Molecules do the triple twist

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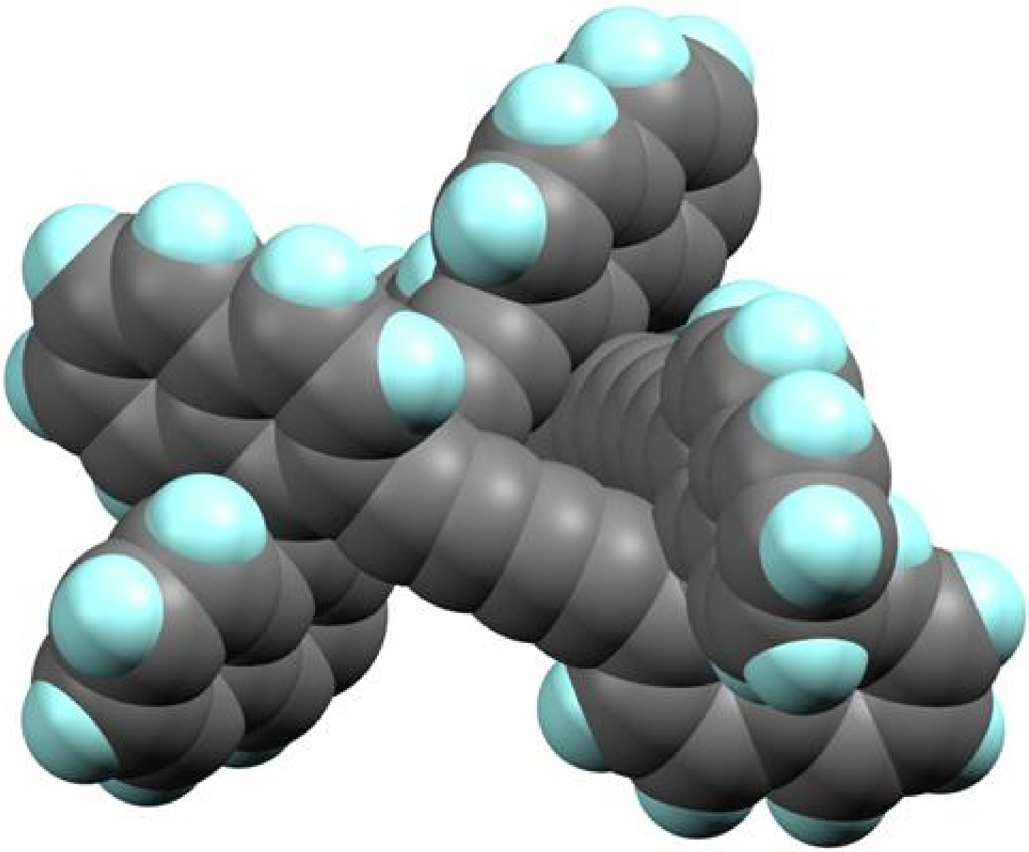


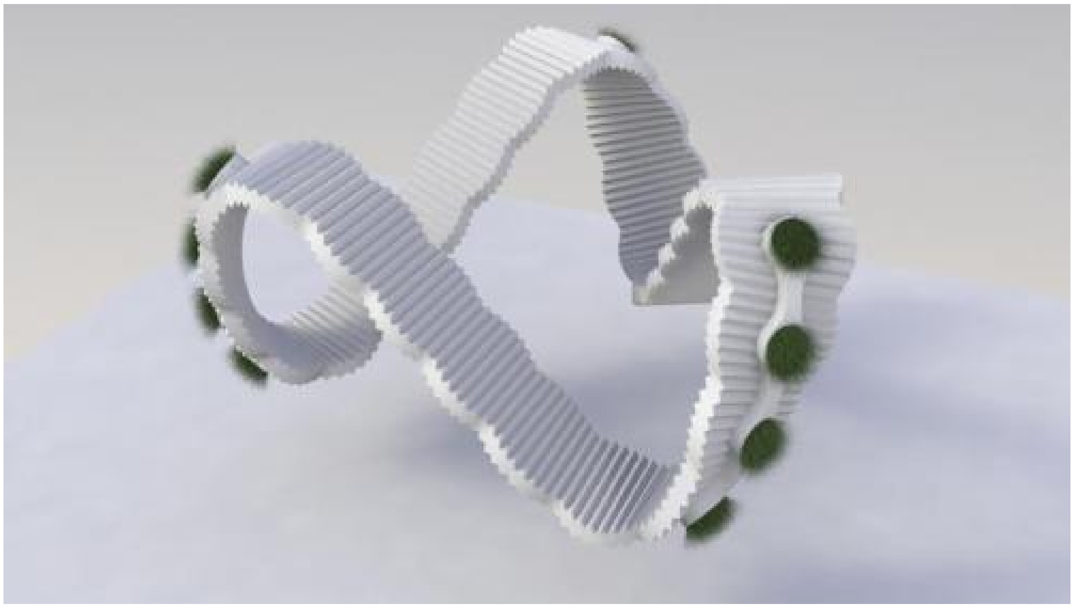
Graphical image of the Moebius molecule Credit: Rainer Herges/Nature Chemistry

