PhD positions: Direct Visualisation of Nucleation: from Fundamentals to New Materials

Understanding the nucleation of crystals is of profound importance both for fundamental and technological reasons. In the simplest material known to self—assemble to form a crystal, hard spheres, state-of-the-art predictions and experimental measurements of nucleation rates differ by over ten orders of magnitude – the “second—biggest discrepancy in physics” [1,2]. Beyond hard spheres, soft particles in the form of colloidal microgels exhibit a wide range of exotic crystal structures, which to date have proven hard to realise.

In this project we will use a novel experiment—computer simulation approach to address the challenges of nucleation and realisation of crystal structures in colloids. We will use

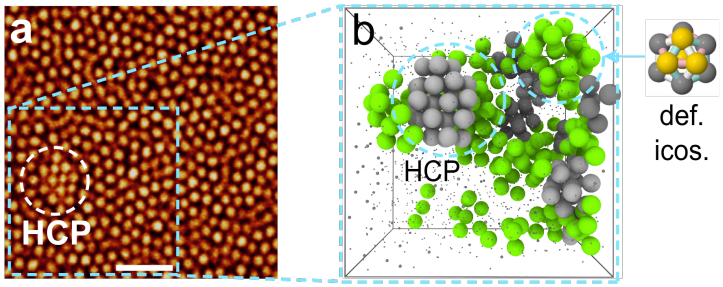
-- A new experimental technique, (Fig. below), to address the challenge of the nucleation rate discrepancy and form the basis for the experimental part of the project.

-- We shall develop a novel feedback method where nano-real space analysis is combined with computer simulations, crystal-prediction methods [3], and free-energy calculation methods [4].

-- Use our methods to develop the assembly of soft particles, which is predicted to massively enhance the range of crystal structures that the system can access.

The project is led by C. Patrick Royall, ESPCI Paris [paddy.royall@espci.fr] (experiments) and Frank Smallenburg [frank.smallenburg@universite-paris-saclay.fr], Paris-Saclay (simulations) and is a collaboration with Dr Nicoletta Gnan, La Sapienza, Roma. PhD positions are available in experiments (CPR) and simulations (FS). The work will be supported by the Agence National de Recherche (ANR).

Candidates should contact CPR (experiments) or FS (simulations). Experience of soft matter experiments or simulations respectively is highly desirable. Further details of the research program of the PIs is available on http://www.padrus.com/ and http://www.frank.smallenburg.nl. The positions are expected to start in fall 2022.



Real–space analysis of self–assembly and mapping experiment to simulation. (a) Birth of a crystal in a colloidal system. The crystal nucleus is highlighted. Bar=10μm. (b) Rendering of coordinates from experimental data with defective icosahedra local structures (green) and particles in crystal environments (grey).

[1] N. Wood, J. Russo, F. Turci, and C.P. Royall, *J. Chem. Phys.* **149** 204506 (2018).

[2] J. Taffs, J. and C. P. Royall, *Nature Comms.* **7** 13225 (2016).

[3] L. Filion, M. Marechal, B. van Oorschot, D. Pelt, F. Smallenburg, and M. Dijkstra, *Phys. Rev. Lett.* **103**, 188302, (2009).

[4] N. P. Kryuchkov, F. Smallenburg, A. V. Ivlev, S. O. Yurchenko, and H. Löwen, *J. Chem. Phys.* **150**, 104903, (2019).