Bottom-up modelling and computer simulations of liquid crystals

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Liquid Crystals (LC) are anisotropic fluids which offer on one hand fascinating fundamental problems, starting with an understanding of the molecular features that lead to their very existence, and on the other are associated with a variety of important technological applications, ranging from displays to sensors and organic electronics. In these lectures we plan to discuss a set of modelling and computation tools that aim to bridge the gap between the essential features of molecules forming liquid crystal phases and the properties of the resulting mesophases. More in details, the plan of the lectures, together with a small list of references, obviously far from comprehensive, but selected because of their relation to the lectures content, is:

- Lecture 1 Microscopic description of molecular organizations in liquid crystals (LCs). Orientational and positional distributions. Order parameters and correlation functions and their determination.[1]
- Lecture 2 Lattice models of LCs: Lebwohl-Lasher [2] and Biaxial [3] models. Introduction to Metropolis Monte Carlo simulations. Determining phase transitions and their character. Topological defects [4, 5].
- Lecture 3 Off lattice molecular level models. Hard particles and attractive -repulsive Gay-Berne models. [6] [7]. Introduction to the Molecular Dynamics method.[8] Applications to nematics, smectics and columnar systems. Liquid crystal elastomers.[9, 10]
- Lecture 4 Atomistic modelling of LCs. Force fields and their importance. Predicting properties such as morphologies, order parameters, and phase-transition temperatures in the bulk[11, 12] and close to surfaces for realistic models.[13, 14]

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