Technology to predict the deformation of DNA origami structures induced by DNA-binding molecules

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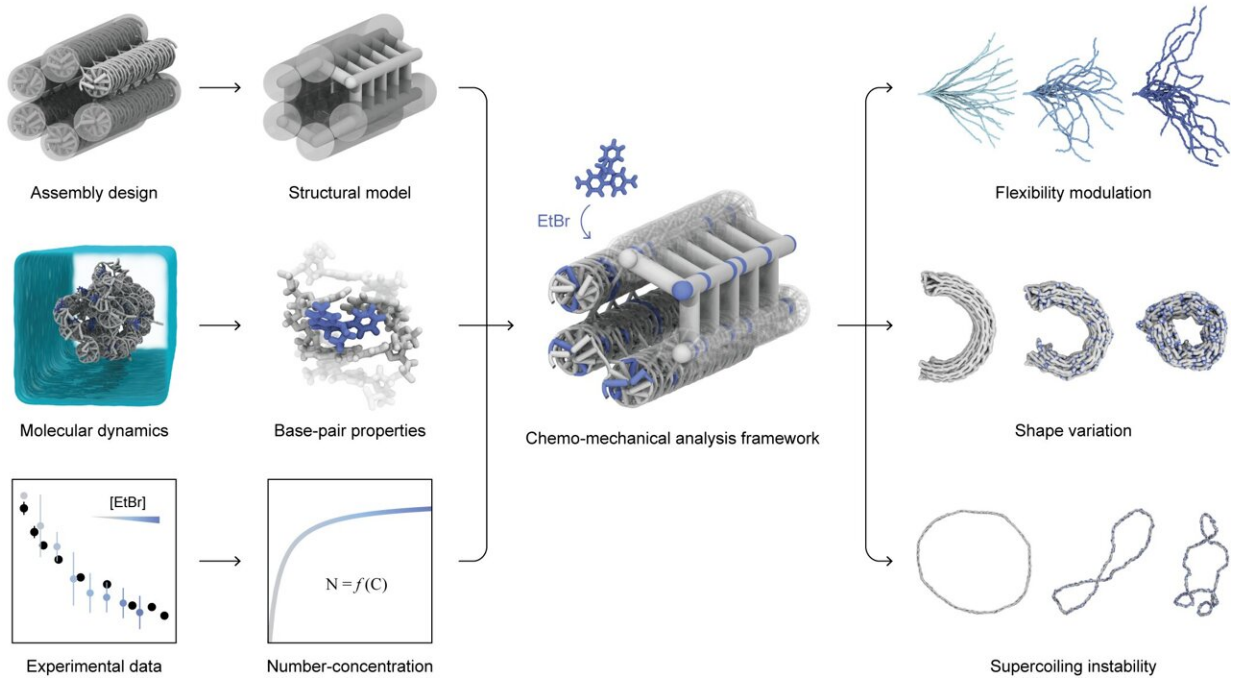


Conceptual Diagram of the Predictive Technology for Mechanochemical Changes in DNA Nanostructures. Credit: Seoul National University College of Engineering

A research team has developed a technology that can quickly predict the mechanochemical shape changes of DNA origami nanostructures. The team includes Professor Do-Nyun Kim's research team from the

