INTERNSHIP PROPOSAL

(One page maximum)

Laboratory name: : Laboratoire de Physique des Solides (LPS)
CNRS identification code: UMR-8502
Internship director surname: Smallenburg
e-mail: frank.smallenburg@cnrs.fr Phone number:
Web page: http://frank.smallenburg.nl https://www.lps.u-psud.fr
Internship location: LPS, Orsay

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

Crystallization of mixtures of polyhedra

Colloidal particles can crystallize into a wide range of different structures. One way of tuning the crystal structure they form is by modifying their shape. Nanoparticles can be created in a huge variety of shapes, often corresponding to simple polyhedra (e.g. Ref. [1]). Polyhedral particles of a single shape and size can form a huge variety of crystal phases [2], and this variety will become even larger if we mix different types of polyhedra together.
Recent experiments at LPS [1] showed the self-assembly of a mixture of tetrahedra and octahedra into a densely packed crystal. To guide future experiments, it would be helpful to know combinations of shapes that readily self-assemble into well-defined crystal phases with interesting structures.
In this project, you will use computer simulations [3] to explore crystallization in mixtures of polyhedra. The goal is to identify candidate structures consisting of polyhedra, and identifying conditions where self-assembly can reliably take place. For interesting structures, you will also probe the thermodynamic stability of the crystal phases using either theoretical approximations or direct coexistence simulations (e.g. Ref. [4]).
The ideal candidate has a strong background in statistical physics, as well as an interest in coding and/or computer simulations.

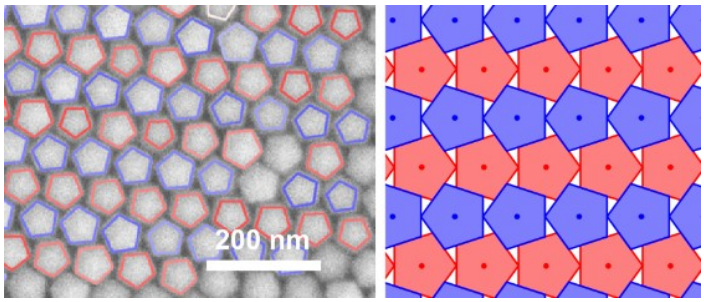


Figure: Nanorod assembly of pentagonal rods and corresponding ideal crystal structure. Taken from Ref. [1].

[1] R. Nag *et al.,* "Depletion-induced tunable assembly of complementary platonic solids." *Nano Letters* **24**,16368 (2024).
[2] P. F. Damasceno, M. Engel, and S. C. Glotzer. "Predictive self-assembly of polyhedra into complex structures." *Science* **337**, 453 (2012).
[3] F. Smallenburg, L. Filion, M. Marechal, and M. Dijkstra, "Vacancy-stabilized crystalline order in hard cubes", *PNAS* **109**, 17886 (2012).
[4] F. Smallenburg, G. Del Monte, M. de Jager, and L. Filion, "A simple and accurate method to determine fluid-crystal phase boundaries from direct coexistence simulations", *Journal Of Chemical Physics* **160**, 224109 (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