Synthesis of Electronic Delocalized Möbius Belt

L. Ye, L. Zhang, Qian Miao*

the Chinese University of Hong Kong, Chemistry Department,

Sha Tin, New Territories, Hong Kong, China

*E-mail: Liping.Ye@oci.uni-heidelberg.de

The Möbius strip, with only one non-orientable surface, was first discovered by August Ferdinand Möbius and Johann Benedict Listing independently in 1858. Due to its captivating topological structure, Möbius strip has garnered significant attention from mathematicians, engineers, and chemists. Herein, we summary two synthetic strategies towards molecular Möbius belt. Strategy I involves introducing a twist (T_w = 1) into a normal carbon nanobelt (CNB),[1] while Strategy II focuses on integrating a writhe (W_r = 1), essentially a helical component, within a normal belt.[2] In this work, we report a successful synthesis of a double-stranded Möbius belt using Strategy II. It exhibits a zigzag molecular backbone featuring 14 linearly fused heteroarene, which is the extended version of Herges's Möbius annulene. The helical moiety in Möbius belt not only significantly alleviates the strain energy by winding the rigid backbone, but also precisely controls the chirality of Möbius belt compared to those formed by Strategy I. The studies with NMR spectroscopy and DFT calculations provide evidence that Möbius belt exhibits a weak global electron communication.

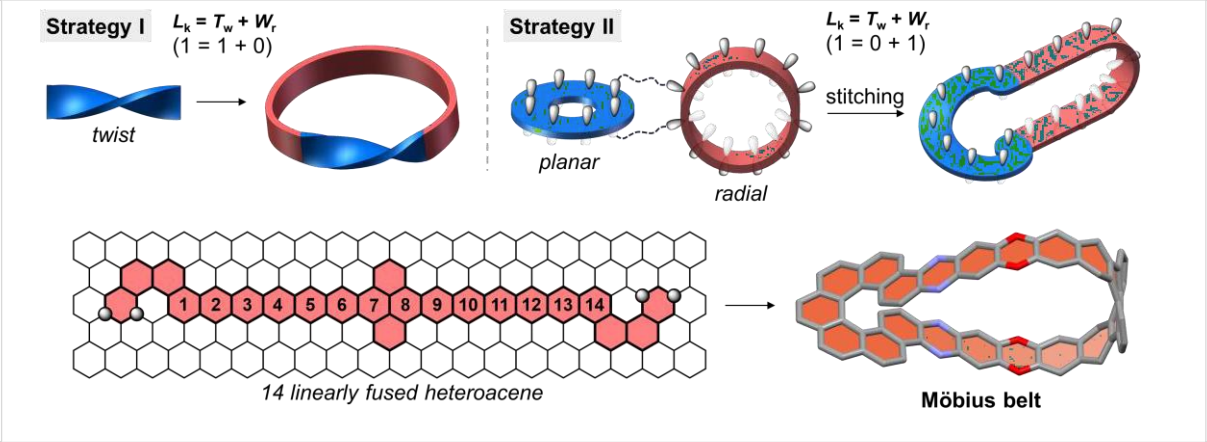

Figure 1: Two synthetic strategies towards molecular Möbius belt, and structure of Möbius belt.

References:

[1] Y. Segawa, T. Watanabe, K. Yamanoue, M. Kuwayama, K. Watanabe, J. Pirillo, Y. Hijikata, K. Itami, Nat. Synth. 2022, 1, 535-541.

[2] D. Ajami, O. Oeckler, A. Simon, R. Herges, Nature 2003, 426, 819-821.