Synthesis of End-Cap Precursor Molecules for the Controlled Growth of Single-Walled Carbon Nanotubes

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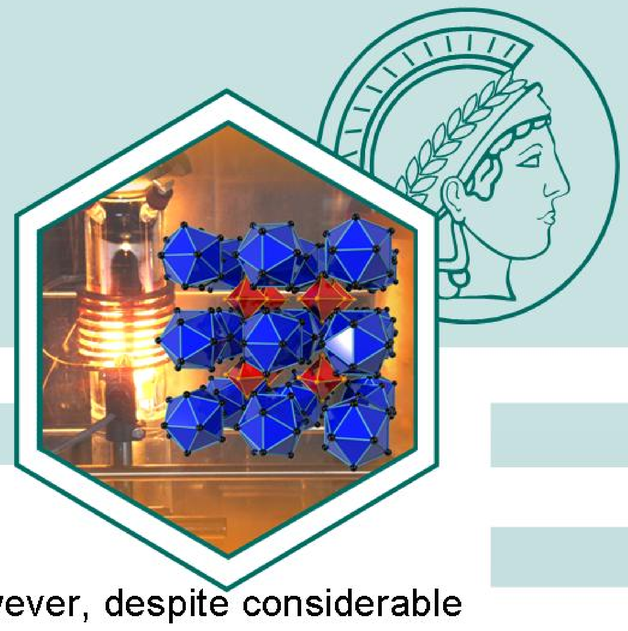
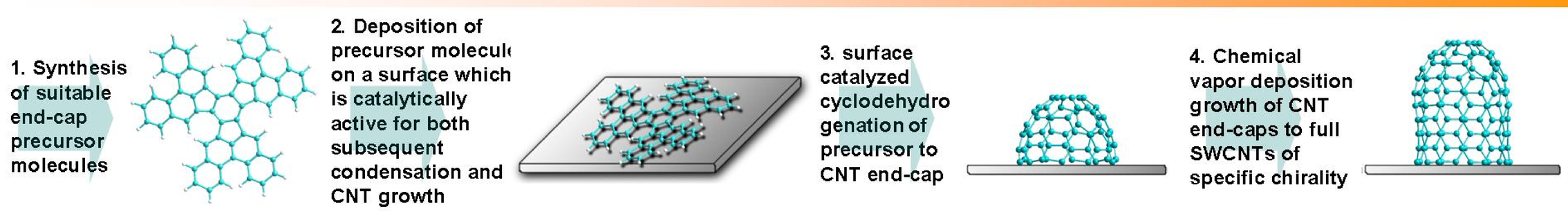


Introduction and approach

Single-walled carbon nanotubes (SWCNT) exhibit very promising properties for future applications. However, despite considerable advance in growth methods for CNTs it is still not possible to rationally control their diameters and chiralities.

