Computer simulation of model colloidal liquid crystals: two novel studies

Giorgio Cinacchi[1], Luca De Gaetani[2], Jeroen S. van Duijneveldt[1]

[1]*School of Chemistry, University of Bristol, Cantock'Close, Bristol BS8 1TS, England;*
[2]*Dipartimento di Chimica, Università di Pisa, Via Risorgimento 35, I–56126 Pisa, Italy*

Abstract

Two novel computer simulation studies on model colloidal liquid crystals are presented. In the first part of this communication, results on a binary mixture of rods and spheres in the dense smectic A phase are reported. Rod-sphere mixtures have recently attracted a great deal of attention. While there are a number of theoretical [1] and experimental studies on the phase behavior and structure of these mixtures [2], dynamics has been less explored so far. Here, the molecular dynamics method has been used to investigate translational and rotational dynamics of rods and sphere in a dense smectic A phase. In particular, notwithstanding the high density and ordered structure of the phase, rods are seen to rotationally relax quite fast, and much faster than in the pure rod smectic A phase at the same density, where reorientations are essentially frozen. In addition, rods prefer to move along rather than perpendicularly to the director, just the contrary of what is occurring in the pure rod smectic A phase at the same value of density. It will be shown that both of these facts are related to the particular microphase separation which is characteristic of this smectic A phase. In the second part, the effect of flexibility on the phase behavior and properties of disc-like particles is studied. This has been done using, as model, hard and infinitely thin discs that are allowed to bend and transform into partial spherical surfaces. The extent of this bending motion is regulated by a harmonic restoring force, which favors the infinitely thin disc conformation. The phase behavior of collections of these particles is studied via Monte Carlo computer simulations. Attention is given to how the isotropic-to-nematic phase transition shifts upon letting the discs bend, a topic relevant to suspensions of clay particles of current interest [3] as well as biological membranes.

References

[1] T. Koda *et al.*, *J.Phys.Soc.Jpn* **65**, 3551 (1996); Z. Dogic *et al.*, *Phys.Rev.E* **62**, 392 (2000); Y. Martinez–Raton *et al. Eur.Phys.J. E* **21**, 175 (2006).

[2] M. Adams *et al. Nature* **393**, 349 (1998).

[3] L. J. Michot *et al.*, *Proc. Nat. Acad.Sci. USA* **103**, 16101 (2006).