INTERNATIONAL SOLVAY INSTITUTES BRUSSELS

Solvay Colloquium

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Bottom up modelling of liquid crystals: from molecules to applications

Liquid crystals (LC), with their unique combination of fluidity and anisotropic physical properties, continue to offer a number of novel fascinating applications, ranging from optical and haptic displays to organic electronics devices, sensors, etc... However, why some molecules form liquid crystals and other apparently similar do not and, more generally, the relation between molecular structure and features of the LC phases formed is still far from being understood. Modelling and computer simulations methods that address this problem at various length scales: mesoscopic, molecular, and atomistic have seen a huge development in the last few years, due also to the impressive increment in computer power. Thus, on one hand, coarse grained models, where molecules or molecular fragments are replaced by simple objects with similar shape endowed with attractive and repulsive interactions can now be employed to handle systems as complex as LC elastomers, explaining some of their unusual mechanical properties. On the other hand, atomistic molecular dynamics (MD) simulations have started to make detailed and fairly reliable predictions of phase transition temperatures, order and other properties of real liquid crystals starting from their chemical structure. An even more exciting development is the possibility of studying the interaction of liquid crystals with solid surfaces. This is particularly important since, for most practical applications, LC are not used in bulk quantities but in micro or nano thick films, where the LC is aligned along a specific direction with the help of surface interactions. In view of this it is somewhat surprising that surface effects are still being described only empirically, and that little is known on their molecular origin. In the talk we plan to show that atomistic MD can now shed some light also on the interfacial behavior of liquid crystals, separating various effects that contribute to alignment, e.g. chemical nature of the substrate, morphology, roughness, surface treatments like rubbing and possibly suggesting way of optimizing devices. A view of the perspectives for future developments of the field will also be briefly discussed.

Tuesday 6 February 2018 at 4.00 P.M.

COFFEE AND TEA WILL BE SERVED AT 3.45 P.M. IN FRONT OF THE SOLVAY ROOM

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