Synthesis and characterization of atropoisomeric pyrene- based dithienylethenes: Optical control of luminescence properties

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Luminescent molecules are present in a wide variety of domains, such as biology (bio-imaging), optoelectronics (data processing, molecular storage) and electroluminescent devices that are now part of our daily lives (OLED screens). In this highly competitive field, our approach aims to bring two additional dimensions:

i) The control of the luminescence by light
ii) The introduction of chirality by atropoisomerism

Based on our expertise in the synthesis and study of photochromic dithienylethenes (DTE), [1] we designed new pyrene-based DTEs that should gather luminescence and chirality, in order to access light-switchable circularly polarized luminescence. [2]

Our strategy toward atropoisomeric DTEs relates on blocking the interconversion between the two antiparallel conformations, by judicious structural modifications of the DTE core (see figure). The obtained racemic mixture of atropoisomeric DTEs will thus be separable upon chiral HPLC. The two pyrenes are positioned in a face to face fashion to produce an excimeric emission, only in the DTE's open form. The photochromic reaction of the DTE will reversibly switch the excimeric luminescence, in a chiral environment. [3] DFT calculations are conducted to study the dynamics of our systems.

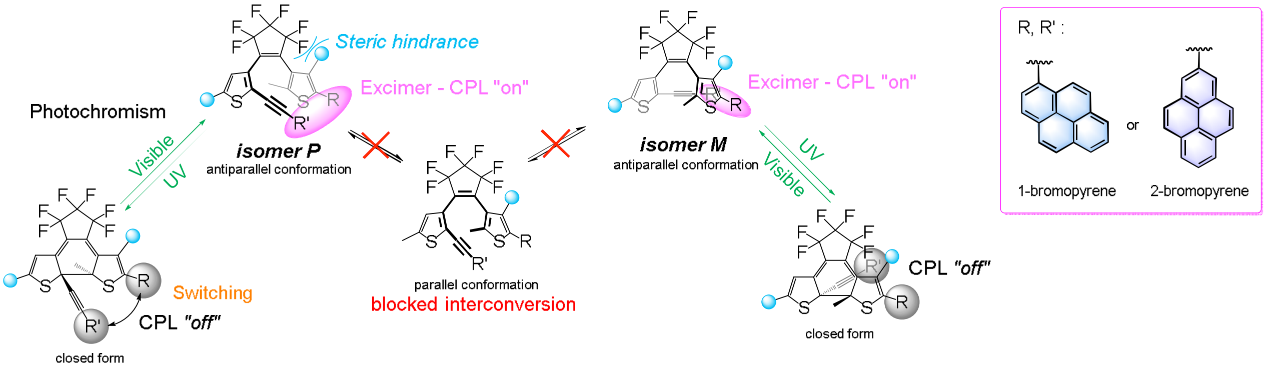

Figure 1. Design of the atropoisomeric pyrene- based DTEs and blocking of the interconversion by atropoisomerism.

The design strategy and the synthetic pathways, along with the optical properties of the synthetized molecules will be presented. The results of the following of the photochromism by ^{1}H and ^{19}F NMR and UV-Visible absorption will be discussed. The dynamic of the system was also studied via variable temperature experiments.

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[2] Hashimoto, Y; Nakashima, T; Shimizu, D; Kawai, T; *Chem. Commun*., **2016**, *52*, 5171 – 5174.
[3] Li, W; Jiao, C; Li, X; Xie, Y; Nakatani, K; Tian, H; Zhu, W; *Angew. Chem*., **2014**, *126*, 4691 – 4695.