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Exploring Charge Transfer Mechanism in Organic NLO (Polymorphic) Materials

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The understanding of nonlinear polarization mechanism and their relation to the structural characteristics of non-linear optical (NLO) materials have been utmost importance considering a surge in the information technology and industrial applications. Some investigations in search of NLO materials have been carried out on organic molecule scaffolds such as stilbene and chalcone having π - e^- donor acceptor substituent which facilitates intermolecular charge transfer; leading to the generation of good frequency conversion materials. Few of such materials are known to exhibit polymorphic characters and most of which crystallize in non-centrosymmetric space group – necessity for a NLO material. It has been realized that the chirality, polymorphic character and NLO activity of the chalcone derivatives are mainly governed by both the substitutions at the para position and the position of sulfur atom in the thiophene ring of thienylchalcone. This presentation will highlight the preliminary results towards the analyses of electron density distributions on NLO active stilbene and chalcone derivatives and their polymorphic forms. Therefore, explore the charge transfer mechanism responsible for the variation of NLO activity across these systems and on their non-centrosymmetric polymorphic forms. Charge densities modelled using both multipole formalism (Hansen & Coppens, 1978) and X-ray constraint wavefunction fittings (Jayatilaka & Grimwood, 2001) will be considered for these studies.

[1] N. K. Hansen, P. Coppens, *Acta Crystallographica*, 1978, A34, 909-921, [2] D. Jayatilaka, D. J. Grimwood, *Acta Crystallographica*, 2001, A57, 76-86

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