Chiral closed- and open-shell molecular systems: From fundamental optoelectronic properties to potential applications in organic electronics

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Chiral π-conjugated materials have recently emerged as a promising direction in material science due to their specific interaction with CP-light and the spin of electron, impacting several domains of applications such as organic light-emitting diodes (OLEDs) for instance, and spintronics.[1]

In this presentation, I will present our contributions regarding this area of research, with firstly the design of covalent and intermolecular chiral luminophores displaying thermally activated delayed fluorescence (TADF) for developing OLEDs with polarized electroluminescence.[2]

I will also illustrate our recent attempts to develop persistent organic chiral mono- and diradicals in which the energy of the singly occupied molecular orbital (SOMO) is below the highest doubly occupied molecular one (HOMO) level, and the impact of these peculiar orbital energetics on both the electronic and photophysical properties of these radicals.[3]

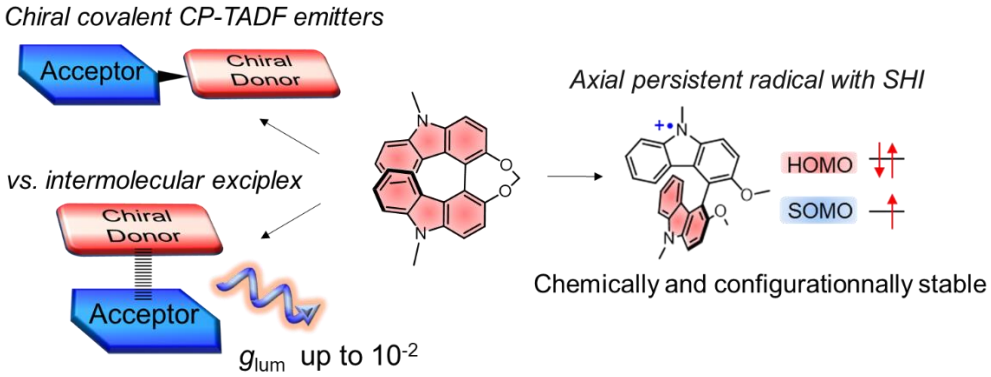

Figure. Chemical structure of chiral bicarbazole compound with an illustration of the approaches explored to develop CP-TADF emitters (left), and a schematic illustration of the SOMO-HOMO Inversion (SHI) obtained for the electronic configuration of the corresponding chiral cationic bicarbazole radical (right).

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(2) P. Sumsalee, L. Abella, T. Roisnel, S. Lebrequier, G. Pieters, J. Autschbach, J. Crassous, L. Favereau, *J. Mater. Chem. C* **2021,** *9*, 11905; P. Sumsalee, L. Abella, S. Kasemthaveechok, N. Vanthuyne, M. Cordier, G. Pieters, J. Autschbach, J. Crassous, L. Favereau, *Chem. Eur. J.* **2021,** *27*, 16505

(3) S. Kasemthaveechok, L. Abella, M. Jean, M. Cordier, T. Roisnel, N. Vanthuyne, T. Guizouarn, O. Cador, J. Autschbach, J. Crassous, L. Favereau, *J. Am. Chem. Soc.* **2020**, *142*, 20409 / **2022**, *144*, 7253; S. Kasemthaveechok, L. Abella, J. Autschbach, J. Crassous, L. Favereau, *Chem. Sci.*, **2022**, *13*, 9833.