DENSITY FUNCTIONAL THEORETICAL INVESTIGATION OF SOME SOLAR CELL MATERIALS

DOCTOR OF PHILOSOPHY

in

PHYSICS

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Abstract

We report density functional theoretical investigation on some solar cell materials namely- dye-sensitized quantum dots, polymers, perovskites and green materials, which are collectively known as the third generation of solar cells.

Chapter 1 of the thesis presents a brief survey of literature related to different generations of solar cell technology [1].

Chapter 2 presents the methodology that is used to calculate the properties of our model systems in this research work. We have used density functional theory (DFT) [2] to calculate structural and electronic properties and time dependent density functional theory (TDDFT) [3] for optical properties. Projected density of states has been calculated using Mulliken population analysis (MPA) [4]. The charge transfer has been studied with the help of natural transition orbitals (NTO) [5]. All the calculations have been performed using Gaussian G09 package [6] based on density functional theory.

In Chapter 3, we have performed a DFT investigation on some factors affecting the nature of charge transfer in CdS quantum dots (QDs) of two different sizes attached to one or two units of dyes among three species viz., coumarine (C343), fluorescein (FLU) and NKX-2388 (NKX). The strength of interaction of the dye and QD depends on the orientation of the dye unit(s) and the type of anchoring group of the dyes and even the direction of charge transfer reverses for different orientation of the dye with respect to the QD in some systems.

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In Chapter 4, we have performed DFT study on some polythiophene and polysilolebased polymers. We found that different pull groups produce direct or

indirect band gaps. Interestingly, there is a phase reversal in LUCO iso-surfaces of direct and indirect band gap polymers.

In Chapter 5, we have studied polymer-PCBM assembly with the help of DFT. The NTO analysis shows that nature of charge transfer varies for different polymers and mode of attachments.

In Chapter 6, DFT studies on all inorganic perovskite, particularly $CsPbBr_3$ quantum dots (QDs) for the investigation of the role of stochiometry, shape and the effect of ligands is presented. It is observed that charge transfers occurs from p-orbitals of Br- ions to p-orbitals of Pb^{+2} ions in all the structures and there is no involvement of Cs+ ions.

In Chapter 7, we report detailed DFT studies on QDs made of three different compositions of "green" materials in the core/shell configuration, viz., CISe/CIS, CISe/ZnS, CISe/ZnSe. The absorption spectrum shows that the frequency range of light absorption can be tuned by varying the core/shell compositions.

References

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