Carbazole and indolcarbazole-based systems: impact of the structural changes on the system properties.

Irene Badía-Domínguez[1], Franktišek Hartl[2], Hongxiang Li[3], Shu Seki[4], Daisuke Sakamaki[4], Fabrizia Negri[5], Juan T. López Navarrete[1], Víctor Hernández Jolín[1], M. Carmen Ruiz Delgado[1].

[1] Department of Physical Chemistry, University of Malaga, Campus de Teatinos s/n, 229071, Malaga, Spain.

[2] Department of Chemistry, University of Reading, Whiteknights, Reading RG6 6AD, United Kingdom.

[3] Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, No.345 Lingling Rd., Shanghai, 200032, China.

[4] Department of Molecular Engineering Graduate School of Engineering, Kyoto University, Nishikyo-ku, Kyoto 615-8510, Japan.

[5] Department of Chemistry "Giacomo Ciamician", University of Bologna, 40126 Bologna, Italy.

π-Conjugated diradical compounds, featuring unique unsaturated valences and radical centres in the ground state, are fundamentally important for understanding the nature of chemical bonds and have potential applications in material science [1]. During the last decade, there has been an increasing interest in the rationalization of how the structural changes stabilize (or destabilize) the diradical system. The tunability of the diradical character has been studied for different structural motifs such as the substitution pattern of lateral groups[2], the elongation of the conjugated core[3] or the molecular isomerism[4], among others. In this sense, we have recently reported an experimental/theoretical study of a family of carbazole-based diradicaloids with dicyanomethylene (DCM) groups incorporated via para (**p-Cz** and **p-ICz**) or meta positions (**m-Cz** and **m-ICz**) aiming to investigate how external stimuli impact on the molecular structure and supramolecular organization, and thus on the resulting optical and electronic properties. In addition, we theoretically investigate at the DFT level a set of ten indolocarbazole-based isomers substituted with DCM groups to disclose how their chemical reactivity and physical properties are affected by isomerism and different substitution pattern.

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