INTERNSHIP PROPOSAL

(One page maximum)

Laboratory name: : Laboratoire de Physique des Solides (LPS)
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Internship location: LPS, Orsay

Thesis possibility after internship: YES
Funding already obtained for a PhD: NO If YES, which type of funding:

Predicting the packing of nanorod mixtures

One interesting feature of nanoparticles is the fact that they can crystallize into a broad array of different crystal structures, depending on their shape and interactions. The experimental team of Cyrille Hamon at LPS is looking into the self-assembly of rod-shaped particles into structures that consist of layers of aligned rods [1]. Within these layers, the particles behave more or less as 2D objects, with a shape corresponding to the cross-section of the rod. Experimentally, this cross-section can be tuned to triangular, square, or pentagonal, such that a slice through one of the layers looks like a packing of polygons.
The question is: what crystal structures could form in such a 2D system of polygons? When all particles have the same shape and size, we know the answer [2], but mixing different shapes or sizes opens the door to a variety of crystals. In this project, you will use specialized computer simulations [3] to explore the packing of mixtures of polygons, and in particular look for regimes where interesting structures emerge. These findings can then help guide future experiments. The ideal candidate has a strong background in statistical physics, as well as an interest in coding and/or computer simulations.

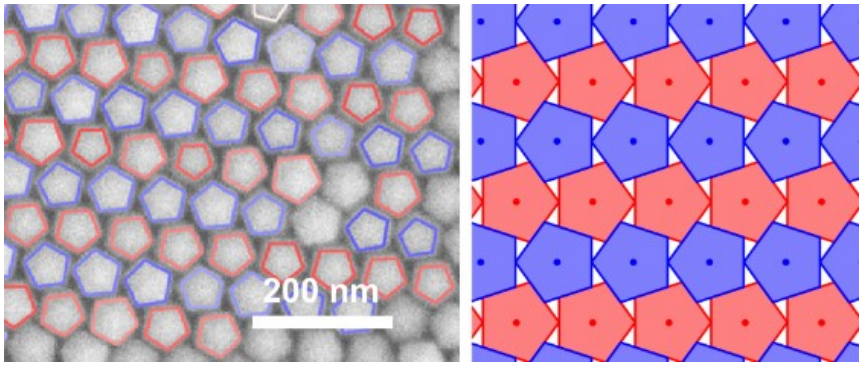


Figure: Nanorod assembly of pentagonal rods and corresponding ideal crystal structure. Taken from Ref. [1].

[1] J. Marcone *et al.*, "Polymorphous packing of pentagonal nanoprisms", *Nano Letters* **23**, 1337 (2023).
[2] J. A. Anderson *et al.*, "Shape and symmetry determine two-dimensional melting transitions of hard regular polygons", *Physical Review X* **7**, 021001, (2017).
[3] E. Fayen, A. Jagannathan, G. Foffi, and F. Smallenburg, "Infinite-pressure phase diagram of binary mixtures of (non) additive hard disks", *Journal Of Chemical Physics* **152**, 204901 (2020).

Please, indicate which speciality(ies) seem(s) to be more adapted to the subject:

Condensed Matter Physics: NO
Soft Matter and Biological Physics: YES
Quantum Physics: NO
Theoretical Physics:YES