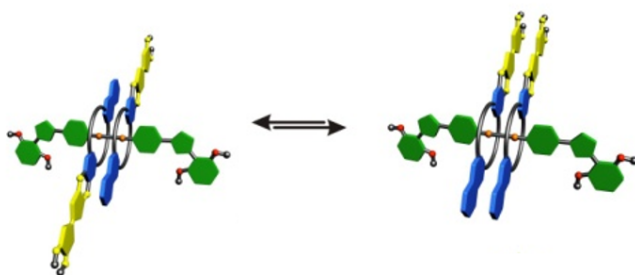


Understanding switchable processes in supramolecular systems

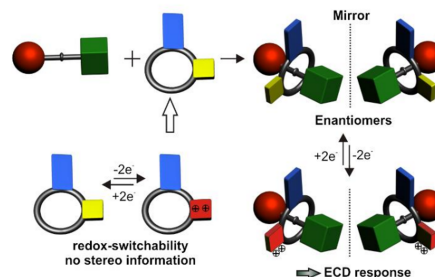
Felix Witte^a, Hendrik V. Schröder^a, Marius Gaedke^a, Christoph A. Schalley^a
and Beate Paulus^a

^aFreie Universität Berlin, BCP - Theoretical Chemistry, Berlin, Germany
jf.witte@fu-berlin.de

The 2016 Nobel prize in chemistry awarded to Jean-Pierre Sauvage, Sir J. Fraser Stoddart, and Bernard L. Feringa "for the design and synthesis of molecular machines" [1] is proof of the broad interest in the creation of new supramolecular architectures capable of converting energy at the nanoscale. The nature of the underlying mechanisms of these "machines" are usually dominated by non-covalent interactions. As long as intermolecular interactions are the target, experimental approaches are often sufficient to obtain a satisfying understanding of the systems' properties. However, the mechanical bond between the different parts of a supramolecule converts most of the originally intermolecular interactions into intramolecular ones, presenting a great challenge for most experimental strategies. In these cases theoretical approaches are indispensable. Here, we study the intramolecular non-covalent interactions in two different kinds of rotaxanes functionalised by TTF (tetrathiafulvalene) units using DFT-based calculations to study and understand their switching mechanisms.



Switchable Co-conformation: A [3]rotaxane performs a controlled rotational motion stimulated by current in a CV setup.



Conformational chirality: A chirally active [2]rotaxane displays a charge-dependent CD signal reversal.

References

1. The Nobel Prize in Chemistry 2016 "for the design and synthesis of molecular machines", Royal Swedish Academy of Sciences.