

Uncommon Molecular Structures for Organic Electronics: Cross-Conjugated Biradical Dianions and Mechano-Made Biradicals

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Significant advances in any field of research often come from unexpected experimental results. We all know that uncommon behaviors are destined to envisage new applications whereas collection of typical features only helps to improve existing ones. There are plenty of examples of this in the field of organic electronics such as the discovery of conductivity in PA, the behavior of PCBM as electron acceptor in bulk heterojunction solar cells or singlet fission for second generation photovoltaics. The two findings I will describe here are not obviously of comparable importance but allow me to introduce the reader in the topic of the talk.

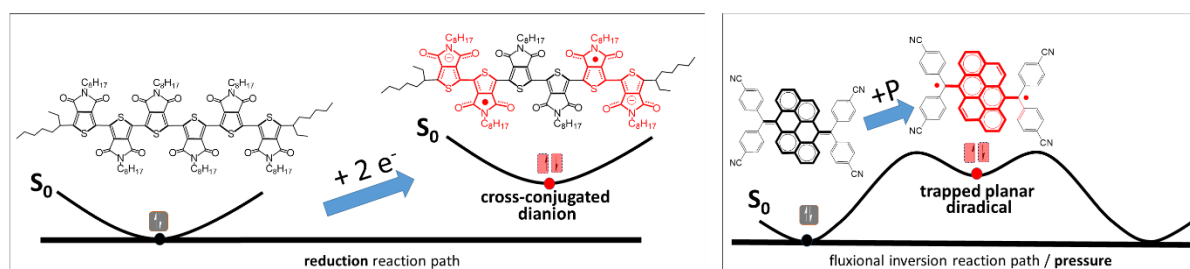


Figure 1. Cross-conjugated dianions of oligothiophenes and acene based quinodimethane biradicals-

The two stories deal with biradical or diradicals, or pairs of unpaired electrons in singlet ground electronic state configurations which allow a series of interesting properties as small singlet-triplet gaps, thermally activated intersystem crossing, magnetic hysteresis in pure organics, etc. The first case concerns with the properties of dianions of oligothiophenes which are stabilized in cross-conjugation regarding the main conjugation path. This structure allows to individual anion electron density to weakly interact each other promoting the small gap with the triplet [1]. The second case is about neutral biradicals generated after pressure application of a closed-shell molecule provoking the rupture of π -bonds and the generation of trapped, kinetically persistent biradicals [1]. Their understanding and implications are discussed.

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References:

- [1] P. Mayorga Burrezo, J.L. Zafra, J.T. López Navarrete, J. Casado, *Angew. Chem. Int. Ed.* **2017**, *56*, 2250 – 2259. Z. Zeng, X. L. Shi, C. Chi, J. T. López Navarrete, J. Casado, J. Wu, *Chem. Soc. Rev.* **2015**, *44*, 6578.