (QuAPI)

### 4.5 Quantum-Classical Path Integral (QCPI)

### 4.6 Evaluating Path Integrals

### 4.7 Calculating Relevant Properties

#### 4.7.1 Mobility

## Appendix A

# Appendix Title Here

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