ARTICLE IN PRESS

+ MODEL

Available online at www.sciencedirect.com

ScienceDirect

Karbala International Journal of Modern Science xx (2017) 1–8
http://www.journals.elsevier.com/karbala-international-journal-of-modern-science/

New organic dyes based on phenylenevinylene for solar cells: DFT and TD-DFT investigation

Aziz El alamy [a,d], Mohamed Bourass [b,*], Amina Amine [a], Mohammed Hamidi [c], Mohammed Bouachrine [d]

[a] *LCBAE/CMMBA, Faculty of Science, Moulay Ismail University, Meknes, Morocco*
[b] *ECIM/LIMME, Faculty of Sciences Dhar El Mahraz, University Sidi Mohamed Ben Abdallah, Fez, Morocco*
[c] *URMM/UCTA, Faculty of Sciences and Techniques of Errachidia, Moulay Ismail University, Morocco*
[d] *MEM, ESTM, Moulay Ismail University, Meknes, Morocco*

Received 5 September 2016; revised 21 March 2017; accepted 22 March 2017

Abstract

In this work, we report five novel organic dyes with donor−π−acceptor (D−π−A) structure, their conjugated bridge is based on phenylenevinylene and thiophene/furan, the acid 2-cyanoacrylic was used as an electron acceptor (anchoring) group and triphenylamine was used as an electron donor group for all compounds. These dyes were studied by Density Functional Theory (DFT) and Time-Dependent DFT (TD-DFT) methods using Becke's three-parameter functional and Lee−Yang−Parr functional (B3LYP) level with 6-31G(d) basis set to investigate their molecular structures, frontier molecular orbitals, optoelectronic properties and absorption spectra as implemented in the Gaussian 09 program. The HOMO (highest occupied molecular orbital), LUMO (lowest unoccupied molecular orbital) levels, gap energy ($E_{HOMO} - E_{LUMO}$) and V_{oc} (open-circuit voltage) of the studied compounds are calculated and discussed. These properties suggest that these compounds as good candidates for use in organic dye-sensitized solar cells.

Keywords: Phenylenevinylene; DFT; Low band gap; Dye-sensitized; Organic solar cells

1. Introduction

Owing to the challenge for searching of renewable energy sources, photovoltaic solar energy is awaited to be a good candidate for this target in the future. The energy provided by the sun in 1 h is more important than the energy consumption globally in an entire year [1]. However, capturing solar energy and converting it to electric with a low cost is still a big challenge. Photovoltaic cells technologies become a topic of interest in the design the solar cell to converting the sun to electrical energy. Different photovoltaic devices based inorganic materials, such as crystalline and amorphous silicon, cadmium telluride (CdTe), gallium arsenide (GaAs), giving efficiencies of 10−32% (under AM (air mass) 1.5 standard sunlight) [2]. But the rarity, toxicity and expensively of these materials brings a lot

* Corresponding author.
E-mail address: mohamedbourass87@gmail.com (M. Bourass).
Peer review under responsibility of University of Kerbala.

http://dx.doi.org/10.1016/j.kijoms.2017.03.002

of researchers to finding and developing new materials cheaper and more efficient. Following this approach, the solar cells based on the organic materials become a very attractive choice, this is attributed to their mechanical flexibility; ease of processing, low-cost production. However, their efficiencies at present are lower than those based on inorganic materials [3]. The power conversion efficiency obtained of these kinds of solar cells still does not warrant for the commercialization: the most efficient devices have an efficiency of 4–5% [4].

Recently, several new materials used in organic solar cells have been studied and developed. Among them, dyes sensitized solar cells (DSSCs) are currently receiving significant attention, due to their potentially low production cost, flexibility and high energy conversion efficiency [5]. Moreover, they present a high power conversion efficiency (PCE) and their devices are easy to fabricate [6]. The photovoltaic cells based on the dye-sensitized solar cell (DSSC) presents several advantages such as their compatibility with various supporting materials and the production under mild conditions make them significantly less expensive compared to others cells. The first DSSCs are based on a ruthenium complex and nanoporous TiO_2 film and have been occurred in 1991 by O'Regan and Grätzel with efficiencies of 7–8% [7]. Later, most research in this field has focused on the sensitization of n-type semiconductors, such as TiO_2 and ZnO (n-type DSSCs), and the obtained conversion efficiencies reached to 11% [8–10].

In this work, we present the results of the quantum studied on five molecules C1, C2, C3, C4, and C5 based on phenylenvinylene and others groups as π-spacer forming D–π–A structure by considering to use them as dyes sensitizers for solar cells (see Fig. 1). In this structure, we used 2-cyanoacrylic as electron acceptor unit (A) and triphenylamine were used as electron donor group (D) for all compounds. To investigate the electronic and optical properties, most favorite method; Density Functional Theory (DFT) is the method of choice according to an accurately describe and less computational cost compared to other high-level quantum approaches as MP2, MP4 ….

Time-Dependent DFT (TD-DFT) has been widely used to investigate the properties of organic compounds in their excited state because its high accuracy is reasonable with the ab-initio method and less computational time cost. In this work, the calculated results obtained by these methods as the optimized geometries, optoelectronic properties and photovoltaic properties (open circuit voltage (V_{oc}), oxidation potential energy, and electron injection force) of all compounds were investigated and reported.

2. Computational methodology

The geometries and optoelectronic properties of new compounds based on phenylenevinylene and thiophene/furan, were determined and investigate using Density Functional Theory (DFT) with Becke's three-parameter functional and Lee–Yang–Parr functional (B3LYP)

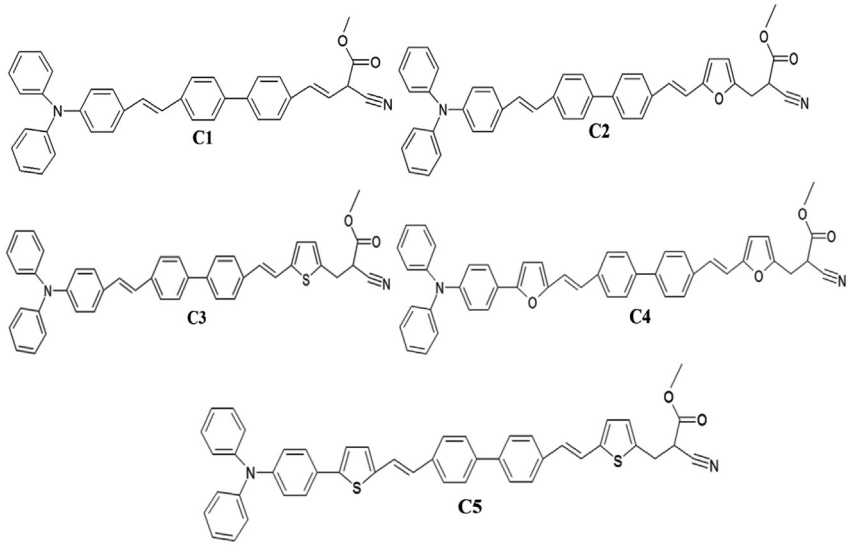

Fig. 1. Studied compounds C1, C2, C3, C4 and C5.

Please cite this article in press as: A. El alamy et al., New organic dyes based on phenylenevinylene for solar cells: DFT and TD-DFT investigation, Karbala International Journal of Modern Science (2017), http://dx.doi.org/10.1016/j.kijoms.2017.03.002