

INTERNSHIP PROPOSAL

(One page maximum)

Laboratory name : Laboratoire de Physique des Solides (LPS)
CNRS identification code: UMR-8502
Internship director'surname: Smallenburg
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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:

Self-assembly in polydisperse mixtures

One interesting feature of colloidal particles is the fact that they can crystallize into a broad array of different crystal structures, depending on their interactions. This process is highly similar to what happens when molecules or atoms crystallize, and is governed by the same statistical mechanics. However, unlike atoms or molecules, colloidal particles are typically polydisperse: they slightly vary in terms of their size, shape, charge, or other microscopic properties.

This polydispersity typically hinders crystallization, but can also lead to the emergence of unexpectedly complex crystal structures [1]. In this project, you will explore how polydispersity with different size distributions leads to the formation of new crystal structures. You will simulate systems of polydisperse hard spheres under different conditions and examine which crystal structures form. Additionally, you will explore the use of modern "inverse design" techniques (e.g. Ref. [2]) to design polydisperse mixtures that self-assemble into a pre-chosen target structure. The ideal candidate has a strong background in statistical physics, as well as an affinity for coding and/or computer simulations.

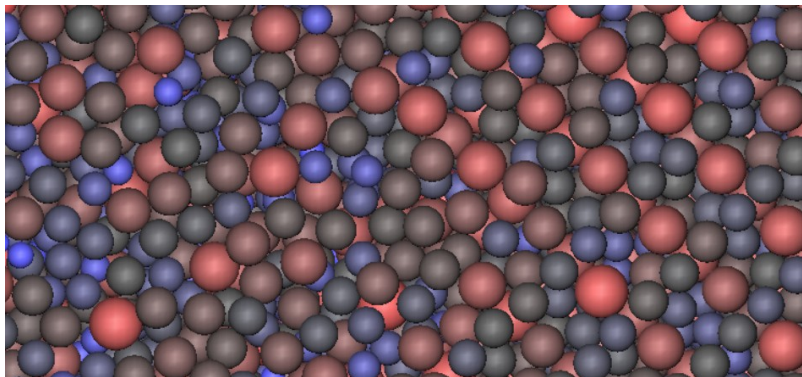


Figure: Polydisperse fluid coexisting with a complex crystal (Laves phase).

- [1] P. K. Bommineni, N. R. Varela-Rosales, M. Klement, and M. Engel, "Complex crystals from size-disperse spheres," *Phys. Rev. Lett.* **122**, 128005 (2019).
[2] Coli et al., "Inverse design of soft materials via a deep learning-based evolutionary strategy", *Sci. Adv.* **8**, eabj6731 (2022)

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