Chapter 2
Proposal

Despite their unique physical, mechanical and electronic properties single-walled carbon nanotube-based technology has commenced slowly. This can be traced back to two major hurdles namely their poor solubility in common solvents on the one hand and the polydispersity of the as-produced material with regard to diameter, length and chirality on the other hand. SWCNT solubilization can conveniently be achieved by the aid of surfactants noncovalently anchored to the SWCNT surface. The resulting dispersion can be subjected to sorting scenarios recently developed. However, up to now, separation efficiencies and yields are poor as sorting is restricted to individualized SWCNTs. Individualization rates by common surfactants are below 25% (after mild centrifugation) so that novel SWCNT surfactants with superior properties are sought for.

Accordingly, the major focus of this thesis is directed towards the evaluation of novel SWCNT surfactants with perylene bisimide (PBI) anchor groups. The desired amphiphilicity that can be considered as prerequisite for an efficient SWCNT dispersion in aqueous media, is generated by peripheral derivatization with *Newkome*-type dendrimers. The dispersion and individualization efficiencies of a variety of perylene bisimide derivatives are to be compared on the foundation of SWCNT absorption and nIR emission spectroscopy, as well as statistical AFM analysis. Since the PBIs are commonly equipped with carboxylic acid functionalities, the influence of the pH value and the counterion is another point which has to be addressed. In order to establish structure property relationships and to elucidate packing densities of the surfactants on the SWCNT scaffold and the underlying interactions, the characterization is to be expanded to alternative methods such as zeta potential measurements, IR spectroscopy, X-Ray photoelectron spectroscopy (XPS) and the hydrodynamic characterization of the SWCNT-PBI complexes by analytical ultracentrifugation.

On the foundation of these findings, potential selective interactions of the PBI dispersants with certain SWCNT species are to be investigated. For this purpose, a characterization routine based on the techniques outlined in Sect. 1.4 is to be developed. The gained insights and the acquired methodologies are then to be

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applied to structural variations of the π-surfactants such as cationic PBIs or pyrene derivatives.

In the second part, the designed surfactants shall be applied for SWCNT separation. Focus is not only to be laid on the use of already established techniques, but also on the design and development of novel separation scenarios accessible by the π-surfactants.

Another obstacle directly related to the polydispersity and poor solubility of the SWCNTs is presented in the characterization of this 1D carbon allotrope. Since no standard protocols can be followed, commonly evidence from multiple characterization techniques is cumulated to gain a comprehensive picture of noncovalently (or covalently) derivatized SWCNTs. Hereby, it is highly challenging to correlate the information obtained from the manifold spectroscopic and microscopic techniques. Accordingly, the improvement of SWCNT characterization and the development of reliable analytical protocols is another topic which is addressed by this thesis.

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Backes, C.
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