MMPS26 **X Oral** **☐ Poster**

Axial and Helical Chiral Bicarbazole Systems: A New Family of Stable Chiral Mono- and Diradical Cations

Sitthichok Kasemthaveechok,[a] Laura Abella,[b] Marion Jean,[c] Marie Cordier,[a] Thierry Roisnel,[a] Nicolas Vanthuyne,[c] Thierry Guizouarn,[a] Olivier Cador,[a] Jochen Autschbach,[b] Jeanne Crassous,[a] Ludovic Favereau[a,*]

a. Univ. Rennes, CNRS, ISCR - UMR6226, 35000 Rennes, France.
b. Department of Chemistry, University at Buffalo, State University of New York, Buffalo, NY 14260, USA
c. Aix Marseille Univ, CNRS, Centrale Marseille, iSm2, Marseille, France.

* email : ludovic.favereau@univ-rennes1.fr

Chiral π-conjugated materials have recently emerged as a promising direction in material science due to their specific interaction with CP-light and the potential of the latter in several domains of applications such as 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] This presentation will illustrate our last result regarding the design of stable organic chiral mono- and diradicals based on C_2-symmetric bicarbazole derivatives.[3] Investigations of their optoelectronic properties revealed a high chemical stability for unprotected carbazole axial radical $\mathbf{1}^{\bullet+}$, in comparison to unstable helical $\mathbf{3}^{\bullet+}$ (Figure 1), owing to an uncommon SOMO-HOMO inversion and a different electronic coupling between the radical center and the electron rich unit bearing the HOMO. Such findings notably allowed us to further design and isolate chemically and configurationally stable chiral diradical $\mathbf{2}^{2\bullet2+}$, which displayed promising near-infrared chiroptical properties and nearly degenerate singlet-triplet ground states (Figure 1).

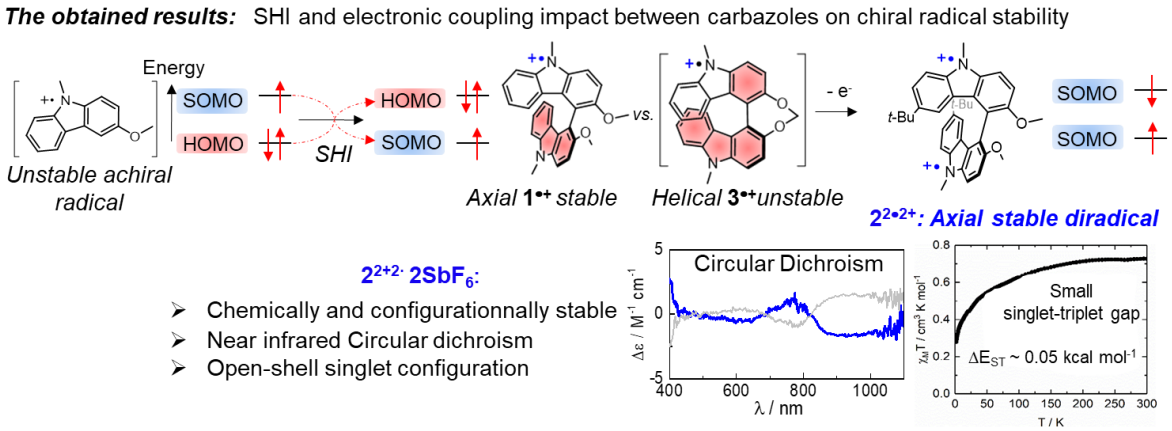

Figure 1. Chiral monoradicals showing a SOMO-HOMO inversion with colors illustrated spin distribution; plot between product of molar magnetic susceptibility (χ) and T vs T of diradical $\mathbf{2}^{2\bullet2+}$ showing curie constant (C) equal to 0.79 cm^3 K mol^{-1}, and g_{abs} of $\mathbf{2}^{2\bullet2+}$ from NIR-ECD.

References: [1] R. Naaman, Y. Paltiel and D. H. Waldeck, *Nat. Rev. Chem.*, 2019, **3**, 250-260.
[2] aA. Rajca, *Chem Rev*, 1994, **94**, 871-893; bJ. R. Brandt, F. Salerno and M. J. Fuchter, *Nat. Rev. Chem.*, 2017, **1**; cY. C. Hsieh, C. F. Wu, Y. T. Chen, C. T. Fang, C. S. Wang, C. H. Li, L. Y. Chen, M. J. Cheng, C. C. Chueh, P. T. Chou and Y. T. Wu, *J. Am. Chem. Soc.*, 2018, **140**, 14357-14366; dC. Shu, H. Zhang, A. Olankitwanit, S. Rajca and A. Rajca, *J Am Chem Soc*, 2019**, 141**, 17287-172943
[3]S. Kasemthaveechok, L. Abella, M. Jean, M. Cordier, T. Roisnel, N. Vanthuyne, T. Guizouarn, O. Cador, J. Autschbach, J. Crassous and L. Favereau, *J. Am. Chem. Soc.*, 2020, **142**, 20409-20418.