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Computational Study of polymeric photovoltaic materials

by

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Declaration

The work described in this thesis was carried out by me under the supervision of Dr. Susil J.Silva, Senior lecturer in chemistry at University of Sri Jayewardenepura and a report on this has not been submitted in whole or in part to any university or any other institution for another Degree or Diploma.

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22/09/2009

I certify that the above statement made by the candidate is true and that this thesis is suitable for submission to the University of Sri Jayewardenepura for the purpose of evaluation for the award of the M.Sc in polymer science and technology.

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Abbreviations

Ac - Alternative current

au – Atomic unit

CB- Conduction Band

CN – Cyano

DC – Direct current

DFT - Density Functional Theory

eV – Electron Volts

HF - Htree- Fock

HOMO – Highest occupied molecular orbital

LUMO - Lowest unoccupied molecular

Oligo - Oligomers

PANI – Polyaniline

PE – Polythene

PPV – Poly Phenylvinylene

PS – Polystyrene

PV – Photovoltaic

PVC – Poly Vinyl Chloride

VB – Valance Band

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ABSTRACT

Quantum-chemical techniques were used to calculate the band gaps in several monomers (Aniline, Acetylene, phenyl vinyl, 1-Cyaono-2 phenyl Ethyne Phenyl Ethyne) oligomers and polymers of these monomers and compared with non photovoltaic monomers, Oligomers and polymers. The band gap calculations on this study was performed by density functional theory (DFT) (B3LYP/3-21G), (B3LYP/6-31G*) and(PBEPBE/6–31G*). Experimental band gap values of photovoltaic materials are less than 1.8eV . The results indicate that calculated band gaps of photovoltaic polymers are in good agreement with the experimental values but some non photovoltaic polymers have also same values.

CHAPTER 01

INTRODUCTION

1.1 Photovoltaics [1], [2]

Due to growing demand of renewable source of energy, manufacture of solar cells and photovoltaics has expanded significantly in recent years. Photovoltaics are field of technology which is converting sun light direct in to the electricity using semi conductors. Solar cells produce direct current (DC) from light, which can be use for many purposes, such as power equipments, recharge the batteries, etc as seen in figure 1.1 below. In power equipments most of the time has to use a inverter to convert DC in to AC. The first practical application of photovoltaics was to power orbiting satellites and other spacecraft, but today the majority of photovoltaic modules are used so many applications,

