QUINOIDIZATION OF REGIOREGULAR OLIGO(THIENO[3,4-*b*]THIOPHENE)S

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The development of high-performance organic electronics has grown exponentially in recent decades, due to their strong impact in society. In this respect, thiophene-based materials occupy a crucial position, owing to their unique palette of colors and amphoteric redox properties with widely tunable energy bandgaps.

In this work, a series of Regioregular Oligo(thieno[3,4-b]thiophene)s in the limit of quinoidal/aromatic conjugation (Figure 1) have been synthesized. Owing to the importance of these molecules for a variety of applications in organic electronics, the establishment of structure-property relationships is strongly pursued. In this sense, we focused on analyzing the electronic structure by different spectroscopic techniques. Moreover the molecular structure of the ground electronic state was studied by vibrational spectroscopy. All experimental analysis was guided and supported by theoretical approaches.

Since these molecules are potential candidates to present the phenomenon of singlet exciton fission (SEF),[1] knowing their deactivation pathways from the excited states will be of great usefulness for the design of more efficient new materials for solar cells.[2]

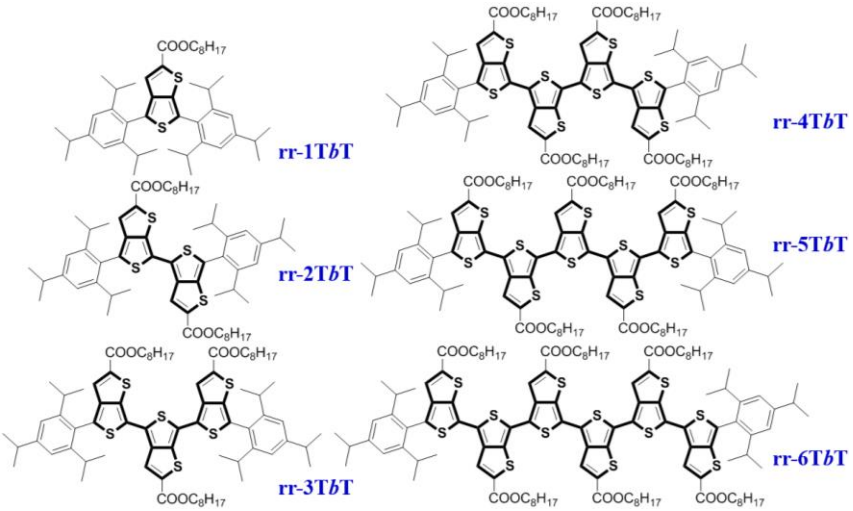

Figure 1. Chemical structures of the compounds object of study.

[1] a) GB, Piland, JJ, Burdett, RJ, Dillon, CJ, Bardeen *J. Phys. Chem. Lett.* **2014**, *5*, 2312-2319; b) BJ, Walker, AJ, Musser, D, Beljonne, RH, Friend *Nature Chemistry* **2013**, *5*, 1019-1024.

[2] a) J, Guo, H, Ohkita, H, Benten, S, Ito *J. Am. Chem. Soc.* **2009**, *131*, 16869-16880; b) AJ, Musser, M, Al-Hashimi, M, Maiuri, D, Brida, M, Heeney, G, Cerullo, RH, Friend, J, Clark *J. Am. Chem. Soc.* **2013**, *135*, 12747-12754.