

(Number of the presentation)

## Diradicals Produce Ambipolar Transistors: What and Why

Juan Casado,<sup>1\*</sup> Sergio Moles Quintero,<sup>1</sup> Shin-ichiro Kato,<sup>2</sup> Fabrizia Negri<sup>3</sup>

<sup>1</sup> Department of Physical Chemistry, University of Málaga, 29071 Málaga, Spain

<sup>2</sup> The University of Shiga Prefecture, 2500 Hassaka-cho, Hikone, Shiga 522-8533, Japan

<sup>3</sup> Dipartimento di Chimica 'Giacomo Ciamician' Università di Bologna, Via F. Selmi, 2, 40126 Bologna, Italy  
casado@uma.es

$\pi$ -organic conjugated diradicals have gaining interest in the recent times given their uses in different formats of electronic applications encompassing OFETs,<sup>1</sup> non-linear optical dyes, chromophores for singlet fission in OPV,<sup>2</sup> etc. Our recent interests have turned into the role of their open-shell structures and their impact in the stabilization of +1, -1 charges. Since the first studies in fused planar diradicals, we were fascinated by the fully reversible and almost perfect oxidation/reduction mirror-like shapes of their cyclic voltammeteries (i.e., uncommon in the organic field, in Fig. 1).<sup>3</sup> This aimed us to test the ambipolar charge transport character of diradicals in OFETs and discovered that some particular diradicals are able to transport both kind of charges, holes and electrons, with similar mobility, or balanced  $p$ - $n$  mobility.

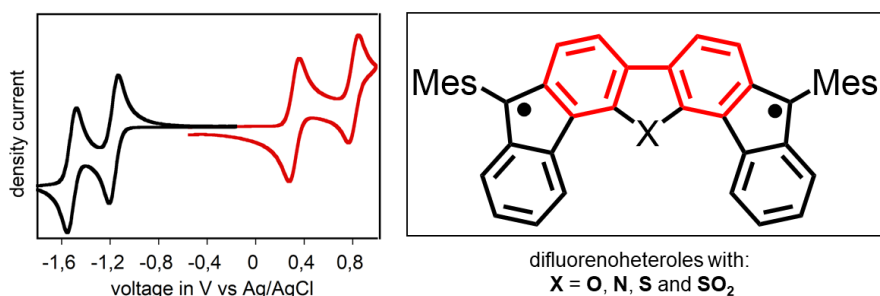


Figure 1. Electrochemical cyclic voltammetry of one of the difluorenoheteroles (X = S) together with their general chemical structures.

Here, we will explore the connection between diradical character and ambipolar charge transport, a relationship that will be put forward through the role of reorganization energies. We will discuss that **medium diradical character** imparts **reduced reorganization energies** either for the exchange of holes and of electrons. Indeed, we found out values of reorganization energies comparable for hole conduction in pentacene, but for both regimes of charging. This suggests that the reduction of the structural changes in molecules with medium diradical character is at the origin of the ambipolar charge transport and of the mirror-like shapes of the cyclic voltammeteries. This communication is focused on the study of the origin of medium diradical character in a set of four difluorenoheterole compounds (Fig. 1) in which the open-shell structure is driven by an amalgam of aromaticity gaining and captodative effects. The experimental  $p$ - $n$  OFET mobilities related with the ambipolar electrical behavior are discussed in terms of reorganization energies.

### References

1. T. Jouselin-Oba, M. Frigoli, *Chem. Sci.* 11 (2020) 12194.
2. S. Lukman, A. J. Musser, *J. Am. Chem. Soc.* 139 (2017) 18376.
3. G. E. Rudebusch, J. Casado, M.M. Haley, *Nat. Chem.* 8 (2016) 753.