In recent years, π-conjugated polymers have been subjected to extensive study as regards their potential applications in transistors, photovoltaic devices, polymer light-emitting diodes, photorefractive devices and in non-linear optical devices. Conjugated polymers continue to fascinate many scientists due to their several advantages such as low cost, processability, high optical contrast, high stability etc. The major goal of the present investigation was to synthesize low band gap polymers possessing both photoconducting and non-linear optical property. Four major objectives of the present study are listed here under:

- Synthesis of the copolymers using direct arylation and Suzuki coupling methods.
- Explore the application of conjugated polymers as active layer in photoconducting devices.
- Explore the application of conjugated copolymers in non-linear optical devices.

The thesis is comprised of seven chapters.

The first chapter consists of a concise introduction to some fundamental principles of photoconducting and non-linear optical (NLO) polymers. The first section begins with the tool box for band gap engineering to produce low band gap conjugated polymers, followed by different polymerization methods for obtaining the D-A copolymers. In the next section, the use of quantum chemical tools for designing the active layer polymers is
explained. This chapter concludes with scope and aim of the work presented in the thesis.

**Chapter 2** deals with theoretical and experimental investigations on the photoconductivity and non-linear optical properties of 3,4-ethylenedioxythiophene (EDOT)-fluorene copolymer. EDOT-fluorene copolymer was synthesized via a simple and facile method, direct arylation polycondensation reaction. Structure of the copolymer was confirmed by FT-IR, $^1$H NMR and XPS. Electronic structure and properties were investigated by DFT theory using periodic boundary condition formalism. Photophysical, electrochemical and thermal properties are also included. Optical limiting property is presented.

**Chapter 3** deals with design, synthesis and third-order non-linear optical properties of 3,4-ethylenedioxythiophene-chalcogenadiazole donor-acceptor copolymers via direct arylation method. Copolymers of EDOT with benzothiadiazole and benzoselenadiazole are investigated by theoretical and experimental (optical and electrochemical) methods. Non-linear absorption and non-linear refraction properties were determined by open aperture and closed aperture z-scan technique, respectively. In addition, suitability of the copolymers for optical limiting application is studied.

**Chapter 4** includes synthesis and third-order NLO properties of low band gap 3,4-ethylenedioxythiophene-quinoxaline copolymers. The effect of structural changes of quinoxaline derivatives on the band gap of EDOT-quinoxaline copolymers are investigated by theoretical calculation (DFT theory) and experimental methods like UV-Visible absorption spectroscopy and electrochemical methods. Third-order NLO properties were evaluated by z-scan technique and are included in this chapter. The optical limiting properties of EDOT-quinoxaline copolymers are also discussed.

**Chapter 5** discusses electronic structure calculation, synthesis and third-order NLO properties of EDOT-thiophene copolymers. Copolymers were
synthesized by direct arylation polycondensation reaction. Structure of the synthesized copolymer was confirmed by FT-IR, ¹H NMR, and XPS. Thermal properties of the copolymer were studied using TG and DSC analysis. Optical studies were done by using UV-Visible absorption spectra and photoluminescence spectra. Third-order NLO properties were determined using z-scan technique and the optical limiting properties are also presented.

**Chapter 6** focusses on the electronic structure, synthesis and third-order NLO properties of novel phenothiazine-triazine copolymer. Copolymer was synthesized via standard Suzuki coupling reaction of phenothiazine with piperidine substituted triazine. The theoretically determined frontier energy levels and energy gap of copolymer agreed with experimentally determined optical and electrochemical results. The third-order NLO properties and optical limiting behaviour of the polymer was also investigated.

The conclusions drawn from each part of the work and references are given at the end of each chapter. The summary and outlook of the work done are presented as the final chapter.