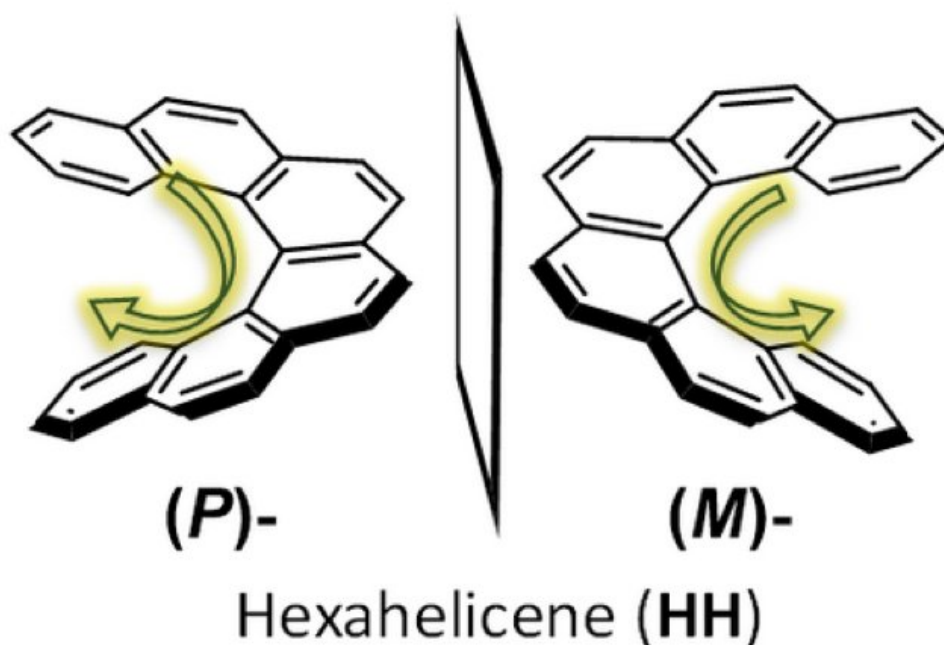


Hope for development of materials for 3-D displays and medical applications

July 6 2018



Enantiomers of hexahelicene. Credit: Osaka University

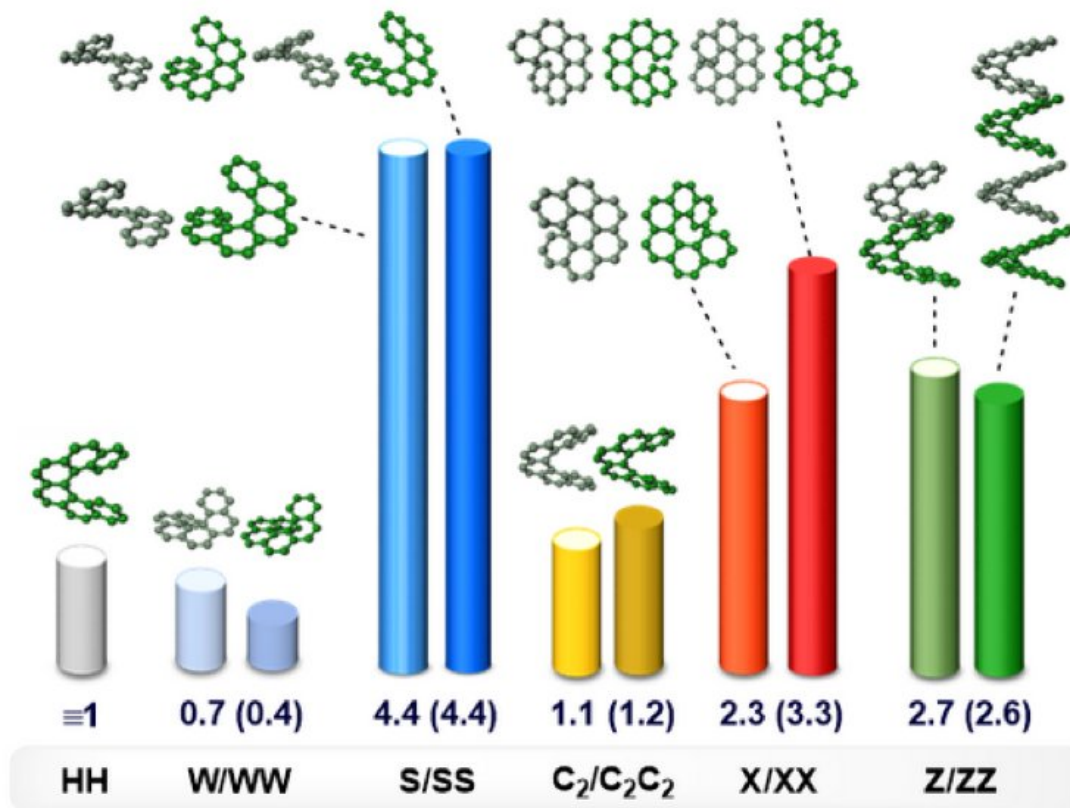
Chiral molecules are mirror images of one another. They are non-superimposable and play a crucial role in advanced materials and technologies. However, there had been no reliable theoretical systems for the design and synthesis of chiral materials. These systems had seen only gradual development, with chemists making progress on the design

and synthesis of chiral materials based on their intuition.

