超分子化学をベースとした高効率半導体性カーボンナノチューブ分離の戦略・メカニズム

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Supramolecular Chemistry-Based One-Pot High-Efficiency Separation of Semiconducting Single-Walled Carbon Nanotubes: Molecular Strategy and Mechanism

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Single-walled carbon nanotubes (SWCNTs) have the potential to revolutionize nanoscale electronics and power sources; however, their low purity and high separation cost limit their use in practical applications. Here we present a supramolecular chemistry-based one-pot, less expensive, scalable, and highly efficient separation of a solubilizer/adsorbent-free pure semiconducting SWCNT (sc-SWCNT) using flavin/isoalloxazine analogues with different substituents. On the basis of both experimental and computational simulations (DFT study), we have revealed the molecular requirements of the solubilizers as well as provided a possible mechanism for such a highly efficient selective sc-SWCNT separation. The present sorting method is very simple (one-pot) and gives a promising sc-SWCNT separation methodology.

Keywords *: Carbon nanotubes; Supramolecular chemistry; High efficient separation; Molecular strategy; Separation mechanism*

As-produced SWCNTs are synthesized as a mixture of semiconducting (sc-) and metallic (m-)-SWCNTs, hence chirality sorting of the SWCNT is highly important, and there has been a strong social demand about this issue from both fundamental and application aspects of the SWCNTs. To date, various methods have been presented for such a separation including surfactant-aided density gradient ultracentrifugation (DGU), gel chromatography techniques, aqueous two-phase extraction method, and the use of polyfluorenes (PFOs) and their analogues.

In this study, we present a concept/molecular design for the (n,m)-chirality separation of SWCNTs and shed light on the mechanism for the sorting chirality of the SWCNTs, in which the method is very simple (one-pot) for the separation of dispersant- free pure sc-SWCNTs with a high efficiency and is scalable. Based on both experimental and computational simulations (DFT study), we have revealed the molecular requirements of the solubilizers as well as provide a possible mechanism for such a highly-efficient selective sc-SWCNT separation.[1)] The present sorting method is very simple (one-pot) and gives a promising sc-SWCNT separation methodology.

Thus the study provides insight for the molecular design of an sc-SWCNT solubilizer with a high (n,m)-chiral selectivity, which benefits many areas including semiconducting nanoelectronics, thermoelectric, bio and energy materials and devices using solubilizer-free very pure sc-SWCNTs.

1)N. Nakashima et al. , *J. Am. Chem.* Soc. **2020**, 142, 11847-11856.