ITI HiFunMat Master Internship Proposal

☐ M 1 ☒ M 2

Title: Nanotubes with controlled diameters: toward a new model of tubular self-assemblies

Internship supervisor

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Laboratory	Institut Charles Sadron
Collaboration with a HiFunMat member (*please indicate their name*)	☐ No ☒ Yes : COMBET

Student profile looked for

Master program (*more than one box can be ticked*)	☒ Material science and engineering ☒ Chemistry ☐ Physics
Other indications if necessary	

Internship description

There are a few organic compounds able to self-assemble in nanotubes.[1] Some theoretical models have been developed for tubes formed by lipids, but concern only large tubes often microtubules. But so far one cannot explain at the molecular level why such self-assembly leads to a nanotubular shape. As a matter of fact, only a few examples of structures of the tubes have been elucidated at the molecular level.[2–4] In our group we have developed simple amide-based molecules, BHPBn (Fig. 1) able to form nanotubes with diameters of a few tens of nm, as shown by freeze fracture TEM and small angle X-ray scattering (SAXS) experiments.[5,6] The diameter depends on the length ***n*** of the ester chain. Recently we have shown that related monoamide compounds also form nanotobes and that in these tubes the compounds form in inner and an outer sheet, with their ester parts turned toward the inner and outer wall, and the amide chains form an interdigitated middle layer like in Fig. 3.[7]

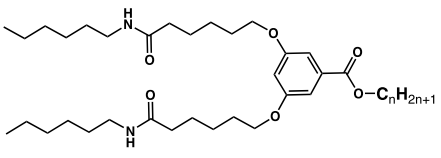

Fig. 1. Chemical structure of BHPBn. n is the number of C atoms in the ester.

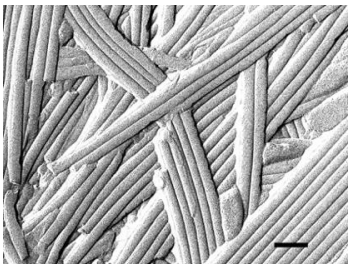

Fig. 2. Freeze fracture TEM of BHPB10 in cyclohexane; Bar is 50 nm

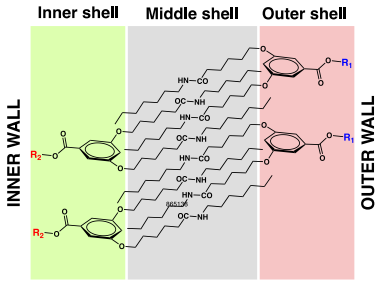

Fig. 3. Possible structure of the self-assembly of BHPBn in the nanotubes.

The project aims at studying the inner structure of the nanotubes of BHPBn, especially to prove and refine the structure proposed in Fig. 3, by small angle X-ray and neutron scattering (SAXS and SANS). The model will be also confirmed by synthesizing analogues of BHPBn with deuterated ester and aromatic parts and studying their self-assemblies by SANS, with the contrast variation method. A second objective is to study

the behavior of binary mixtures BHPBn/BHPBm and to measure the variations of the structures with the mixture ratios. We will first verify that they form solid solutions by DSC and that also form tubes. Then, we will analyze with deuterated analogues how the BHPBn and BHPBm are distributed. Are they equally located on the inner and outer walls of the tubes or do they selectively occupy one face? The latter case would explain why the self-assembly induces a curvature.

The hired student will 1) synthesize a homologous series of BHPBn and the deuterated analogues of BHPB8 and BHPB10, 2) study the structure of the self-assemblies by freeze fracture TEM, in collaboration with M. Schmutz and by SAXS in collaboration with J. Combet. The binary mixtures will be studied by microDSC.

We are looking for a motivated student with a background in organic or polymer chemistry eager to learn physicochemical techniques; or with a background in physical chemistry able to conduct few chemical syntheses. A good proficiency in English is a plus. The applicant should send her/his resume and material to mesini@ics-cnrs.unistra. All acceptation, enrolment and paperwork has to be done by October 8th, because the Institut Charles Sadron is a ZRR lab (restricted access area).

1 Shimizu, T. *et al. Chem. Rev.* 105, 1401–1444 (2005)
2 Valéry, C. *et al. Proc. Natl. Acad. Sci.* 100, 10258–10262 (2003)
3 Tarabout, C. *et al. Proc. Natl. Acad. Sci. U. S. A.* 108, 7679–7684 (2011)
4 Oda, R. *et al. J Am Chem Soc* 130, 14705–14712 (2008)
5 Diaz, N. *et al. Angew Chem Int Ed* 44, 3260–3264 (2005)
6 Simon, F.-X. *et al. Soft Matter* 9, 8483–8493 (2013)
7 Zapién-Castillo, S. *et al. Int. J. Mol. Sci.* 21, 4960 (2020)