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**RECENT ADVANCES IN CHARACTERIZATION,
PROCESSING, DESIGN AND MODELLING OF
STRUCTURAL AND FUNCTIONAL MATERIALS**

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Universidade Técnica de Lisboa . PORTUGAL

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Sociedade Portuguesa de Materiais

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Materials Symposium**

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A DFT STUDY ON THE SONLO PROPERTIES OF OLIGO-THIOPHENE ACETYLIDE Ru COMPLEXES

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The search on organometallic compounds for the development of novel nonlinear optical (NLO) materials with large second-order nonlinearities (SONLO) is currently the subject of significant interest in view of their potential application in the area of integrated optics [1]. Experimental and computational systematic studies were made on half-sandwich organometallic complexes presenting the typical push-pull feature in which the metal centre, bound to a highly polarizable conjugated backbone, acts as an electron-releasing or withdrawing group. The results revealed that η^5 -monocyclopentadienylruthenium moiety can be very efficient electron-donor group in complexes presenting thiophene-based ligands with a nitro group as an electron acceptor [2,3]. Nevertheless, the understanding of the relationship between the structure and experimental molecular NLO phenomena is not completely clear, namely the effect of the conjugation length of the chromophores. Theoretical studies using time-dependent density functional theory (TD-DFT) method has been used to calculate first hyperpolarizabilities of organometallic complexes. These theoretical studies are very useful for a better understanding on the electronic factors that may be responsible for the SONLO properties.

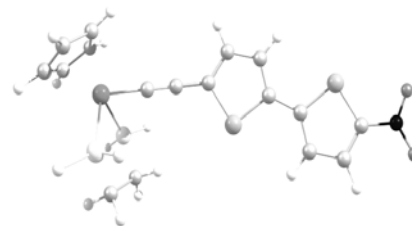


Figure 1

In order to contribute to a clarification on the molecular organometallic structure-SONLO properties of half-sandwich complexes with substituted thiophene ligands, we report therein the results of TD-DFT calculations, using the Gaussian03W program package, on the model complexes $[\text{RuCp}(\text{H}_2\text{PCH}_2\text{CH}_2\text{PH}_2)(\text{CC}\{\text{SC}_4\text{H}_2\}_n\text{NO}_2)]$ ($n=1-4$). For instance, Figure 1 shows the optimized structure for $[\text{RuCp}(\text{H}_2\text{PCH}_2\text{CH}_2\text{PH}_2)(\text{CC}\{\text{SC}_4\text{H}_2\}_2\text{NO}_2)]$. The role played by the conjugation length of the thiophene ligands on the SONLO properties of these complexes will be evaluated.

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