They are three-dimensional and yet single-sided: Moebius strips. These twisted objects have only one side and one edge and they put our imagination to the test. Under the leadership of Kiel University's chemist Professor Rainer Herges, an international team of scientists has succeeded in designing the world's first triply twisted molecule. Because of their peculiar quantum mechanical properties these structures are interesting for applications in molecular electronics and optoelectronics. In the scientific journal *Nature Chemistry* the scientists report that they used a topological trick when making these intricate molecules.

In 1858, the mathematicians Johann Benedict Listing and August Ferdinand Moebius independently discovered the twisted bands with only one side and edge. Ever since, Moebius strips inspired architects, artists and natural scientists alike. Anyone can make a simple model. Just twist a strip of paper by 180 degrees and join both ends to form a band. The topological properties are mind blowing. For example, if cut lengthwise, the band does not give, – as with an ordinary strip – two strips but instead one band, with twice the diameter and twisted fourfold.

In the 1960s, chemists also became interested in this peculiar topology because theoretical calculations had predicted properties, which would violate one of the most important laws of chemistry concerning the stability of molecules. But it took almost 50 years to create a simple twisted molecule and to confirm these predictions. And here, too, it was Rainer Herges and his PhD student Dariush Ajami of Kiel University who succeeded in this project. The difficulty was to twist the molecules: like strips made from cardboard or steel, they would resist twisting and start to "untwist" when released at the "ends". Therefore, the scientists constructed their molecule from two parts: One part was an ordinary, strip-like component, the other was pre-shaped and in the form of a belt. Merging these two components unevitably creates a twisted ring

Triply twisted rings, however, are far too strained to be made like this. In this quandary hope comes from topology. It's an everyday life observation that, to relieve tension, twisted bands wind around themselves – best seen in twisted telephone cords or garden hoses. "The building blocks to construct our triply twisted Moebius molecule are three helical components. They look like short sections of a DNA helix", explains Rainer Herges.



Artistic depiction of a triple twisted Moebius molecule for Kiel University in form of a staircase Credit: Copyright: Herges

Unlike twisted components, helical molecules are stable. Still, it was not easy to combine these spiral units to a Moebius molecule, because they are chiral. This means that the mirror image cannot be superimposed on the original and that they rotate in a different direction. The researchers had to find the right way of combining the three components in order to design the desired molecule. In the end, they succeeded.

"With our strategy, it is in fact simpler to fabricate triply twisted or other multiply twisted molecular systems than singly twisted units", Herges sums up. The Moebius molecules from Kiel have very interesting electronic and optical properties. They could eventually be used as components to build quantum computers. The "quantum bits" would be defined by the topological states "twisted" and "untwisted" instead of a voltage on and off. Due to their peculiar quantum mechanical properties, currents induced by a magnetic field in Moebius molecules flow in the direction opposite to that they would take in normal rings.

More information: Gaston R. Schaller, Filip Topic, Kari Rissanen, Yoshio Okamoto, Jun Shen and Rainer Herges. "Design and synthesis of the first triply twisted Möbius annulene." *Nature Chemistry*; DOI: 10.1038/nchem.1955 (Advance Online Publication)

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