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


a Dipartimento di Scienza e Alta Tecnologia, Università degli Studi dell’Insubria, Via Valleggio 11, 22100 Como.
b Department of Physical Chemistry, University of Málaga, 29071 Málaga (Spain).
c IPOC-Functional Polymers, Institute of Polymer Chemistry, University of Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart.
d Dipartimento di Chimica, Università degli Studi di Milano, Via Golgi 19, 20133 Milano.
e Istituto per lo Studio delle Macromolecole, Consiglio Nazionale delle Ricerche (ISMAC-CNR), Via E. Bassini 15, 20133 Milano, Italy.

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 BT2T4 (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 FeCl3 oxidation of the enantiopure BT2T4 produces 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 BT2E4 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 spectrophotometry and CV coupled with in-situ conductance measurements. [5]

![Figure 1 Compounds under study.](image-url)