Comparison between Quantum Mechanical Computations of NLO Properties and Experimental Data of Selected Functionalized Azo-Dyes

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Résumé en anglais	Nonlinear optical (NLO) materials have been extensively studied for many years. The search of new materials with NLO properties is an important research field. Significant interest still exists in the design and development of materials exhibiting large second and third-order NLO response because of the potential application in optoelectronics devices. In this talk, comparison between quantum mechanical computations of NLO properties and experimental data in selected azo-dyes will be done. Particularly we will focus on correlation between macroscopic level and microscipic one. To reveal the microscopic second-order NLO properties of a family of azo-azulenes, the electric dipole moments (μ) and static first hyperpolarizabilities (ß) have been evaluated by using density functional theory (DFT) quantum mechanical calculations at B3LYP/ 6-311+G (d, p) level. The calculation results with non-zero values on first hyperpolarizabilities indicate that the title molecules might possess microscopic second-order NLO phenomena. The maximum one-photon absorption (OPA) wavelengths obtained by theoretical computations using the configuration interaction (CI) method are located in the visible region, supporting the $\pi \rightarrow \pi^*$ transitions. We have also calculated the dynamic second (χ^2) and third-order (χ^3) susceptibilities using the time-dependent Hartree-Fock (TDHF) method.
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