A research group led by Tadashi Mori at Osaka University aligned two hexahelicenes (Figure 1) in various orientations, theoretically examined, and proposed that S- and X-shaped double hexahelicene aligned in right symmetry were a key to improve the properties of helicenes. The researchers then synthesized double hexahelicenes to demonstrate their improved chiroptical properties as chiral materials: circular dichroism (CD) and circularly polarized luminescence (CPL). Their research results were published in *Communications Chemistry*.

They aligned multiple chiral hexahelicene units to thoroughly examine how their chiroptical properties would be enhanced by [quantum chemical calculations](#). (Figure 2) The results suggested that chiroptical performances were enhanced in S- and X-shaped helicenes aligned in right symmetry.

The researchers also examined the number of molecules to be aligned and the space between molecules and found the possibility that double helicenes, in which two helicenes are merged, could become ideal chiral materials.



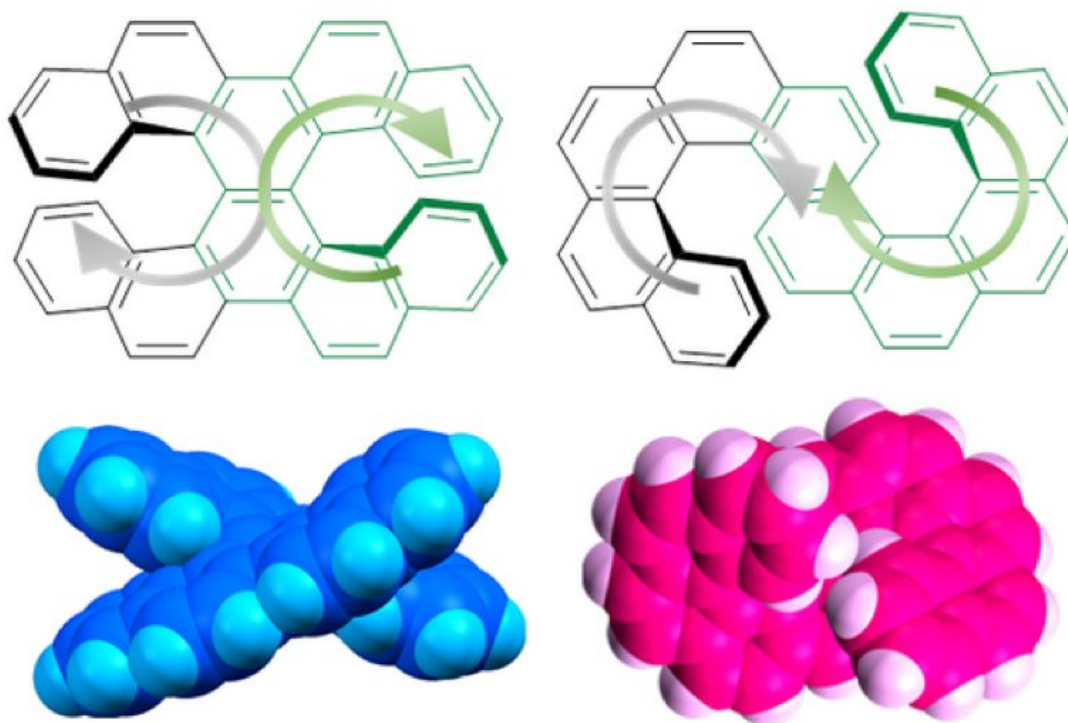
In their theoretical prediction using hexahelicenes aligned in various orientations, the S (blue) and X (red) assemblies with high molecular symmetry had higher chiroptical performance than the properties of native helicenes, demonstrating that they could become ideal chiral materials. Credit: Osaka University

Based on the discussion stated above, employing X- and S- shaped pristine double hexahelicenes (DNH and DPC) as representative molecular models, this group synthesized both double hexahelicenes, demonstrating drastic improvement of their chiroptical properties. (Figure 3)

They sought to determine which factors control chiroptical responses

and found that both intensity and orientation of the electric and magnetic transition dipole moments of the molecules were important.

This group demonstrated a new logical protocol for designing chiral [materials](#)—how to rationally align and design [molecules](#). By using strategies beyond conventional ways of material development that were based on researchers intuition, the group drastically improved material development costs. Polarized light can be used for next-generation optical information technology, so this study will accelerate technical innovation in the development of [advanced materials](#) for 3-D displays and endoscopes in medical applications, as well as security paint in information and communication fields.



Chemical structures and crystal structures of X- and S-shaped double helicenes. They showed high chiroptical properties due to their high symmetry. Credit:

Osaka University

More information: Hiroki Tanaka et al, Symmetry-based rational design for boosting chiroptical responses, *Communications Chemistry* (2018). [DOI: 10.1038/s42004-018-0035-x](https://doi.org/10.1038/s42004-018-0035-x)

Provided by Osaka University

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