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## The perspectives of modelling and simulations for device and non-device applications of liquid crystals

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The physical properties of soft materials vary significantly with their phase organization and morphology [1] and thus a key aspect in the development of new materials of this kind rests on the possibility of controlling their molecular assemblage from the nano scale, e.g. for organic electronics applications [2], up to the much larger micro-scale, e.g. for photonic applications [3]. Corresponding to this range of length scales of interest the modelling and simulation problem has also to be tackled at different resolutions: atomistic, molecular and coarser grain lattice models. In this talk we plan to show some examples of each, highlighting the current state of the art and perspectives.

At atomistic level, we demonstrate the current possibilities of predicting the organization and properties of low molecular mass liquid crystals starting from their molecular structure and in particular the prediction of transition temperatures and observable properties (e.g. dielectric constant, NMR dipolar couplings) for nematic liquid crystals [4]. We also discuss the realistic prediction of Resonant Energy Transfer, in systems of interest for light harvesting devices [5].

At the molecular resolution level we show, in particular, structured organizations obtained from fullerene containing mesogens [6].

Finally, we discuss the possibility, first hinted in a seminal paper by Nelson [7] of using colloidal particles coated with a layer of nematic liquid crystals to build complex micro-scale architectures [7]. As shown in [7,8], trying to cover the sphere leads to four half-strength tetrahedrally placed topological defects, potentially suitable for a chemical attack yielding a tetravalent “colloidal atom”. Using Monte Carlo simulations we show that the number and position of these valence spots can be varied by the application of suitable multipolar fields [8], leading to a potentially powerful approach to new meso-scale organizations.

*References*

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