Density functional theory of smectic and columnar liquid-crystal phases in systems of hard helices
(Giorgio Cinacchi, giorgio.cinacchi@uam.es)

In systems of hard rod-like particles nematic and smectic liquid-crystal [1] phases can form. In the former case, particle centroids are uniformly distributed while particle main axes tend to orient along a preferred direction **n**. In the latter case, this orientational order combines with a partial positional order in that particle centroids are now forming layers, often perpendicular to **n**. There is also another liquid-crystal phase that may form, namely a columnar phase, characterised by, as the name suggests, particle centroids organising into columns [1]. This phase organisation is typical in systems of disc-like particles. It may also form in multicomponent systems of rod-like particles and this phenomenon is well-understood. Its formation in systems of single-component rod-like particles is however rarer and the mechanism responsible for it unclear. In fact, numerical simulation studies on hard rod systems, so successful in reproducing nematic and smectic phases observed in experiments, have so far not provided any evidence of a stable columnar phase in a single-component system of hard rods [2]. However, experiments on colloidal suspensions of DNA [3] and elongated virus particles [4], the latter guaranteed by nature to be highly mono-sized, did report columnar phases. In the case of virus colloidal particles in particular, the sequence of phases observed on increasing density is as follows: nematic → smectic → columnar. One possible explanation is that the virus colloidal particles can be assimilated to hard rods only on a first approximation, as electrostatic interactions will also play a role, ultimately stabilising the columnar phase at high density. Quantifying reliably electrostatic interactions and their role is however not straightforward. Rather, one should not forget that both DNA and virus colloidal particles are chiral and that at high density particle shape play a very subtle role.
By using a statistical mechanical density functional theory, this project seeks a possible alternative explanation to the formation of a columnar phase in a single-component hard rod system only based on particle shape. It will investigate the effect of progressively changing the shape of a hard particle from being that of a straight rod to that of a helix, inherently chiral, on to the stability of smectic and columnar phases. That is, it will aim at exploring whether twisting a straight rod in to a helicoidal rod will favour the formation of a columnar phase over a smectic phase.
The student will be introduced to the basics of classical density functional theory formalism, one of the most important theoretical technique in (soft) condensed matter physics, and then be able to apply it to a problem of current interest [5].

[1] P.G. de Gennes, J. Prost, *The Physics of Liquid Crystals*, Clarendon Press, Oxford (1993).

[2] P. Bolhuis, D. Frenkel, *J. Chem. Phys.* 106, 666 (1997).

[3] e.g. F. Livolant, A. Leforestier, *Prog. Polym. Sci.*, 21, 1115 (1996).

[4] E. Grelet, *Phys. Rev. Lett.* 100, 168301 (2008); *Phys. Rev. X* 4, 021053 (2014).

[5] H.B Kolli , E. Frezza , G. Cinacchi, A. Ferrarini, A. Giacometti, T. S. Hudson, *J. Chem. Phys.* 140, 081101 (2014) ; H. B. Kolli, E. Frezza, G. Cinacchi, A. Ferrarini, A. Giacometti, T. S. Hudson, C. De Michele, F. Sciortino, *Soft Matter* 10, 8171 (2014).