Theoretical spectroscopic studies on [6]helicene-based chiral conjugated oligomers

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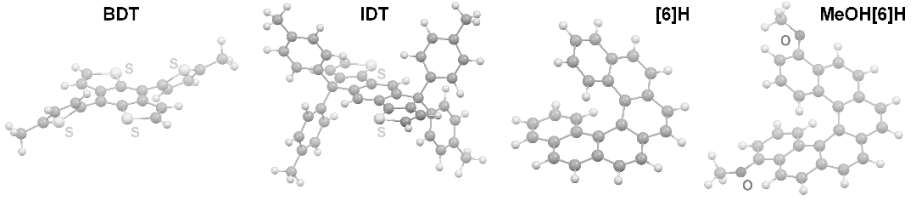
Conjugated polymers are the object of increasing scientific interest as many of them find applications in areas such as chemical sensing, bio-imaging or optoelectronics including organic light-emitting diodes and photodetectors. One of the most appealing features of chemical systems envisioned as materials for a development of efficient optoelectronic devices is currently the ability to emit circularly polarized light, which in the case of conjugated polymers can be achieved by incorporating a chiral component into their structure. Recently, chiral conjugated oligomers based on benzodithiophene (BDT) and indacenodithiophene (IDT) with (dimethoxy) carbo[6] helicene (see figure below) as a chiral inducer have been obtained and experimentally studied as circularly polarized luminescence (CPL) emitters [1].

The goal of the presented theoretical studies was to create (employing density functional theory and its time-dependent variant calculations) a structural and spectroscopic characterization of the newly synthesized helicene-based conjugated polymers, using model systems with 1:1 and 2:2 BDT/IDT-to-helicene ratio, and thus shed a light on their experimentally observed photophysical and chiroptical properties and identify significant structure-to-property correlations. The research involved a conformational analysis of the proposed motifs, their UV-vis and electronic circular dichroism simulations, and modelling of emission features via S1 excited-state geometry optimizations, showing important role of both building blocks and geometric (rotameric) structure of the model on computed properties.



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1] Gedeon C., Del Rio N., Furlan F., Taddeucci A., Vanthuyne N., Gregoriou V. G., Fuchter M. J., Siligardi G., Gasparini N., Crassous J. and Chochos C. L. (2024) Adv. Mater., 2314337.

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