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

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. The main goal of the project will be to develop original simulation techniques based on Monte-Carlo and Molecular Dynamics to study nucleation/growth processes of crystals and to deploy them on either gas hydrates, cementitious hydrates or colloidal crystals for which we have a large set of experimental data [1-3]. The work will benefit from the recent and original development of enhanced sampling techniques and analysis tools [4-6].

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

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