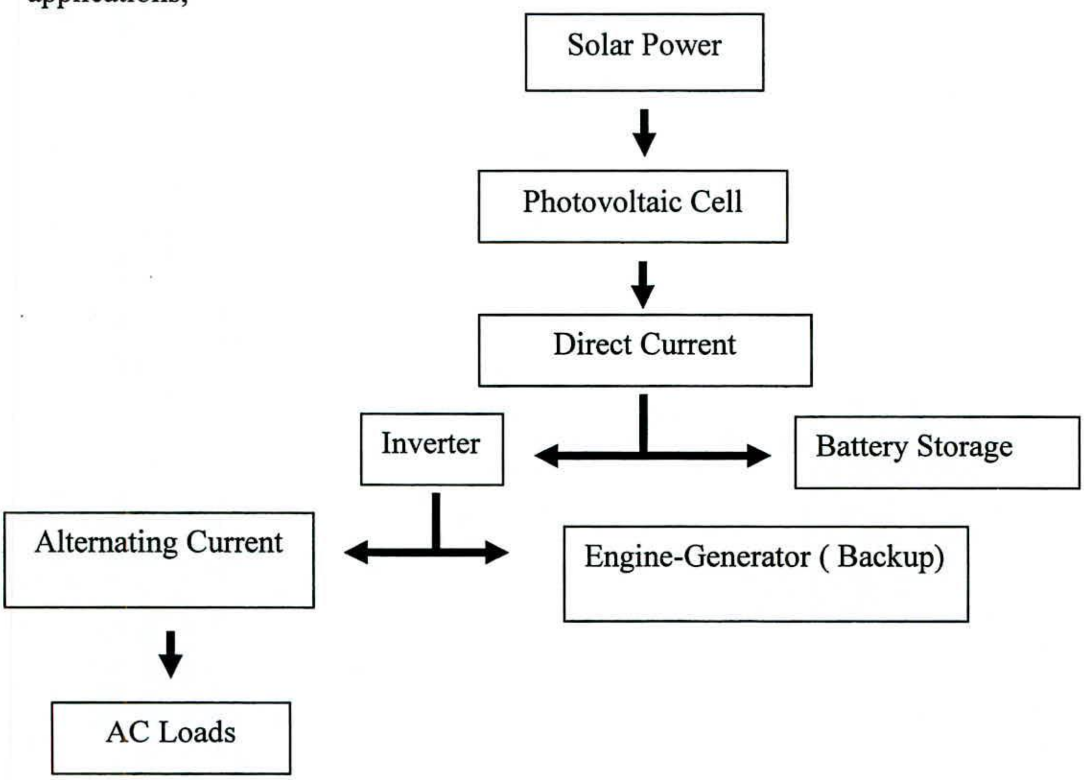

Figure 1.1 – Conversion of sunlight in to electricity by photovoltaic effect

Mainly there are two types of photovoltaics.

- Inorganic photovoltaics – Silicon based devices
- Organic photovoltaics / Polymeric photovoltaics

1.2 Silicon based inorganic photovoltaics [3]

Modern solar cells are based on semiconductor physics. They are basically P-N junction photodiodes with a very large light-sensitive area. The photovoltaic effect, which causes the cell to convert light directly into electrical energy, occurs in the three energy-conversion layers as seen in figure 1.2.

- 1st Layer - Top junction layer
- 2nd Layer – Absorbing layer
- 3rd Layer - Back junction layer

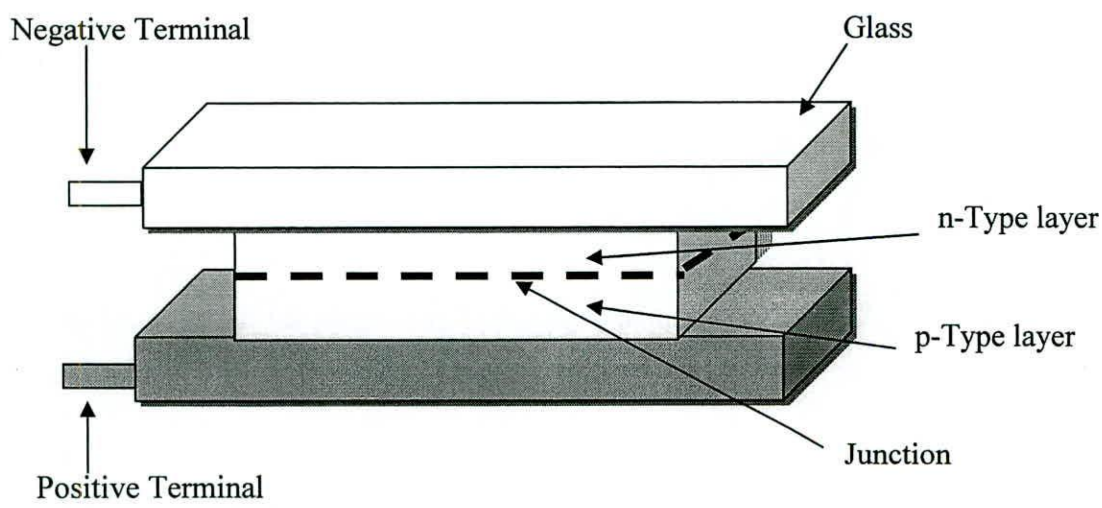

Figure 1.2 – Three energy conversion layers of a photovoltaic cell

1.2.1 Top junction layer[4]

The first of these three layers necessary for energy conversion in a solar cell is the top junction layer which is made of N-type semiconductor .This semiconductor type in which the density of holes in the valence band is exceeded by the density of electrons in the conduction band. N-type behavior is induced by the addition of donor impurities, such as arsenic or phosphorus, to the crystal structure of silicon. In N-type semiconductors, electrons are the majority carriers, and holes are the minority carriers.

1.2.2 Absorbing layer

The next layer in the structure is the core of the device; this is the absorber layer (the P-N junction). The basic structure formed by the intimate contact of P-type and N-type semiconductors. The important characteristic of a P-N junction is that it will conduct electric current with one polarity of applied voltage (forward bias) but will not conduct with the opposite polarity (reverse bias).

1.2.3 Back junction layer

The last of the energy-conversion layers is the back junction layer which is made of P-type semiconductor. This semiconductor type in which the density of electrons in the conduction band is exceeded by the density of holes in the valence band. In P-type semiconductors, holes are the majority carriers, and electrons are the minority carriers. This type of semiconductor is used acceptor impurities, such as boron, to the crystal structure of silicon.