PREPARATION OF Π-CONJUGATED POLYMERS AND EVALUATION OF THEIR
PHOTOVOLTAIC PROPERTIES

ABSTRACT

The present thesis deals with synthesis, characterization and evaluation of thermal, electrochemical, photoluminescence properties of a few new 1,1'-bis-2-naphthol based polyurethanes, side chain and main chain azomethine linkage containing polythiophenes and polycarbazole derivatives. A considerable effort has been devoted to the synthesis of polymers with special emphasis on the solubility, optical and electrochemical properties of π-conjugated polymers. The thesis also provides an account of photovoltaic performances exhibited by the polymers. The contents of the thesis have been compiled into five chapters.

Chapter 1 deals with the general introduction of π-conjugated polymers and their application in photovoltaic devices. A brief review of synthetic procedures, optical properties, electrochemical properties of conjugated polymers is presented. General aspects of the device, device characterization and different types of device architectures for polymeric photovoltaic cells have been described in this chapter. This chapter also describes objectives along with the plan and methodology.

Chapter 2 describes the synthesis and characterization of monomers and polymers and thermal properties of polymers. We have synthesized the following polymers.

i) Poly [N,N-bis-(2-thienylmethylene)-o-dianisidine] (PBTD)
ii) Poly [(3-phenyl azomethine ethyl) thiophene] (PPAET)
iii) Poly [(3-phenyl azomethine butyl) thiophene] (PPABT)
iv) Poly[(9-dodecylcarbazole)] (PDDC)
v) Poly[(9-dodecylcarbazole)-co-thiophene] (PDDCT)
vi) Poly(tolyl-1,1'-binaphthyl carbamate) (PU₁)
vii) Poly(hexamethylene-1,1'-binaphthyl carbamate) (PU₂)

The synthetic procedures of monomers and polymers are discussed in this chapter. The monomers were characterized by FTIR, ¹H NMR and CHN analyzer. The synthesized polymers
were also thoroughly characterized by FTIR, $^1$H NMR, and molecular weights of polymers were
determined by GPC analysis. The physical parameters and thermal properties of the polymers
were also evaluated and are discussed in detail.

Chapter 3 reports the electrochemical and the optical properties of synthesized polymers.
The oxidation and reduction potential of polymers were assessed in cyclic voltammetry method.
Furthermore, band gap of polymers was measured by electrochemically and compared with the
optical method. The relative PL quantum yield of polymers with respect to Rhodamine B dye
was measured. The PL quenching of the polymers in the presence of TiO$_2$ nanoparticles in
solution have been observed. This explains the suitability of TiO$_2$ nanoparticles as electron
acceptor in hybrid photovoltaic devices indicating ultrafast electron transfer from donor polymer
to acceptor.

Chapter 4 includes the study of photovoltaic performance of the synthesized polymers.
Single layer, bulk heterojunction, hybrid organic-inorganic and host-guest approach of solar cells
for the developed conjugated polymers have been reported. The polymers show the power
conversion efficiency in the range 0.019-0.38%.

Chapter 5, the last chapter of the thesis includes the concluding remarks, highlights of
the findings and future scopes of the present investigation. 1,1'-bis-2-naphthol based
polyurethanes, side chain and main chain azomethinic linkage containing polythiophens, and
polycarbazole derivatives have been synthesized using condensation and oxidative coupling
methods. The polymers are soluble in organic solvents and found thermally stable. The optical
and electrochemical properties showed that the polymers bear the potentiality to be used in
photovoltaic devices. The optical band gap of the polymers calculated was in the range of 2.1-3.4
eV. The utility of the polymers as photovoltaic materials has been studied by fabricating the
devices with different structural approaches and showed significant performance.