Is chirality always needed to obtain twisted molecular organizations?

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Twisted molecular organizations are typically originated by chiral constituent particles, like in cholesteric or smectic C* liquid crystals obtained from chiral mesogens or by seeding an achiral phase with chiral dopants [1]. On the other hand, similar structures can be obtained in sufficiently thin films by the effect of suitable external boundaries, like in Twisted Nematic displays^[2], or by a chiral surface inducing twist in a nematic. The situation is much less obvious if the confining surfaces are just those of a hybrid film [3] or even not present, like in a isolated nematic nanodroplet that can become chiral [4, 5]. Computer simulations are currently very useful for examining the relation between molecular and overall chirality, both for simple rigid molecules [5] and for realistic atomistic simulations [3]. However, a problem that has to be solved, and that is often neglected in published literature, is that of assessing and objectively quantifying the instantaneous and average chirality, both of the constituent molecules, particularly when they have conformational freedom [6, 7] and, even more importantly, of the resulting self-assembled structures. In the talk we discuss various examples of chirality assessment from the computer simulation of various model Gay-Berne based systems [2, 5] and realistic systems like chiral islands of sexithiophen [8] and odd cyanobiphenyl dimers [9] that are experimentally found to form heliconical phases [10].

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