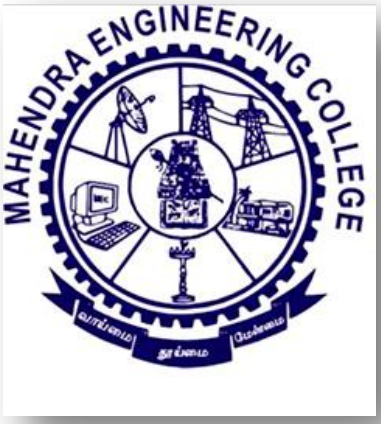
MAHENDRA ENGINEERING COLLEGE, MALLASAMUDRAM, TAMIL NADU, INDIA

Identification of new solar cell materials

2. Project Report



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Abstract

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Abstract

The solar irradiation of the sun is an infinite energy source. This source is available at any place on the planet and almost for free. Nowadays a lot of different solar applications are discovered and their efficiency is constantly improved. Due to the solar devices the mankind can reduce the CO2 emissions and moreover match the growing power demand in the world. One of the photovoltaic devices, namely dye sensitized solar cells (DSSC), are discussed in this project. In particular this technology offers a lot of advantages. The cost of production is in comparison to the silicon based solar cells very less. Moreover the energy input for the manufacturing is on a very low level. A further aspect is, that in the DSSC application can be used the direct and furthermore the diffuse solar irradiation in comparison to the silicon based solar cells, which are prefer to use the direct irradiation.

The nucleus of the DSSC technology is the dye sensitizer. Indeed, there is already an intensive research going on to discover and develop a strong, high efficient dye sensitizer. Some DSSC are already in the market but still on a small scale. The most promising dyes are the ruthenium doped metal-organic compounds. They reach efficiencies over 11%. For the deeper understanding of the different interactions, happening in a dye during the excitation, and evaluation of various dyes this project shows a way, how the dyes theoretically can be investigated and be improved. For this approach it is necessary to study the geometries, electronic structures, polarizabilities and hyperpolarizabilities of dye sensitizer based on Density Functional Theory (DFT) using the hybrid functional B3LYP. The Ultraviolet-Visible (UV-VIS) spectrum was investigated by using a hybrid method which combines the properties and dynamics of many-body systems in the presence of time-dependent (TD) potentials, i.e. TDSCF-DFT(B3LYP). Features of the electronic absorption spectrum in the visible and near-UV regions were plotted assigned based on TD-DFT calculations.

Due to the absorption bands of the metal-organic compound are n · π* present. In this project henna dye, 3-(5-((1E)-2-(1,4-dihydro-1,4-dioxonaphthalen-3-yloxy)vinyl)thiophen-2-yl)-2-isocyanoacrylic acid and anthocyanin are investigated. It is essential that the used dye sensitizer includes a strong donator group, a π-conjugation bridge and a stout acceptor group. The donator group can be improved by using a molecule with more atoms, i.e. naphthalocyanin. For the conjugation bridge a large thiophene compound is advantageous. The anchoring group can be strengthening by using an acid. To put it in a nutshell, for the further research are a lot of starting points available to develop sufficient dye sensitizers.