Dissipative particle dynamics simulation of multi block bolaamphiphiles

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Dissipative Particle Dynamic (DPD) simulations have been employed to explore the nature of tri and quaternary block bolaamphiphiles[1]. These molecules are composed of a rod-shaped core, with polar groups at each end and one or two laterally attached chains (figure 1). In condensed phases the different groups microphase segregate to produce ordered liquid phases different from the standard nematic or smectic phases associated with liquid crystalline systems. Typically, bolaamphiphiles show columnar ordering, where the rigid rod component forms the walls of the column and the laterally attached chains form the body of the column. The cross sectional area of the column can be controlled by adjusting the length of the laterally attached chain and in this way different columnar phases can be produced (figure 1). We show how simulations[2] can reproduce the established relationships between molecular dimensions and phase behaviour in ternary bolaamphiphiles. We then predict the phase behaviour of more complex quaternary bolaamphiphiles, with a relatively simple micro-phase segregating model. The quaternary bolaamphiphiles present a curious problem in that some of expected columnar phases can be non-commensurate with complete micro-phase segregation, these complex columnar phases necessitate a frustrated structure. The DPD simulations can be used to supplement experimental data and aid in the characterisation of some of these more complex, frustrated phases.

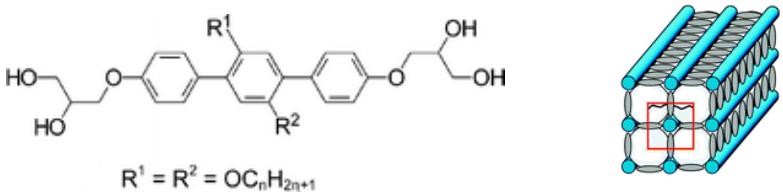

Figure 1. Quaternary block bolaamphiphile molecule (left). Schematic of condensed phase structure (right).

(1) C. Tschierske, *Chem. Soc. Rev.* **2007**, *36*, 1930 – 1970.
(2) M. A. Bates and M. Walker, *Soft Matter* **2009**, *5*, 346-353.