Self-assembled artificial microtubule like LEGO building blocks

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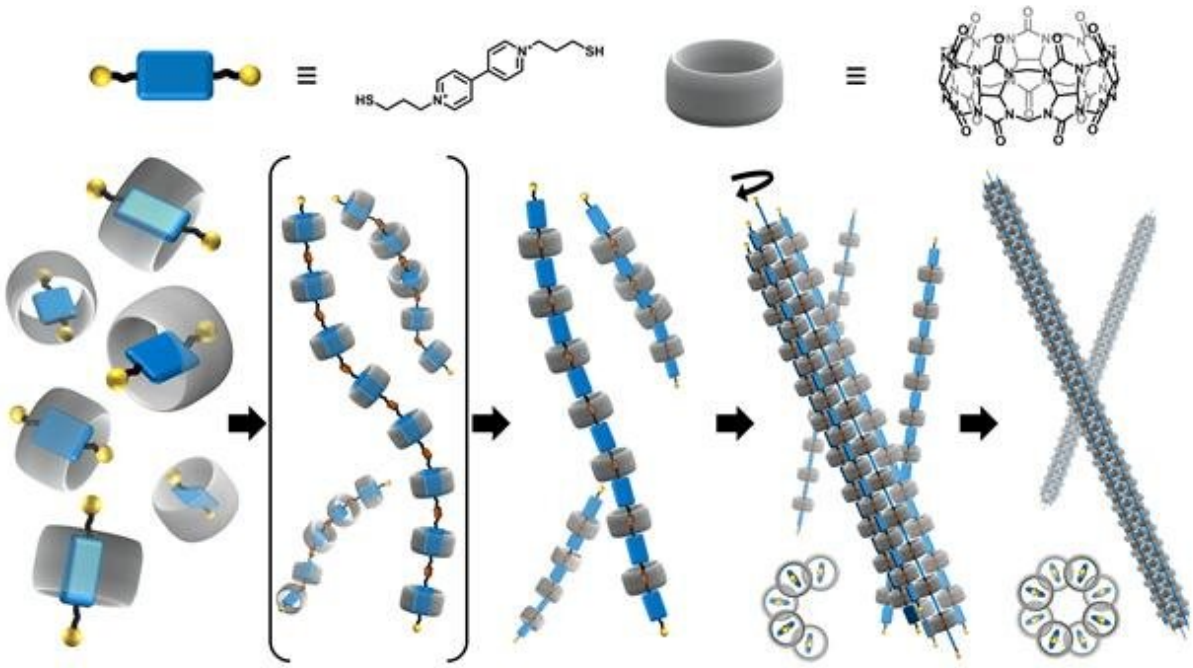

Hierarchical self-assembly of polypseudorotaxanes into artificial microtubules. Credit: Kimoon Kim (POSTECH)

Simple LEGO bricks can be assembled to more complicated structures, which can be further associated into a wide variety of complex architectures, from automobiles, rockets, and ships to gigantic castles and amusement parks. Such an event of multi-step assembly, so-called

'hierarchical self-assembly,' also happens in living organisms.

Professor Kimoon Kim (Department of Chemistry, POSTECH) and his research team (Center for Self-assembly and Complexity, Institute for Basic Science) discovered that a cucurbituril-based host-guest complex polymerized into a linear polymer chain, which was further associated with each other into a hollow microtubule via van der Waals interactions arising from their shape self-complementarity. Their novel findings are introduced as breaking news in *Angewandte Chemie International Edition*, which is one of the world's renowned journals in Chemistry.

Microtubules exist in living cells of plants and animals and they are essential in maintaining cellular structures, migration of cells, intracellular transport and more. In other words, essential cellular functions such as cellular divisions and intracellular transport cannot be performed when problems occur in formation or dissociation of microtubules.

These microtubules are formed via hierarchical self-assembly of globular proteins in nanometer size tubulins, which grow into linear protofilaments. Subsequently, these protofilaments are assembled together to build a multi-stranded tubular structure with a length over tens of micrometers.

Before the researchers' findings, many attempts were made to mimic the self-assembly of microtubules in depth for years. However, the formation mechanism of natural microtubules at the molecular level is still ambiguous.

To make artificial microtubules, the research group utilized the cucurbituril-based host-guest complex with two thiol groups attached at the both ends as a building block. This building block assembled into one-dimensional linear polymers by disulfide bond formation. Then, these

polymers were laterally associated into a hollow cylindrical architecture similar to natural microtubules through van der Waals interactions. The formation of artificial microtubules was characterized by various spectroscopic and microscopic studies including X-ray diffraction at Pohang Light Source.

The research team found that the polymer chain became straight and stiff by itself, and eventually LEGO brick-like shape self-complementarity emerged during the growth of polymer. Strikingly, the convex structures of one chain matched well with the concave parts of the neighboring chains, which allowed lateral association of polymer chains.

The first author of the paper, Wooseup Hwang explained, "Studies before our discovery were focused on mimicking architecture of microtubules. What differentiates our research from the conventional ones is that we attempt to mimic the formation mechanism of microtubules as well as architecture."

Dr. Kangkyun Baek, the other co-corresponding author commented, "We are planning to extend our study to mimic dynamic behaviors and various biological functions of natural microtubules," and "This novel approach based on the shape self-complementarity will make a step forward to understand the formation mechanism of natural microtubules and offer new opportunities to explore unconventional hierarchical self-assemblies and novel functional materials."

More information: Wooseup Hwang et al, Hierarchical Self-assembly of Polypseudorotaxanes into Artificial Microtubules, *Angewandte Chemie* (2019). DOI: 10.1002/ange.201913384

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