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Optoelectronic properties of four azobenzene based iminopyridine ligands for photovoltaic application

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Abstract

Thanks to their optoelectronic properties and potential applications in a wide range of electronic and optoelectronic devices such as organic solar cells, the research in the organic π-conjugated materials encompassing both polymers and oligomers have been widely studied over the last years. In this work, a theoretical study using the DFT method on four azobenzene based iminopyridine is reported. The theoretical ground-state geometry, electronic structure and the optoelectronic parameters (the highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO) energy levels, the open-circuit voltage (Voc) and the oscillator strengths (O.S)) of the studied molecules were obtained by density functional theory (DFT) and time-dependent (TDDFT) approaches. The effects of the structure length and the substituents on the geometries and optoelectronic properties of these materials are discussed to investigate the relationship between molecular structure and optoelectronic properties. The results of this study are in agreement with the experimental ones and suggest these materials as good candidates for use in photovoltaic devices.

***Keywords**:* π-conjugated materials, azobenzene, optoelectronic properties, DFT calculations, HOMO-LUMO gap.

1. Introduction

In the last decade, organic electronic devices represent an important part of the electronic research; these electronic devices need special polymers and molecules with specific and adapted properties. ΠI conjugated materials have much attention for optoelectronic and photovoltaic applications such as batteries [1,2], electroluminescent devices like light-emitting diodes (LEDs) [3], organic field-effect transistors [4] and organic photovoltaic cells (OPCs) [5-16].