A 3-years Ph.D. position is opening, starting in September 2019, on

Nucleation and growth processes by molecular simulations
Application to molecular and colloidal crystals

Location: Laboratoire Interdisciplinaire Carnot de Bourgogne, UMR 6303 CNRS, Univ. Bourgogne Franche-Comté, FR-21000 DIJON, FRANCE

Research Department: INTERFACES

Project description: Crystals, composed of a regular and periodic arrangement of either atoms/molecules or nanoparticles, are ubiquitous in Nature but are also an important component in many field of applications, from optics to energy storage to construction materials. Understanding and controlling their formation is thus of paramount importance. It proceeds through the nucleation of small nuclei which further grow/crystallize to lead to the final crystalline material. The nucleation, thus, plays a crucial role in the control of the microscopic properties (size, purity, structure, morphology) which directly affect the physical chemistry of the crystalline material formed at the macroscopic scale. However, this process is still far from being well understood and is a field of intensive research. This is because experiments still struggle to characterize crystal nucleation, which happens on exceedingly small/short length/time scales (ns/nm). Conversely, molecular simulations, which could indeed provide invaluable insight, are hampered by the fact that nucleation is a rare event, as seconds, or days or even weeks are typically needed for a crystalline nucleus to reach its critical size and proceed toward crystallization. Thus, the development and use of enhanced sampling techniques are needed to tackle the time scale problem via molecular simulations.

At the INTERFACES Department, of the University of Bourgogne Franche-Comté, an important research effort is put on the nucleation and growth of solid crystalline materials and thin films of oxides for applications in catalysis, energy storage, construction materials, photonics and environment see e.g [1-3]. At present, it is the subject of concern in five PhD thesis, one junior fellowship, several master internships, one ANR project on gas hydrates (MI2C) and one European consortium project on cementitious hydrates (NANOCEM core project 15). The PhD project fits into this research effort.

The main goal will be to develop original simulation techniques based on Monte-Carlo and Molecular Dynamics to study nucleation and growth processes of crystals and to deployed them on either gas hydrates, cementitious hydrates or colloidal crystals for which we have a large set of experimental data. The work will benefit from the recent and original development of enhanced sampling techniques allowing the calculation of the Gibbs free energy and surface free energy[4-6] as well as from a large set of simulations and numerical analysis tools for crystals and nuclei [7].

Application:
To apply, please, email a note of interest, your CV, and 2-3 professional references including complete contact details to christophe.labbez@u-bourgogne.fr and jmsimon@u-bourgogne.fr

References

[1] Krautwurst, N; Nicoleau, L ; Dietzsch, M ; Lieberwirth, I ; Labbez, C ; FernandezMartinez, A ; Van Driessche, AES ; Barton, B ; Leukel, S ; Tremel, W, TwoStep Nucleation Process of Calcium Silicate Hydrate, the Nanobrick of Cement, Chemistry of Materials (2018) 30 28952904
[2] Picker, A ; Nicoleau, L ; Burghard, Z ; Bill, J ; Zlotnikov, I ; Labbez, C ; Nonat, A ; Colfen, H Mesocrystalline calcium silicate hydrate: A bioinspired route toward elastic concrete materials, Science Advances (2017) 3 e1701216
[3] Cabane, B ; Li, J ; Artzner, F ; Botet, R ; Labbez, C. ; Bareigts, G ; Sztucki, M ; Goehring, L Hiding in Plain View: Colloidal Self-Assembly from Polydisperse Populations, Physical Review Letters (2016) 116 208001
[4] Delhorme, M ; Labbez C.; Turesson, M ; Lesniewska, E ; Woodward, CE ; Jonsson, B, Aggregation of Calcium Silicate Hydrate Nanoplatelets, Langmuir (2016) 32 2058-2066
Bonnaud, PA ; Labbez, C. ; Miura, R ; Suzuki, A ; Miyamoto, N ; Hatakeyama, N ; Miyamoto,
[5] A ; Van Vliet, KJ, Interaction grand potential between calcium-silicate-hydrate nanoparticles at the molecular level, Nanoscale (2016) 8 4160-4172
[6] Labbez C., Jönsson B., Woodward C., Nonat A., Delhorme M., The growth of charged platelets, Physical Chemistry Chemical Physics (2014) 16 23800-23808
[7] Bareigts G., Interactions and Structures in Polydisperse Suspensions of Charged Spherical Colloids, PhD Thesis, Dijon, France, 14th of December 2018.