
Abstract

Introduction

In the recent years, the predicted exhaust of fossil fuels actuated the world to search for an alternative source of energy for their increased necessity. Only the renewable energies will be able to compensate the demand. Optoelectronics is the best alternative of energy which includes photovoltaics, OLEDs, etc. The sun is the infinite source of renewable energy. So the most affordable technology to get more energy is the photovoltaics, the emerging technology in the field of optoelectronics. Another way of conserving the energy is to use it efficiently with less energy to produce more light. Here OLEDs comes into the picture. Developing efficient materials for Optoelectronics is the challenging task. Theoretical methods have been playing significant role to model efficient optoelectronic material. This thesis is organised in to five chapters.

Chapter 1

This Chapter includes introduction and classifications of various optoelectronic devices such as silicon solar cells, DSSC and OLED and materials involved in these devices. Further various DFT methodologies which are used to successful design of the materials for these applications are discussed in detail. The main role played by these materials and computational explanation for the suitability of the molecules for the applications are discussed.

Chapter 2

This chapter describes a study of the molecules TCNQ and F4-TCNQ surface doped on hydrogen-terminated Si (111) surface [H-Si(111)], with emphasis on the role of van der Waals interactions in stabilizing the molecular adsorption orientations and the binding energy using density functional theory(DFT).

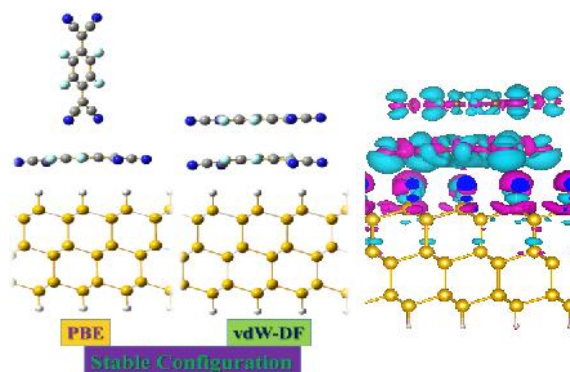
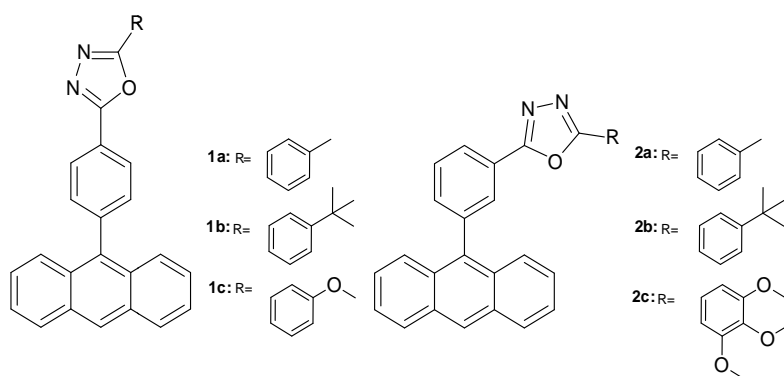
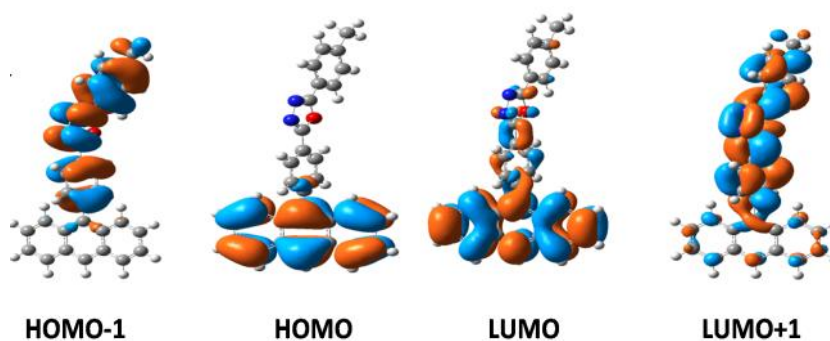


Figure 1

The most stable spatial configuration of the adsorbed molecules predicted with and without including the dispersion energy in a low concentration dopant system is same though the magnitude of the binding energy is much larger in the former case. On the other hand in the case of increased dopant concentration the adsorption orientations predicted with and without the inclusion of dispersion energy are different and so is the magnitude of the binding energy. It is concluded that inclusion of dispersion energy term is important for correct prediction of the spatial configurations of the adsorbed molecules in surface transfer doping of semiconductors. Finally it is observed there is a charge transfer from H-Si(111) to dopant as shown in **Figure 1**.

Chapter 3

In this chapter, opto-electronic and charge transport properties of the six Anthracene-Oxadiazole derivatives (**1a-1c** and **2a-2c**) (Scheme 1) which show promising charge transport properties in OLED are studied using DFT and TD-DFT methodologies. Estimated reorganization energies, charge transfer integrals witness the importance of these molecules as emitters and charge transporters in the OLED device development. For a good charge transporter well stacked crystal structure is required.

