# Modelling the phase behaviour of nematic liquid crystals by Molecular Dynamics simulation

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Liquid crystals (LCs) are a fascinating state of matter with properties in between those of crystalline solids and liquids. They are employed in a wide spectrum of applications, including smart windows and lens and, especially, in displays. LCs flow like liquids, but exhibit a degree of internal order that resembles the organisation typically found in crystals. If this ordering is only orientational, nematic LCs are observed, otherwise a degree of positional ordering in one or two dimensions leads to more complex systems, such as smectic and columnar LCs. In particular, uniaxial nematics ($N_U$) are characterised by the presence of a single optic axes, whereas biaxial nematics ($N_B$) exhibit two optic axes. The $N_B$ phase has been observed experimentally in micellar [1] and colloidal [2] systems, but its existence at the molecular scale is still debated.

Motivated by the impact that molecular $N_B$ phases would generate on display technology and in light of our recent work on colloidal biaxial nematics [3], in this contribution we discuss the phase behaviour of a family of molecules that have been indicated as promising candidates to form $N_B$ phases [4]. More specifically, these molecules consist of a rigid anthraquinone core decorated by four heavily substituted groups with lateral and/or terminal aliphatic chains. By employing an atomistic model and the General Amber Force Field (GAFF), we perform Molecular Dynamics simulation to map the pressure *vs* temperature phase diagrams of these systems and locate the order-to-disorder phase transition. We characterise the LCs observed at equilibrium by computing positional and orientational pair correlation functions to assess the eventual presence of positional and orientational ordering, respectively. Our results indicate that, in a range of temperatures and pressures, these molecules are able to form especially aligned $N_U$ phases, with an especially large nematic order parameter [5] and in qualitative agreement with experimental results.

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