QUANTUM CHEMICAL INVESTIGATIONS OF NEW CONJUGATED COMPOUNDS BASED ON DITHIOBITHIOPHENE AS SOLAR CELLS MATERIALS

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***Abstract*— Thanks to their specific properties, The research in the organic π-conjugated molecules and polymers has become one of the most interesting topics in the fields of chemistry physics and materials science., these compounds have become the most promising materials for the optoelectronic device technology such as solar cells. In this work, The theoretical ground-state geometry and electronic structure of the studied molecules were investigated by the DFT method at B3LYP level with 6-31G(d) basis set has been performed to explore the optical and electronic properties of a series of different compounds based on bithiophene. Different electron side groups were introduced to investigate their effects on the electronic structure. The effects of the ring structure and the substituents on the geometries and electronic properties of these materials were discussed with the aim to evidence the relationship between molecular structure and optoelectronic properties. The theoretical knowledge of the HOMO and LUMO energy levels of the components is basic in studying organic solar cells so the HOMO, LUMO, Gap energy and Voc (open circuit voltage) of the studied compounds have been calculated and reported. These properties suggest these materials as a good candidate for organic dye-sensitized solar cells.**

***Keywords*— π-conjugated molecules, bithiophene, organic solar cells, DFT, low band-gap, electronic properties, Voc (open circuit voltage)**

I. INTRODUCTION

Since their discovery, materials based on conjugated molecules have attracted continuing interest as a result of their suitability in a broad range of applications, such as batteries (Nalwa, 1999; Lim *et al*., 2006) , electroluminescent devices (Dimitrakopolous *et al*., 2002), field-effect transistors (Kraft *et al*., 1998; Kim *et al*., 2006) and photovoltaics (Manoj and Narayan, 2003; Wienk *et al*., 2003). Conjugated polymers containing carbazole or (and) thiophene moieties either in the main or side chains have attracted much attention because of their unique electronic properties, their high photoluminescence quantum efficiency, thermal stability and also their facile color tenability (Müllen *et al*., 1998; Cornil *et al*., 1998). Thanks to its important specific properties, these new compounds became the most promising materials for the optoelectronic device technology (Sariciftci *et al*., 1992). These properties depend on the degree of electronic delocalization in these materials and on the modification of chemical structure through the incorporation of charge carriers into the molecule backbone. One of the most important factors of controlling physical properties is the band gap, which is a current topic of research. In particular, organic materials with a low gap are desired in optoelectronic applications. Many ways have been used to modulate this parameter the best one is the modification of chemical structure through the incorporation of charges carriers in the polymer backbone. Most of recent papers have focused on the synthesis of short-chain conjugated compounds. These compounds became the most promising materials for the optoelectronic device technology (Brabec *et al.*, 2001a; Zhou *et al*., 2007). Recent work in this area has been focused on the synthesis and design of new molecules combining donor and acceptor blocks, or conjugated systems with narrow band gaps (Cravino and Sariciftci, 2002; Roquet *et al*., 2006). In order to obtain materials with more predominant capability, the development of novel structures is now being undertaken following the molecular engineering guidelines, theoretical studies on the electronic structures of these materials have made great contributions to the rationalization of the properties of known ones and the prediction those of unknown ones (Bouzakraoui *et al*., 2006; Mondal *et al*., 2010; Bundgaard *et al*., 2007). We note that theoretical knowledge of the HOMO and LUMO energy levels of the components is crucial in studying organic solar cells. So, we can save time and money in choosing the adequate organic materials to optimize photovoltaic devices properties. The HOMO and LUMO energy levels of the donor and of the acceptor components for photovoltaic devices are very important factors to determine whether effective charge transfer will happen between donor and acceptor. The offset of band edges of the HOMO and LUMO levels will prove responsible for the improvement of all photovoltaic properties of the organic solar cells.