Computer simulations of soft self-organising molecular materials

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A rapid rise in computer power, coupled with multi-processor computers and improved simulation algorithms has led to significant improvements in the capability of molecular simulation to provide answers to the problems of molecular design. Computer simulation of soft matter has progressed rapidly in the last decade, moving from a point where researchers aimed purely to "see" mesophases within the computer, to a situation in which state-of-the-art simulation can now be used as a tool in aiding the understanding of the structure of mesophases and in improving the design of new materials [1,2].

This talk discusses recent results in two areas of molecular simulation: atomistic and coarse-grained studies. Work presented includes;

- Atomistic studies of molecular ordering in a biaxial liquid crystal; including the use of NMR probes to study biaxiality in a host phase [3].
- Atomistic studies of nematic mixtures; including the calculation of bulk material properties [1].
- Coarse-grained models for the study of polyphilic macromolecular liquid crystals; including simulations of polymers, dendrimers and multipodal liquid crystals [1].

[1] Progress in computer simulations of liquid crystals. Wilson M. R., *Int. Rev. Phys. Chem.,* 2005, 24, 421-455.
[2] Molecular simulation of liquid crystals: progress towards a better understanding of bulk structure and the prediction of material properties. Wilson M. R., *Chem. Soc. Rev.*, 2007, 36, 1881.
[3] Atomistic Simulations of a Thermotropic Biaxial Liquid Crystal. Pelaez J. and Wilson M. R., *Phys. Rev. Lett.*, 2006, 97, 267801.