

	INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI SHORT ABSTRACT OF THESIS	
	Name of the Student	: MOHD SHAVEZ
Roll Number	: 166122041	
Programme of Study	: Ph.D.	
Thesis Title: Designing donor-acceptor oligomers and small molecules for photovoltaic applications: Insights from computational studies		
Name of Thesis Supervisor(s)	: Prof. Aditya Narayan Panda	
Thesis Submitted to the Department/ Center	: Department of Chemistry	
Date of completion of Thesis Viva-Voce Exam	: 02-02-2022	
Key words for description of Thesis Work	: Organic Solar cell, Charge transport and Charge transfer properties, DFT and TDDFT	

SHORT ABSTRACT

The thesis entitled “Designing donor-acceptor oligomers and small molecules for photovoltaic applications: Insights from computational studies” describes how small changes in the molecular architecture can have significant effect on the photovoltaic properties. In particular, design strategies of new donor-acceptor oligomers and small molecules with promising photovoltaic applications are presented, and their structural, optoelectronic, charge transport, and charge transfer properties are reported. The thesis has been divided into seven chapters as follows:

Chapter 1 introduces the field of organic solar cells, and discusses the working methodology and various parameters used to characterize the solar cells.

Chapter 2 reports the theoretical and computational methodologies including the Hartree-Fock, DFT and TDDFT methods and the Marcus theory for charge transfer in detail.

Chapter 3 reports a detailed DFT study on the structural, optoelectronic and charge transport properties of a series of BDT-TAZ based conjugated oligomers.

Chapter 4 shows effects of halogenation on structural, optoelectronic and charge transfer properties of a series of BDT based small molecules as donors and PCBM as acceptor.

Chapter 5 describes the effects of insertion of various Π bridge units on structural, optoelectronic and charge transfer properties of BDTT-TT-F based oligomers and their blends with PCBM.

Chapter 6 explores the effects of Π bridge units in a random oligomer-based donor. In addition, charge transfer properties are also explored by making blends with a non-fullerene acceptor.

Chapter 7 presents the summary of the thesis work.