Synthesis of end-cap precursor molecules for the controlled growth of single-walled carbon nanotubes

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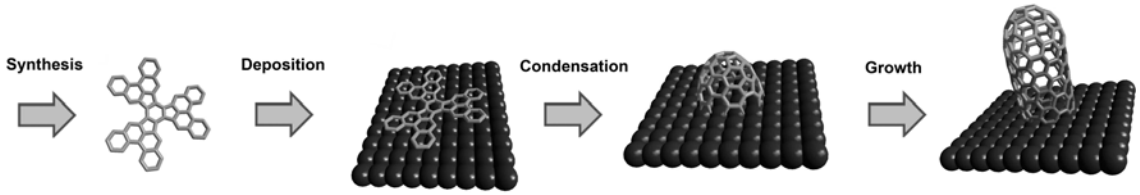
Despite considerable advance in growth methods for single-walled carbon nanotubes (SWCNTs) it is still not possible to rationally control their diameters and chiralities.

According to recent theoretical and experimental work, growth of SWCNTs starts by nucleation of an end-cap fragment on the catalyst particle followed by subsequent growth through incorporation of carbon atoms.[1, 2] Considering this growth mechanism of CNTs, it appears prospective to avoid the usual nucleation step of CNTs leading to the formation of an end-cap with accidental geometry by introducing a predefined end-cap molecule, the structure of which can be fully controlled. Subsequent growth will lead to the desired SWCNT species as determined by the end-cap geometry.

Several precursor molecules for different SWCNT species, including armchair, zigzag or chiral type have been prepared.[3] Such polyaromatic hydrocarbons can then be condensed to the corresponding bucky bowls by catalyzed cyclodehydrogenation on a metal surface. [4]

The synthesized precursors were used for the growth scenario shown in the scheme below and their influence on the carbon nanotube growth was investigated.



General scheme for the cyclodehydrogenation of the SWCNT end-cap precursor molecules and the subsequent growth of the CNT.

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