Abstract

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# Electronic Absorption Spectra of Platinum (II) Complexes Used for Sensitized Solar Cells: DFT/TDDFT Study

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## Abstract

Using the time dependent density functional theory, we studied in this work the electronic absorption spectra of a series of heteroleptic complexes using ferrocene based dithiocarbamate complexes involving Pt(II) in the form [M(dppf)L] [where dppf =1 10-bis(diphenylphosphino)ferrocene, M=Pt(II) and L= p-tolylsulfonyl dithiocarbimate, p-CH3C6H4SO2NCS2 (1). M=Pt and L= p-chlorobenzene sulfonyl dithiocarbimate, p-ClC6H4SO2NCS2 (2). M=Pt and L= p-bromobenzene sulfonyl dithiocarbimate, p-BrC6H4SO2NCS2 (3). M=Pt andL=1-ethoxycarbonyl-1-cyanoethylene-2,2 ithiolate(ecda)(4).

These complexes have been synthesized and characterized experimentally using the spectroscopy methods (IR, 1H, 13C and 31P NMR and UV-Vis) and crystal X-ray diffraction. Due to their photo-physical and photo-chemical properties, they have been used as photosensibilisator in the DSSC (Dye Sensitized Cell Solar). For each complex our contribution was made in two main steps. The first is a geometry optimization to find the optimal structure with the density functional theory (DFT). We using the CAM-B3LYP density functional and PBE0, using 6-31G (d,p) and 6-31+G(d) basis as implemented in Gaussian09. The study of HOMO, LUMO has been used to explicate information about charge transfer in molecules. Lastly, from the frontier molecular orbitals we elucidate the UV-vis spectra and electronic absorption proprieties. The calculated spectrums have been compared with the experimental result. We have chosen to improve the efficacy of the dye in DSSC by introducing an anchor ligand –COOH with a thiophen auxiliarygroupin M(dppf) NCS2 (M=Pt(II), and substitute the ligand L=p-XC6H4SO2 (X=CH3, Cl, Br) with 2-Thiophene carboxylic acid which has a hypsochrome effect on the absorption spectrum due to the π-conjugation and the strong auxochrome resulting from the thiophene.

## Biography

Sefia BRAHIM, graduated from the University of Saida, Algeria in 2011 with a Bachelor of Science in Chemistry with a specialization in Physical Chemistry. In 2013, I received a Master of Science degree in Computational Chemistry. In 2015, I started my Ph.D. work in degree in Computational Chemistry in the Laboratory of Modeling and Methods of calculation (LMMC), University of Saida. My thesis focused on the study of electronic absorption spectra of organometallic complexes used as photosensitizers in DSSC.