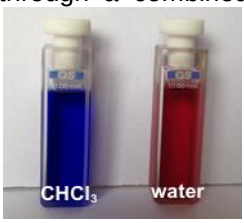
Photoinduced charge transfer, negative solvatochromism and hyperpolarizability of push-pull pyridinium and quinolinium derivatives.

B. Carlotti[1], E. Benassi[2], F. Elisei[1], V. Barone[2], C. G. Fortuna[3], A. Spalletti[1]
[1]*University of Perugia, Italy*
[2] *Scuola Normale Superiore, Pisa, Italy*
[3] *University of Catania, Italy*

Some stilbene and butadiene derivatives bearing an electron deficient pyridinium or quinolinium group and an electron donor aromatic portion have been investigated through a combined experimental and theoretical approach, by using steady-state and femtosecond resolved spectroscopies and DFT calculations.[1] The spectra resulted significantly affected by the solvent polarity: a large blue shift of the absorption band was observed in the polar solvents implying a clear change in the solution colour. The negative solvatochromism was comprehended thanks to the help of the calculations considering the variation of the dipole moment under excitation. A significant quenching of the fluorescence was observed upon increasing the solvent polarity. The photobehaviour was interpreted considering the ground and excited state optimized geometries as a function of the solvent. The ultrafast measurements allowed an insight into the excited state dynamics revealing an interesting competition among solvent relaxation and photoinduced intramolecular charge transfer (ICT), whose efficiency was modulated by the solvent and the molecular structure. The hyperpolarizability was estimated by the solvatochromic method[2] from the collected experimental data and compared with that predicted by the QM calculations. The findings for the investigated compounds (interesting molecular structure/ICT/NLO properties relationships) indicate their potential application in optoelectronics and photonics as NLO materials.



1. B. Carlotti, C. G. Fortuna, G. Consiglio, U. Mazzucato, A. Spalletti and F. Elisei, *J. Phys. Chem. A*, submitted; B. Carlotti, E. Benassi, A. Spalletti, C. G. Fortuna, F. Elisei and V. Barone, *Phys. Chem. Chem. Phys.*, submitted.

2. R. L. Sutherland, Handbook of Nonlinear Optics, 2nd edition, Marcel Dekker, Inc., 2003, and references therein.