Institut Ruđer Bošković

XCV. Kolokvij Zavoda za organsku kemiju i biokemiju,

Sekcije za organsku kemiju, Sekcije za teorijsku i računsku kemiju

Hrvatskog kemijskog društva i Fakulteta kemijskog inženjerstva i

tehnologije, Sveučilišta u Zagrebu .

Professor Fausto Elisei
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University of Perugia
Perugia, Italy

Utorak, 19. 06. 2012. godine
Predavaonica **III.** krila IRB

15.00-16.00 sati

Dielectric Controlled Photophysics of Representative Push-Pull Compounds

Organic molecules with delocalized π-electron bridges and electron-donor (D) and electron-acceptor (A) groups at the two opposite ends (push−pull systems) have been widely investigated owing to their ability to absorb light and to generate charge separation. These properties are particularly interesting to perform useful photoinduced functions such as fluorescent sensing of ions and molecules, solar energy conversion, optical information storage and effects of non−linear optics. An increasing interest has been devoted to organic compounds, particularly for non-linear optics.[1,2] owing to their higher applicative potential, easier synthesis and lower cost compared to the inorganic materials.

After the first observation of photoinduced intramolecular charge transfer (ICT) in 4−(N,N−dimethylamino)benzonitrile,[3] a wide series of push−pull systems have been studied in different solvents.[4]

Recent studies were carried out in our laboratory on distyryl− and ethynyl−aromatics bearing electron−acceptor/electron−donor side groups with the aim to characterize the photophysics of the substrates in fluid media.[5−9] Experimental (steady−state and time−resolved techniques with nanosecond and femtosecond resolution) and quantum−mechanical (TDDFT) approaches were used to investigate the solvent effect on the main deactivation processes of the lowest excited singlet states, such as intramolecular charge transfer (ICT), fluorescence (F), singlet−triplet intersystem crossing (ISC) and internal conversion (IC). Particularly interesting is the solvent effect on the ISC rate constant which changes drastically with the LE/CT nature of the S_1 state.

The effect of molecular structure and solvent polarity on dynamics of the lowest excited singlet and triplet states allowed a complete picture of their deactivation pathways to be obtained.

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