One crucial aspect of designing organic energy materials is understanding the role of molecular structures and their impact on their properties. In this thesis, an attempt has been made to develop the structure-property relationship by considering examples of different organic electronic materials with application potential in harvesting solar energy and organic light-emitting diodes through computational chemistry methods. Fundamental challenges in the design and development of organic electronic materials and the scope of the investigation are presented in **Chapter 1**.

The possible development of a structure-aromaticity-conjugation spectroscopy relationship (SACSR) is presented in **Chapter-2**.

Chapter 3 presents the design of a series of organic dye molecules using ullazine and perylene employing D-π-A topology, with ullazine analogs as donors and perylene dicarboxylic anhydride as an acceptor along with acetylene linker as π-bridge for DSSC applications. The findings will be beneficial in designing efficient and cost-effective organic dyes for solar energy conversion.

A comprehensive investigation into the optoelectronic properties of electron donor-based molecules, having Isoindigo (IIG) moiety for their potential application in efficient OSCs is described in **Chapter 4**. Findings highlight the potential of central group modifications and spacer effects in enhancing the efficiency of organic solar cells for the D_2-A-π-D_1-π-A-D_2 framework. These findings contribute to the ongoing development of sustainable and efficient solar energy technologies based on organic materials.

Chapter 5 focuses on the design and characterization of a series of triazine-based systems for OLED applications utilizing the TADF mechanism. The molecules investigated include diphenylamine (DPA), triphenylamine (TPA), carbazole (Cbz), indolocarbazole (ICbz), dimethyl acridine (DMAC), phenoxazine (PXZ), phenothiazine (PTZ), diphenyl acridine (DPAC), diphenyl azasiline (DPAS), spiro acridine fluorene (SAF), and spiro silole azasiline (SSiAS). The findings point out the potential of these molecules as blue emitters and underscore the importance of further investigations to optimize their performance and efficiency. The insights gained from this research contribute to the advancement of organic electronics, specifically in the development of high-performance OLED devices.

Chapter 6 summarizes the primary results and conclusions that were derived from the present investigation.