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Understanding Cross-Conjugation for Organic Electronics

Samara Medina,[a] Jean-François Morin,[b] Xiaozhang Zhu[c], Juan Casado[a]

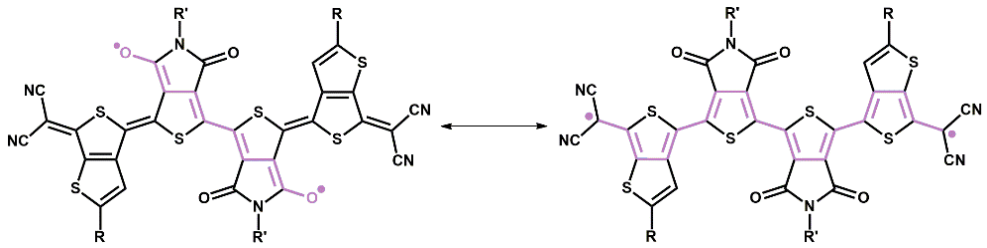
[a] *Univ. Malaga, Dept. Phys. Chem., Campus Teatinos S-N, E-29071 Malaga, Spain, samara@uma.es.*
[b] *Département de Chimie, Université Laval, 1045 Ave de la Médecine, Québec, G1V 0A6, Canada.*
[c] *Chinese Acad. Sci., Inst. Chem., CAS Key Lab Organ Solids, Beijing 100080, Peoples R China.*

Abstract:

π-Conjugated organic molecules have been the focus of interest since they have been probed as potential semiconducting materials,[1] suitable for replacing the widely used silicon technologies. Their structural, optical and conductive properties are now under study to improve their application in organic electronics and to make possible their *ad hoc* synthesis. In this sense, the knowledge of the π-electron delocalization is crucial to stablish the relation between the properties and the function, enabling the development of a synthesis guide based on the specific application.

The most acknowledged conjugated organic materials are those which present extended, linearly-conjugated π-systems.[1,2] However, this is not the only way of π-electron delocalization: homoconjugation, cross-conjugation, curved-conjugation, etc. constitute different electronic designs to achieve new organic materials.

There is a relative high abundance in the organic world of cross-conjugated but limited comprehension.[1,2,3] Thus, the understanding of how cross-conjugation works in π-electronic systems is of importance. Following this idea, in this project we show 4 different structures which present two perpendicular π-conjugated paths and how the cross-conjugated property is revealed. On the one hand, two molecules based on thieno[3,4-c]pyrrole-4,6-dione quaterthiophenes[2,3] allow us to accomplish the subject from the aromatic/quinoidal outlook, and, on the other hand, two molecules with an anthanthrone core make possible the study from the perspective of the substituent groups.[4]



Cross-conjugated paths in a quaterthiophene-based molecule.

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