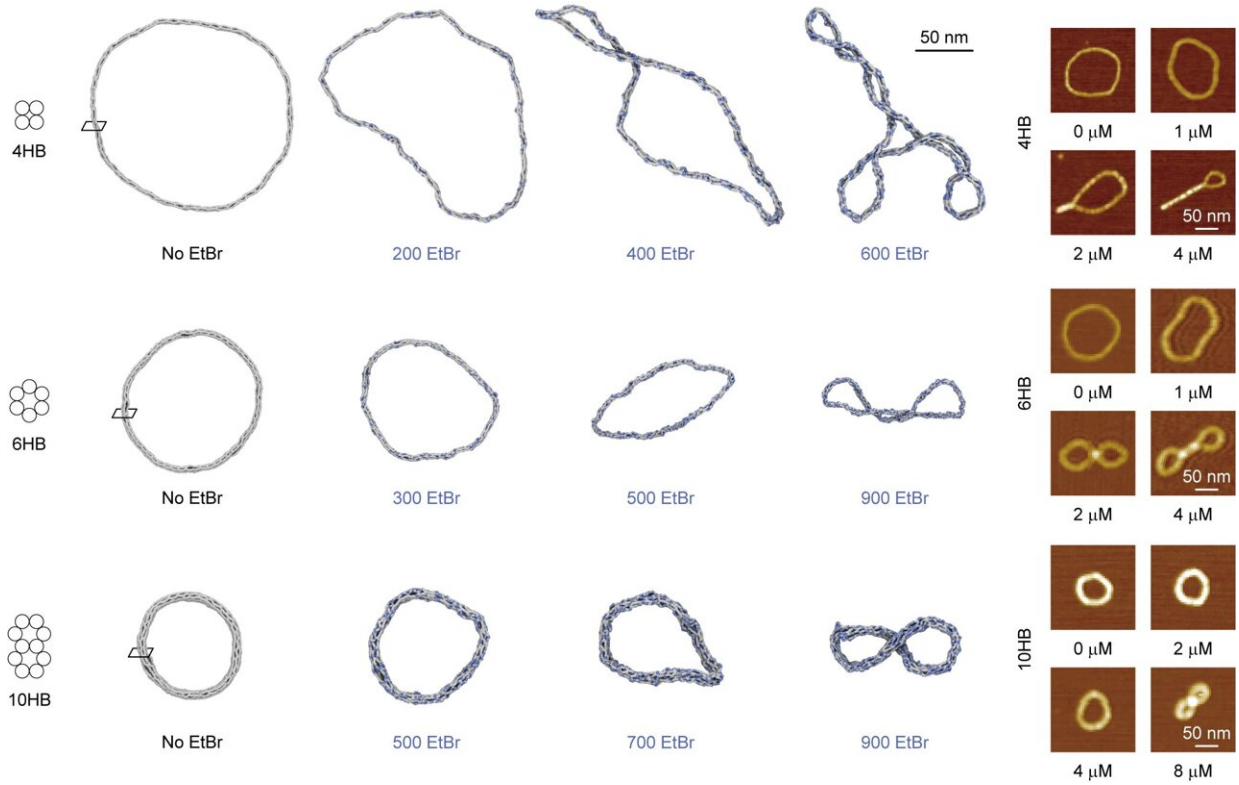
Department of Mechanical Engineering at The College of Engineering of Seoul National University.

The results of this study were published on July 31 in the journal *Nature Communications*.

DNA origami technology, which uses the self-assembly characteristics of DNA to design and fabricate structures of desired shapes with nanoscale precision, has high applicability and is being actively researched in advanced bio-convergence fields. Especially, technology to utilize environmental changes within the body to alter the shape of structures to perform necessary functions is attracting attention.

However, due to the lack of modeling and computer simulation technology that can design these variable mechanisms with understanding, implementing variable technology has relied on repetitive experiments and trial and error. There has been a rising need to study effective methods to rapidly analyze the deformation mechanisms of structures based on the geometric and mechanical properties of DNA, which change with environmental conditions.

Starting from this problem awareness, the research team discovered a way to quickly predict how the shape of DNA origami structures changes depending on the concentration of molecules binding to DNA. The team first quantitatively analyzed the geometric and mechanical changes in DNA caused by binding with a representative DNA-binding molecule, Ethidium Bromide (EtBr), through molecular dynamics simulations.



Prediction and Experiment of DNA Ring Structure Supercoiling Phenomenon with Varying EtBr Concentrations. Credit: Seoul National University College of Engineering

Then, they constructed a relationship between the concentration of binding molecules and changes in DNA properties using this molecular-level calculated information and applied it to DNA structure analysis. Through this process, they were finally able to quickly determine the mechanochemical deformation of DNA origami structures according to changes in EtBr concentration.

This technology can be easily extended to predict DNA property changes due to binding with other DNA-binding molecules. It can also be used to design tunable DNA origami structures that can change shape based on

the concentration of binding molecules or according to the type of binding molecules, thereby significantly contributing to the advancement of related DNA nanotechnology and various application research.

Meanwhile, this study, led by Professor Do-nyun Kim of the Department of Mechanical Engineering at Seoul National University and conducted by Research Professor Lee Jae-young and Researcher Kim Yang-kyun.

More information: Jae Young Lee et al, Predicting the effect of binding molecules on the shape and mechanical properties of structured DNA assemblies, *Nature Communications* (2024). DOI: 10.1038/s41467-024-50871-3

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