Theory and molecular simulations of biaxial nematics: long standing challenges and recent advancements

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The notorious elusiveness of the biaxial nematic phase, particularly in low molar mass thermotropic liquid crystals, has been stimulating intensive research efforts in synthesis, physical measurement, theory and molecular simulations over the last four decades. These efforts have led recently to new insights into the richness of possible hierarchical structures[1-7] which can appear in the nematic phase and which underlie a broad diversity in the response of various nematic LCs to external stimuli. An overview of the present status in the theory and molecular simulations will be given, with emphasis on the domain structures and symmetries of the biaxial nematic phase both in thermotropic[1-4] and in colloidal systems[5-7]. New results will be presented on (1) the phenomenological theory of the nematic phase, where account is taken of the hierarchical structures, and an analogy between the respective nematic-nematic and liquid-gas transition; (2) the response of locally structured nematic phases to external electric and magnetic fields, both by phenomenology and by Monte Carlo molecular simulations and (3) entropy driven cybotaxis in purely hard-body molecular models of mesogens studied by Monte Carlo simulations.

References:

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