Theoretical insights into the Electronic and Structural Properties of New, Low-band Gap Inherently Chiral Ethylendioxythiophene-based Oligothiophene

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In the last years, conjugated oligothiophene macrocycles have attracted increasing scientific interest due to some peculiar properties related to their cyclic structure [1-3]. T. Benincori et al. synthesized the 2,2′-bis(2,2′-bithiophene-5-yl)-3,3′-bithianaphthene nicknamed BT_2T_4 (Figure 1) that represents the first member of a new class of chiral oligothiophenes in which chirality results from a tailored torsion produced in the polyconjugated backbone and not from the presence of stereogenic centres, external to it. Interestingly, the $FeCl_3$ oxidation of the enantiopure BT_2T_4 produce a mixture of chiral macrocycles, like dimers and trimers. [4]
Recently, also thanks to DFT and TD-DFT calculations, we have studied the new monomer BT_2E_4 in order to investigate the role of the insertion of 3,4-ethylenedioxythiophene (EDOT) units on the electronic and molecular properties of neutral and charged monomer and oligomer species. Furthermore, the electroactive films were evaluated by cyclic voltammetry (CV), UV/vis spectroelectrochemistry and CV coupled with *in-situ* conductance measurements. [5]

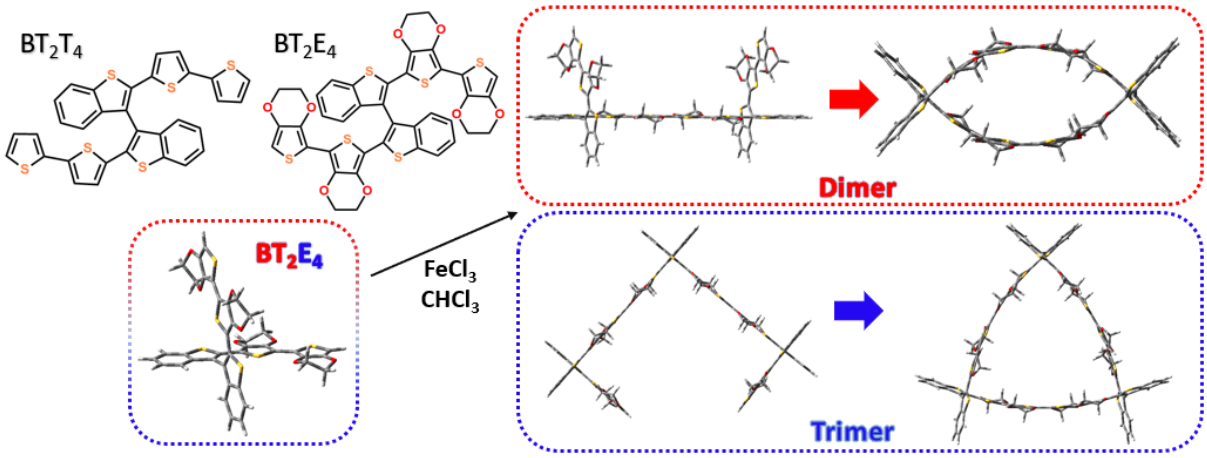

Figure 1 Compounds under study.

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