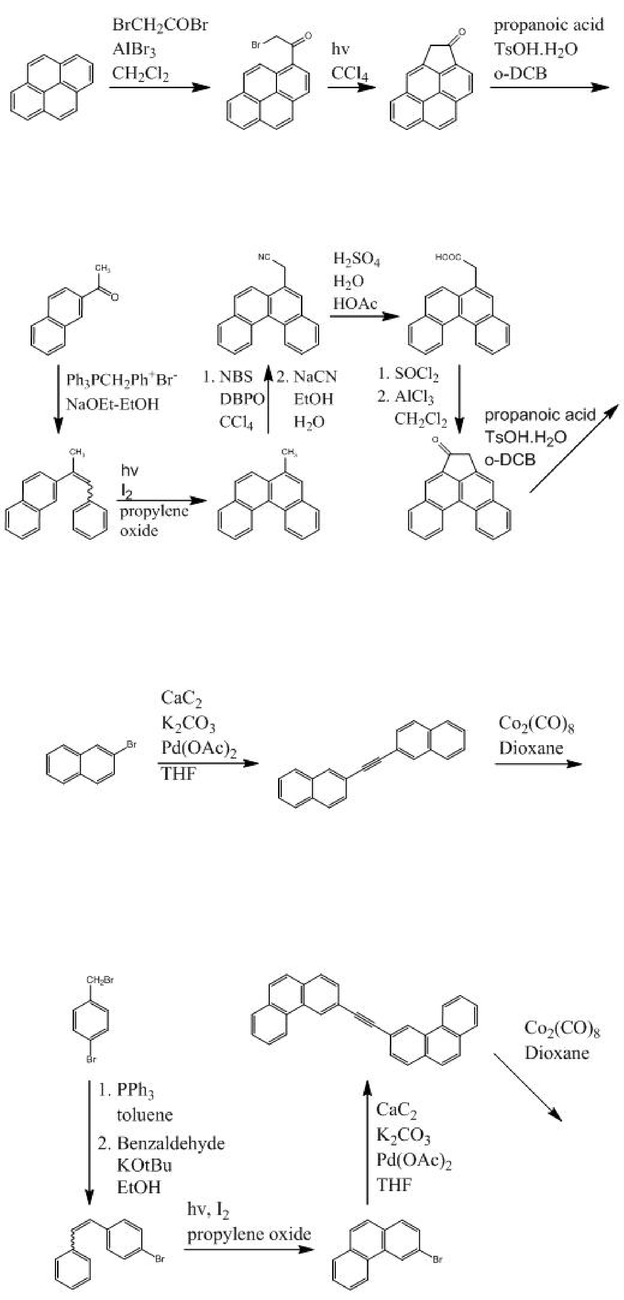
According to recent theoretical and experimental work by several groups investigating the very first steps of CNT synthesis, growth of SWCNTs starts by nucleation of an end-cap fragment on the catalyst particle followed by subsequent growth through incorporation of carbon atoms from the metal surface or bulk.[1, 2] Considering this growth mechanism of CNTs, it appears to be attractive 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. Further, specially designed polyaromatic hydrocarbons can be condensed selectively to the aimed bowl or fullerene structure on catalytically active surfaces.[3, 4]

