Insights into the dynamics of chiral supramolecular polymers based on benzene-1,3,5-tricarboxamides

Sinan Kardas, Mathieu Fossépré, Mathijs F. J. Mabesoone[1], Rafael Martín-Rapún[2], Anja R. A. Palmans[1], Mathieu Surin

Laboratory for Chemistry of Novel Materials, University of Mons, Place du Parc 20, 7000-Mons, Belgium

(corresponding author: S. Kardas, e-mail: sinan.kardas@umons.ac.be)

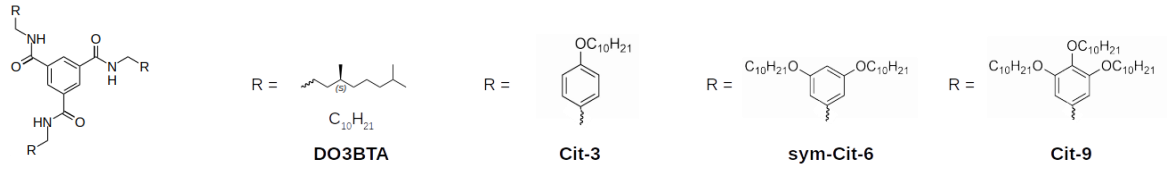
[1] *Institute for Complex Molecular Systems, Eindhoven University of Technology, P. O. Box 513, 5600-Eindhoven, The Netherlands*

[2] *Institute of Chemical Research of Catalonia, Avgda. Paisos Catalans 16, 43007-Tarragona, Spain*

Detailed understanding of the supramolecular polymerization of small molecules is of crucial importance to establish the design rules for the non-covalent synthesis of well-defined supramolecular architectures. Although impressive progress has been achieved in recent years [1], unraveling the molecular origin that governs the self-assembly of the supramolecular polymers remains a challenging question.

The helical self-assembly of benzene-1,3,5-tricarboxamides (BTAs) decorated with a wide variety of side groups has been extensively studied [2]. The incorporation of chiral side groups was shown to induce a preferential helicity in their supramolecular architectures, resulting from a transfer of the chiral information to the central benzene core.

Here we use molecular dynamics (MD) simulations to evaluate the influence of side groups and stacks length on the dynamics of BTA stacks. For this, we compared the dynamics of a model compound (DO3BTA in Scheme 1) with a series of compounds designed in this study (Cit-3, sym-Cit-6 and Cit-9 in Scheme 1). All BTA derivatives under study incorporate a phenyl group in between the amides and the representative chiral *(S)*-3,7-dimethyloctyl side chains. We investigated the effects of the number and position of alkoxy side groups present at the phenyl units on the stability and geometry of BTA stacks. Our computational study aims at rationalising the influence of alkoxy groups on bulk and solution behaviour of the different BTA derivatives.



DO3BTA Cit-3 sym-Cit-6 Cit-9

Scheme 1 – Chemical structures of the benzene-1,3,5-tricarboxamides (BTAs) monomers investigated in this study.

[1] D. Bochicchio et al., Adv. Phys. X **3**, 1436408 (2018).

[2] C. Kulkarni et al., Acc. Chem. Res. **50**, 1928 (2017).