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:

Free energies of quasicrystals

Quasicrystals are exotic aperiodic structures, that can exhibit symmetries forbidden by the normal rules of crystallography. While typically found in metallic alloys, over the past decades a number of soft-matter systems – both experimental and simulated – have been developed that are capable of forming quasicrystal phases.

In most cases, these self-assembled quasicrystal can be interpreted as being constructed out of a limited set of tiles, such as squares and triangles in 2D, that are mixed together to produce an aperiodic pattern. Interestingly, there are usually many ways these tilings can be rearranged in order to form similar patterns. This degeneracy leads to a so-called configurational entropy contribution to the free energy of the quasicrystal, which helps stabilize the quasicrystal phase. In some of our past work [1], we have examined the free energy of quasicrystal tilings in a simple model system, in order to map out the phase diagram. Interestingly, in that model system, it turned out that all different variations of the same quasicrystal tiling provided essentially the same contribution to the free energy. While this greatly simplified our calculations, this is likely not a typical case.

In this project, you will explore methods to predict how likely a given quasicrystalline tiling is in a model system consisting of two-dimensional patchy particles. You will perform simulations of this model system, calculate free energies for specific tiling patterns, and use regression and/or machine learning techniques in order to train models that can predict the free energies of different tilings. The ideal candidate has a strong background in statistical physics, as well as an affinity for coding and/or computer simulations.

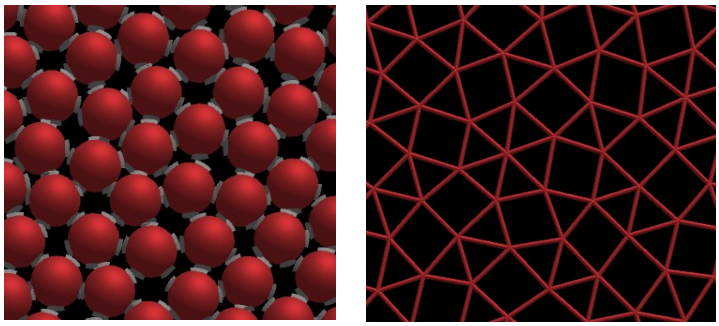

Figure: Quasicrystal made of patchy particles and the corresponding tiling pattern.

[1] E. Fayen, L. Filion, G. Foffi, and F. Smallenburg, *Physical Review Letters* **132**, 048202 (2024).

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