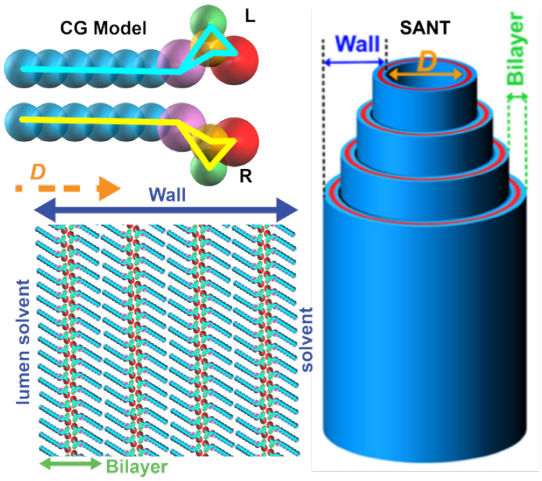
M2 INTERNSHIP PROPOSAL

Title: SCAM: Simulating **C**hirality-Driven Self-Assembly of Nanotubes in **A**polar **M**edia.

Laboratory: Institut Charles Sadron, Strasbourg - TSP and SyFOS teams.
Supervisors: William S. Fall (william.fall@cnrs.fr) and Philippe Mésini (philippe.mesini@ics-cnrs.unistra.fr)

Proposal: Self-assembled nanotubes (SANTs) are fascinating objects in soft matter science, valued for their well-defined inner diameters, high aspect ratios, and hollow cores, which make them promising candidates for applications such as filtration, selective capture, encapsulation, and drug delivery. While most SANTs form in aqueous media from chiral amphiphilic compounds—where molecular chirality drives a symmetry-breaking twist that bends flat ribbons into tubes—far fewer systems assemble in apolar media, where the tube architecture is instead governed by strong, specific short-range interactions such as hydrogen bonding and π–π stacking. Experiments have shown that a chiral amphiphilic system self-assembles into micrometer-long nanotubes in oils and alkanes, with tube formation depending critically on the enantiomeric composition of the building blocks. A key open question is how each enantiomer is distributed across the tube wall—experiments cannot resolve this partitioning, yet it likely controls curvature and morphology. The small diameter of these nanotubes makes them uniquely suited to large-scale coarse-grained molecular dynamics simulations, which are generally limited to a few hundred nanometers. By running many parallel "computer experiments," simulations can map the phase behaviour across key parameters, narrowing the vast phase space and allowing experimental efforts to be targeted towards the most informative conditions.



Objectives: The objectives of the internship are as follows:

- Retune pre-existing coarse-grained models to accurately represent the amphiphilic system [1,2], capturing both the conformational freedom of flexible tails and the enantiomeric state of head groups.
- Validate models and perform preliminary simulations of spontaneous nanotube self-assembly.
- Map the phase diagram as a function of enantiomeric excess with parallel "computer experiments"
- Quantify how enantiomer partitioning across the bilayer drives the transition between tubular and flat ribbon morphologies
- Extract effective chiral potentials of mean force to inform and refine continuum models of chiral self-assembly.

Candidate Profile: Masters or final-year student in physics, materials science, or physical chemistry with an interest in molecular simulations, polymer physics or mechanics. Candidates should have a firm grasp of statistical physics. Candidates with existing experience with molecular simulations (LAMMPS), HPC clusters of the CNRS (Adastra/Jean-Zay) and programming (Python/C/C++) are highly sought after.

References: [1] Fall, W. S. et al. *ACS Macro Lett.* **2023**, *12*, 808–813. [2] Fall, W. S. & Wensink, H. H. *Phys. Rev. Lett.* **2025,** 135 (26), 268101.

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