

# Estimation of Hyperpolarizabilities of Organometallic Complexes by DFT

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The research of nonlinear optical (NLO) materials has grown in the past decades due to the potential application in optical device technology, like data storage, communication and bio-sensing. For obtaining large molecular second-order nonlinear optical (SONLO) responses, i.e. large hyperpolarizabilities ( $\beta$ ), molecules have to possess typical “push-pull” asymmetric structures.  $\eta^5$ - Monocyclopentadienylruthenium(II) and iron(II) complexes presenting heterocyclic organic chromophores have proven to be promising systems in this field. Also the presence of a transition metal suggests that it is possible to switch the SONLO response of the material by changing its oxidation state, by electrochemical means for example. In this case, two distinct forms would be expected: the “switched on” form, with high  $\beta$  value; and the “switched-off” form, with negligible or substantially lower  $\beta$ . Herein, we show the application of Density Functional Theory (DFT) to the studies of SONLO properties of several organometallic complexes bearing thiophene based organic ligands as active NLO chromophores.

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