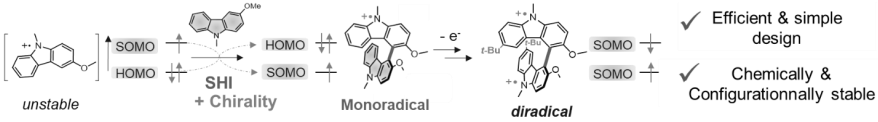
REACHING HIGH-SPIN CHIRAL MOLECULAR MATERIALS

Rysich A., Favereau L., Boixel J.
ISCR, UMR CNRS 6226 – Université de Rennes, Rennes, France
anastasiia.rysich@univ-rennes1.fr

Chiral π-conjugated materials have recently emerged as a new direction in material science due to their specific interaction with circularly polarized light and the potential of the latter in organic light-emitting diodes (OLEDs), organic field-effect transistors (OFETs) and magnets [1]. While extensive researches have been focusing on organic closed-shell chiral dyes, a few attention has been given to their open-shell counterparts due to their low configurational stability and high chemical reactivity [2]. Despite this immense challenge for synthetic chemists, we recently developed the first example of enantiopure chiral monoradicals displaying SOMO-HOMO inversion (Fig. 1, a), which allows us to further discover extended helical mono- and diradicals with interesting properties [3]. Thus, the objective of this work is to design new families of chiral materials, based on preliminary results in our group, investigate the impact of SHI in favouring high-spin chiral di- and polyradicals and bring new findings in chiroptoelectronic applications due to the expected synergy between chiroptical and magnetic properties, which are currently unexplored (Fig. 1, b).

a) **SOMO-HOMO inversion impact on classically unstable radical**



b) **Design of new high-spin radicals with possible SOMO-HOMO inversion**

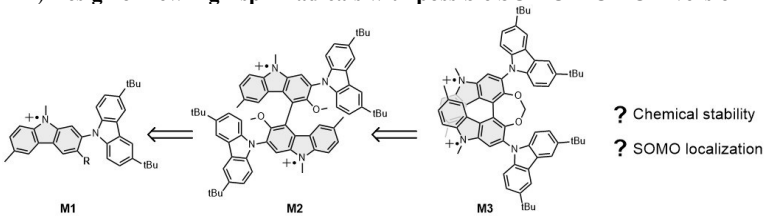


Fig. 1. a) Examples of developed chiral organic monoradicals showing SHI, previously reported in our group; b) Design of new high-spin radicals based on carbazole moieties, possibly leading to SHI

References

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3. a) Kasemthaveechok, S. et al., *J. Am. Chem. Soc.* **2020**, *142* (48), 20409–20418; b) Kasemthaveechok, S. et al., *J. Am. Chem. Soc.* **2022**, *144*, 7253–7263.