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For immediate release

Press release

HKU Chemists Develop Compact Catenane with Tuneable Mechanical Chirality, Offering New Possibilities for the Design and Application of Mechanically Interlocked Molecules



Figure 1. Diagrammatic representation of the isostructural desymmetrisation strategy to transform an achiral catenane into a chiral structure.

A team of chemists from The University of Hong Kong (HKU), in collaboration with international scientists, has made significant strides in the field of mechanically interlocked molecules (MIMs). Their work, recently published in the prestigious journal *Nature Synthesis*, showcases the development of a compact catenane with tuneable mechanical chirality, offering promising applications in areas such as material science, nanotechnology, and pharmaceuticals.

The research was a collaborative effort led by the late Nobel Laureate Professor Fraser STODDART, alongside Research Assistant Professors Dr Chun TANG and Dr Ruihua ZHANG from HKU's Department of Chemistry. Contributions also came from researchers at HKU, Northwestern University and other global institutions.

Catenanes and Mechanical Chirality

Catenanes are unique molecular structures formed by the mechanical interlocking of two or more rings, akin to chain links. Unlike covalent bonds, these rings are held together by mechanical forces. Mechanical chirality



refers to the chirality arising from the non-superimposable spatial arrangement of interlocked molecular rings, which can significantly impact their properties and functions.

In this study, researchers demonstrated that two achiral rings with specific symmetrical features can create a catenane with mechanical chirality through an innovative isostructural desymmetrisation strategy. This allows the catenane to adopt a compact co-conformation, similar to its achiral counterpart. When interlocked in this compact form, the rings lose their individual symmetry and form chiral structures that cannot overlap with their mirror images, a property known as chirality in chemistry.

Technical Innovation and Methodology

The research team has developed a catenane with tuneable chirality, achieved through chiral induction and advanced synthetic techniques. By introducing chiral disulfonate molecules, they can favour one mirror-image form over the other, allowing precise control over the catenane's behaviour in solutions and solid crystals. This tunability, driven by a compact design and strategic molecular geometry adjustments, suggests promising applications in smart materials, and nanotechnology and novel drug design. Computational modelling and experimental validation have enabled the manipulation of chirality by controlling the interaction and mechanical movements of the interlocked rings, allowing transitions between different chiral states. The researchers also revealed that the equilibrium between these enantiomers can be adjusted by introducing certain chiral molecules, inducing chirality and optical activity.

Potential Applications

In nanotechnology, these catenanes could be used to create molecular machines with specific chiral functionalities that perform tasks such as molecular recognition or targeted drug delivery. In materials science, the tunable properties of these structures could lead to the development of new materials and composites with customisable mechanical and optical characteristics for sensing and other applications.

"The ability to create and control mechanical chirality in catenanes opens up new avenues for the development of advanced functional materials and artificial molecular machines," said Dr Tang. "Our findings highlight the potential of using mechanical bonds to create chirality, which could have important implications for the field of chemistry and materials science."

The Research Team and Collaborators

This research not only showcases the innovative capabilities of HKU's Department of Chemistry but also underscores the importance of international collaboration in advancing scientific knowledge. The study was supported by the University Research Committee of HKU, the US Department of Energy, and the Starry Night Science Fund of Zhejiang University Shanghai Institute for Advanced Study.



This research is a collaboration among Professor Fraser Stoddart, Research Assistant Professors Chun TANG and Ruihua ZHANG from The University of Hong Kong, Professor Michael R WASIELEWSKI and Professor Evan A SCOTT from Northwestern University in the United States, and Professor Zhi Li from ShanghaiTech University. The international team also includes Drs. Han HAN, Guangcheng WU, and Yong WU, as well as Professor Aspen X-Y CHEN, Paige J BROWN, Ryan M YOUNG, Xueze ZHAO, Arthur H G DAVID, Bo SONG, Alexandre ABHERVE, Yu-Meng YE, Yuanning FENG, and Charlotte L STERN, all of whom made significant contributions to this research project. Professor Fraser STODDART passed away on December 30, 2024. At the time of submission, he was one of the corresponding authors.

The journal paper "A Compact Catenane with Tuneable Mechanical Chirality" can be accessed from here: <u>https://www.nature.com/articles/s44160-025-00781-z</u>

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