

From Generic to Atomistic Models. How relevant are the details?

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Generic microscopic models both of lattice (e.g. Lebwohl-Lasher) and off-lattice (e.g. Gay-Berne) type have a long history and have greatly helped our understanding of the molecular origins of the macroscopic properties and of the phase organization of various types of liquid crystals (LC) and, as we shall see in the talk are still of great value. For instance lattice models simulations can be used to study defects in fairly complex systems such as thin nematic film coatings of colloidal particles of different shape [1,2] and molecular resolution models can be applied in the study of biaxial phases [3] and of model display devices [4]. More recently, fairly realistic atomistic models have been put forward [5] in an effort to predict some of the important features of real mesogens like phase transition temperatures [6] and NMR observables for molecules in the bulk or at the nano-scale. In the talk we present recent relevant examples of applications of the various models and, following the indications coming from realistic models, we discuss which details of the generic models should be included in a next generation of simple or hybrid [7] models.

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