One-dimensional molecular nano-structures inside single-walled carbon nanotubes

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One of the most interesting features of molecular materials is the fact that their physical properties change with the molecular arrangement as well as the properties of the molecule itself. Self-organization is an efficient pathway through which organic molecules assemble to form well-ordered nanometre-scale objects that are hardly synthesized by conventional chemical reactions. In these systems, two or more molecules are held together and assembled by means of intermolecular (noncovalent) bonding such as ion-dipole or dipole-dipole interactions, hydrogen bonding, hydrophobic interactions, or π - π stacking.

Single-walled carbon nanotubes (SWCNTs) can offer a suitable interior space for accommodating molecules. The nanostructures produced by incorporating such molecules into SWCNTs are expected to exhibit several superior features. For example, because the diameter of SWCNTs can be adjusted to the size of the molecules, well-ordered molecular arrangements beyond a micro-metre long can be easily produced. The synthesized molecular arrangements are also expected to be strong and flexible against mechanical strain because the nanotube templates sustain the structure. Furthermore, the synthesized nanostructures are isolated from active molecules by the tube wall, which leads to the superior durability of the encapsulated molecules.

In this conference, we will report several characteristic nanostructures formed inside SWCNTs. For example, planner π -conjugated molecules, coronenes form nano-scale columns in a way that differs from 3D solid coronenes, resulting in electronic and optical properties peculiar to the 1D structure (Fig. 1) [1]. The basic properties of the produced 1D molecular crystal will be discussed in detail.



Figure 1. (a) Molecular structure of coronene. (b) HRTEM images of coronenes encapsulating SWCNTs. (c) Schematic illustration of coronenes encapsulating SWCNTs.

[1] T. Okazaki, Y. Iizumi, S. Okubo, H. Kataura, Z. Liu, K. Suenaga, Y. Tahara, M. Yudasaka, S. Okada, S. Iijima, *Angew. Chem. Int. Ed.*, in press.