A COMPUTER SIMULATION STUDY OF MESOPHASES FROM DIPOLAR BANANA-SHAPED MOLECULES

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We report the results of a Monte Carlo (MC) computer simulation of a system of N=1000 banana-shaped molecules with dipolar interactions.

Banana-shaped liquid crystalline systems have been studied widely recently, due to their biaxiality and novel chiral phase ordering, despite the constituent molecules are achiral. On the other side many liquid crystal molecules posses polar groups that may have an influence on the type of phase observed. As such it becomes crucial to understand the role of polar forces on the phase behavior of a banana liquid crystal model. In particular, the object of this computer simulation study is to investigate how the addition of a tranverse point electric dipole can effect the mesophase organization as well the phase transitions.

The banana-shaped molecule is modelled by joining three Gay-Berne (GB) sites with a bending angle of $\phi=120^{o}$. We consider three different polar cases: 1) one electric point dipole embedded in the central site and oriented along the molecular transversal axis; 2) two dipoles with orientations $\theta_1=30^{o}$ and $\theta_2=-30^{o}$ on respect to the molecular transversal axis, embedded in the terminal site centers, and 3) in intermediate positions between centers and ends of terminal sites.

We have investigated several temperatures corrisponding to nematic and smectic liquid crystal phases in the isobaric-isothermal (NPT) ensemble,

paying attention to the characterization of the smectic phase. The simulations show that at low temperature an untilted smectic phase with large biaxiality is found. Each smectic layer show local polarization, but layers are arranged in an antiferroelectric fashion and the overall sample is not polarized.

Dipoles in terminal sites centers seem to induce a softening of the disorder-ordered transition with the appearance of a nematic phase, which is absent in the previous case, as well in the corresponding pure GB systems. Again, an untilted smectic phases with pronunced biaxiality and antiferroelectric order in layers are observed.

Moving dipoles towards the terminal site ends has the effect of broadening the nematic phase, which is slightly biaxial. At low temperatures tilted smectic layers are formed. Layers are only partially polarized showing domains with different dipoles orientations. This wider variety of orientations is reflected also in the decrease in phase biaxiality.

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