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Editorial

Fundamental Properties of the Smallest Carbon Nanotubes Identified by a Newly Synthesized Chemical Compound

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EDITORIAL

Chemical rings of carbon and hydrogen atoms bend to form very stable structures capable of transporting electricity and other functions, but how do these curved systems alter as additional components are added? Researchers in Japan discovered that by changing the properties of a chemical molecule with just a few subatomic additions, they may change the system states and behaviors. "Open-shell molecules have gotten a lot of interest in the last decade, not just in the field of reactive intermediates, but also in materials science," stated the main author. Open-shell molecules can add or subtract molecules, allowing them to modify their chemical bonds. Carbon and hydrogen atom rings, for example, form a strong connection in carbon nanotubes.

However, the more rings added, the more the tube's properties can alter. The open-shell molecules were exposed to systems with molecular orbits containing two electrons in various states, in addition to the carbon and hydrogen atoms, known as curved paraphenylenes, or CPPs. This team investigated how the CPP might change if the open-shell molecules were exposed to systems with molecular orbits containing two electrons in various states, in addition to the carbon and hydrogen atoms. The introduction of these diradical systems to the CPPs resulted in the formation of a new type of azoalkane, which is a nitrogen-based molecule with a group of weakly linked hydrogen and carbon atoms. The researchers discovered that the states and features of CPPs with embedded diradicals varied depending on the number of CPPs in the final system, such as the intrinsic description of a particle known as spin.

Spin, or a particle's angular momentum, can help or hurt a system's stability depending on how the energy is balanced. Because the spins of the unbonded electrons are opposite in a singlet state, the system remains stable. The ground-state spin multiplicity is mostly determined by the ring size, which refers to the possible spin orientations that can signal a system's stability. For smaller CPP derivatives, the singlet ground state was preferred. The smaller singlet states diradical CPPs with narrower energy ranges between orbital shells also showed aromaticity or more stable alignment in a single plane, which is a desirable property for carbon nanotubes. Because the carbon-hydrogen rings create the tubes at unique angles, they can be driven out of alignment, causing system instability.

A system grows more strained as additional rings are added to it. The rings align in one plane for smaller singlet state systems, resulting in increased stability. The researchers hope to examine this in-plane aromaticity more in the future; with the goal of building the largest structure feasible with strong bonds that nevertheless exhibits this stable feature.

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