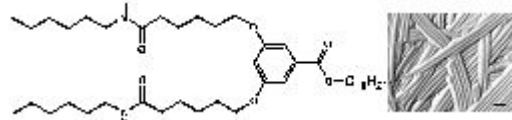


Project B4: Self-assembled nanotubes sheathing semiconducting wires

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Current state of research. Only few molecules self-assemble spontaneously in solution to form nanotubes. Several phenomenological physical models have been proposed to explain the formation of helical coils based on the chirality of the molecules involved, however without account for structural effects induced molecular interactions. This is particularly obvious when achiral molecules form chiral tubular structures (see Figure on the right: an achiral diamide ester forms nanotubes). In addition, some systems change their assembly behavior qualitatively when changing the solvent. The dynamics of the self-assembly process and of the transition from one morphology to another, e.g. from tubes to ribbons, is still unknown. Interestingly, the chemical reactivity within such nanotubes can be tuned by functionalizing the interior through self-assembly of suitable molecules. However, often the packing in the nanotube is disrupted by the functional groups, leading to the disintegration of the tube.



Contributions of the principal investigators. The Strasbourg group has developed a series of aromatic nonchiral diamides which self-assemble in organic solvents into nanotubes with diameters of up to ca. 30 nm and lengths of many micrometers. These compounds can be derivatized, which potentially allows to carry out reactions inside the nanotube. The Freiburg group has long-standing experience in the structural analysis of polymers near surfaces. Arranging the nanotubes in an ordered fashion on surfaces allows the study of their structure by microscopy (e.g. AFM, STM), including also different levels of organization at different length scales and functionality. Preliminary results show that such an approach is promising.

Research project and collaborations. This project aims at understanding the self-assembly of the aforementioned functional diamide compounds in solution and on surfaces. We want to identify the molecular parameters influencing the shape and size of the self-assembled aggregates. The impact of “external” parameters, like concentration, temperature, solvent composition, etc., will also be explored. Furthermore, dynamic aspects can also determine the size and shape of the aggregates and thus control the growth and morphology of the self-assembled structures. Ultimately, with the help of the theory group at the ICS in Strasbourg, we aim at modeling the processes relevant for the formation of the ordered objects.

A series of analogs with varying sizes of ester or with amide groups at various positions will be synthesized. We also plan to introduce a chiral group on the ester. Moreover, the two amide groups may have an anti-parallel orientation. The resulting self-assembled structures will be characterized by various microscopy techniques, yielding e.g. internal and external radii. The controlling influence of chirality and of various interactions, e.g. H-bonds or π -stacking, in various aromatic solvents will be elucidated. Finally, also in collaboration with M. Brinkmann (ICS), we will try to direct self-assembly on patterned and functionalized polymeric substrates, and to use the functional interior of the nanotubes for a subsequent filling stage, yielding e.g. nanotubes having a conductive or semiconducting interior, i.e. nano-wires encapsulated in an insulating tube.

Work plan. The doctoral researcher will spend a significant time of his thesis in Strasbourg, contributing to the synthesis and characterization of the compounds. Electron microscopy studies on the formed aggregates will also be performed in Strasbourg. In Freiburg, functionalized aggregates on substrates will be studied by AFM and STM. By condensing vapors of different solvents, in the presence of complementary compounds, onto these deposited nanotubes, reorganization dynamics and filling or co-assembly processes will be studied.