**Scheme 1****Figure 2 FMOs of 1a**

Chapter 4

This chapter dealt with the two A-D-A type TPA derivatives (**TPA1** and **TPA2**) with different number of anchoring carboxylic acid groups showing different efficiencies in DSSCs. Their photo voltaic performance difference is explained by DFT, TD-DFT and periodic DFT calculations. TD-DFT data is well harmonized with experimental UV-Vis absorption data. Periodic DFT calculations were carried out on nanocrystalline TiO_2 modeled with a slab of 5×8 super cell of $\text{TiO}_2(101)$ anatase phase and the dyes were tethered on to the surface in different adsorption modes such as bi-dentate bridging mode(BB), mono-dentate(BB) and two mono-dentate modes (M-M) (Figure 3) among which two mono-dentate mode(M-M) show strong adsorption energy which could be reason for high efficiency in DSSC. From the isosurface plots of highest occupied molecular orbital (HOCO) and least unoccupied crystal orbital (LUCO) of the dyes adsorbed on to the $\text{TiO}_2(101)$ there is a charge transfer clearly observed from dyes to $\text{TiO}_2(101)$ surface.

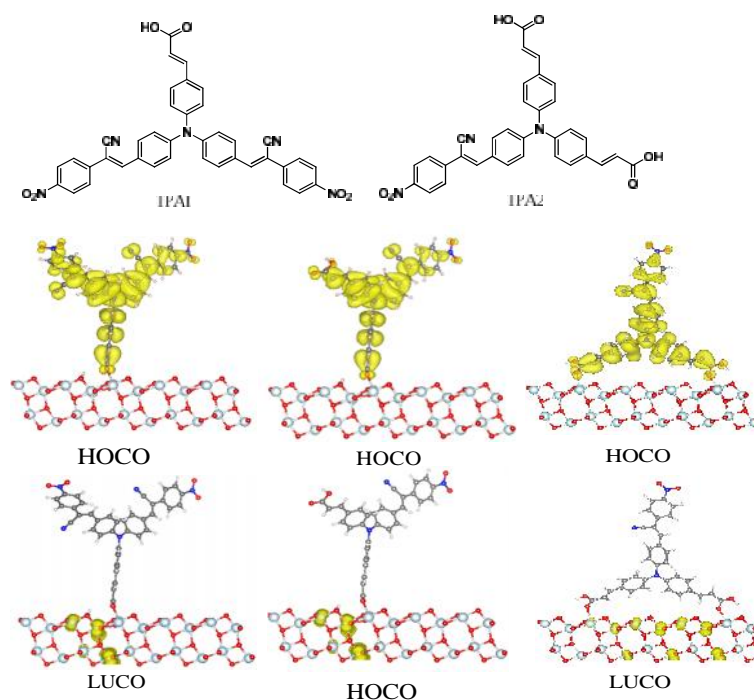
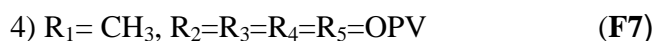
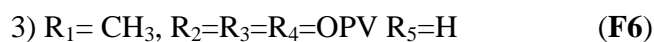
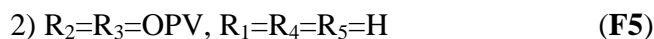
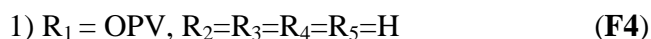
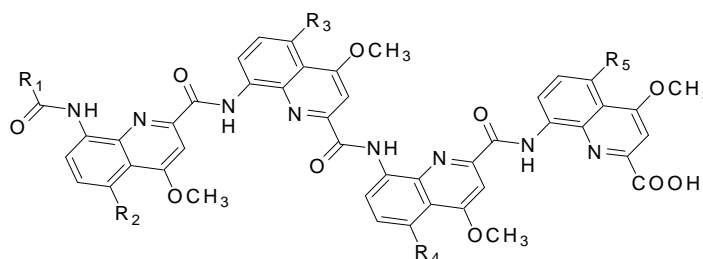


Figure 3 Crystal orbitals of **TPA1** (BB mode) and **TPA2** (BB and M-M mode)

Chapter 5

In this chapter, a new class of helically folded quinolinemolecules has been suggested possessing the charge transfer property. Five quinoline derived tetramer molecules **F4- F7** (Scheme 2) has been designed appended with donor OPV (oligo(p-phenylene vinylene) as donor

varying in number and position on Q4 ring and –COOH group as acceptor. The detailed computational investigation has been carried out to predict the charge transfer and charge delocalization behavior of folded molecule and its corresponding linear form. The folded form of each molecule shows the higher intensity of charge transfer as compare with corresponding linear form. LUMO in folded form is delocalized over the entire quinoline tetramer unlike the linear form where it is localized only on the fourth quinoline ring and –COOH region. This theoretical investigation demonstrates that helical quinoline ring act as a conjugate bridge during the charge transfer from donor to acceptor which breaks in the linear form. Owing to a higher intensity and presence of conjugation in charge transfer for such kind of foldamers may have significant use in the field of material science.



Scheme 2