Proposed scenario for the controled growth of single walled carbon nanotubes

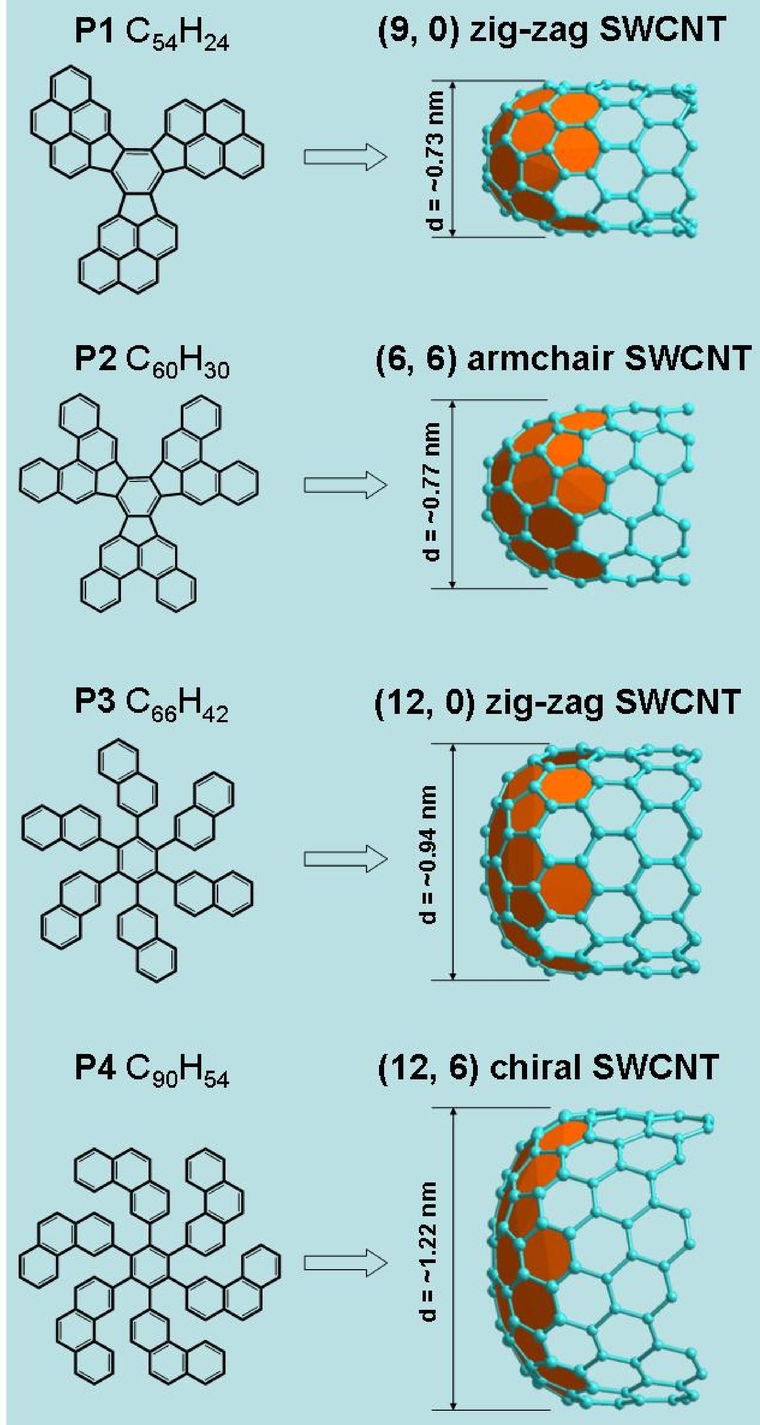


Results

Synthetic routes



Synthesized SWCNT end-cap precursors and corresponding SWCNTs

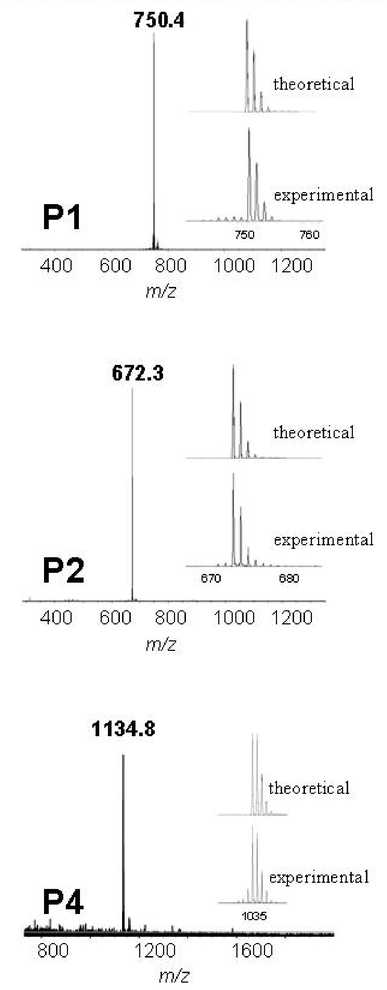


Four precursor molecules for single-wall carbon nanotube end - caps were synthesized. P1 and P2 contain 3 of the required 6 pentagons in their precursor structure while the remaining 3 have to be formed during condensation to the CNT end-cap (step 3 of the growth scenario). For P3 and P4 all 6 pentagons must be formed during the condensation step.

It is to note that all four precursors lead to different nanotube diameters and chirality types (armchair, zig-zag and chiral) but all of metallic electronic structure as can be determined from the equation: (n – m)/3 = integer which is true for metallic single-wall carbon nanotubes with arbitrary chiral indices (n, m).

MS analysis indicates a high purity of the synthesized products suitable for the subsequent steps of our growth scenario.

Analysis of final synthesis products and purity



Molecular structure of $C_{60}H_{30}$ precursor **P2** as determined from single-crystal X-ray diffraction data

Conclusions and future work

Four precursor molecules for CNT end-caps of different sizes, from 0.73 to 1.22 nm were synthesized.
All molecules would lead to metallic SWCNTs of different chiralities, namely zig-zag, arbmchair and chiral,
As the molecules can be obtained in high purity and are stable under conditions used for sublimation, they will be used for the further growth scenario steps.
Their influence on the SWCNT growth will be investigated.

References

[1] Y. Ohta, Y. Okamoto, S. Irle, K. Morokuma, *J. Phys. Chem. C* **2009**, 113, 159-169. [2] S. Hofmann et al., *Nano Lett.* **2007,** 7, 602-608.
[3] K. T. Rim et al., *Angew. Chem. Int. Ed.* **2007**, 46, 7891-7895. [4] K. Amsharov, S. Stephanov, S. Rauschenbach, M. Jansen K. Kern, N. Abdurakhmanova Angew. Chem. 2010, submitted. [5] A. Mueller, K. Amsharov, M. Jansen, *Tedrahedron Lett.* **2010**, 51, 3221-3225.

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