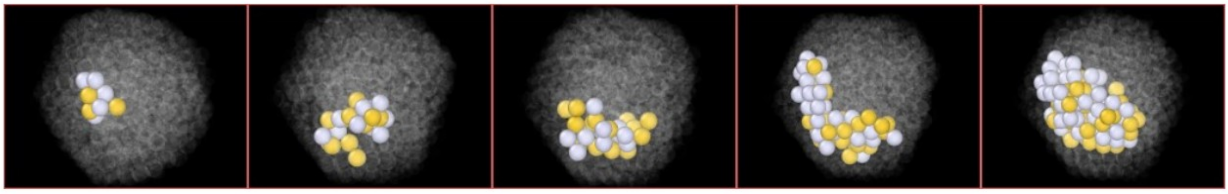
Machine-learning approaches for nanoparticle simulations

Keywords Atomistic simulations, machine-learning, nucleation, crystallization, nanoparticles

Short description The formation of a crystal is triggered by the emergence of a nucleation core. Classical nucleation theory (CNT) is widely employed to discuss its nature and its origin. In CNT, the thermodynamically stable phase is always the one that grows first and its size is then driven by the free energy competition between how much it costs to build a liquid-crystal interface and the gain from growing the crystal. Yet, following Ostwald's rule, another structure may emerge beforehand if it is closer in free energy to the mother phase. Then, structural and also chemical reorganizations happen during the growth. This multi-stage nucleation mechanism already appears in bulk systems but can be amplified in nanocrystal nucleation where surface effects and chemical reactivity are enhanced. For nanoscience to be inspired by the practical applications instead of still being driven by the synthesis possibilities, it is crucial to reach a better understanding of the unique crystallization mechanisms leading to nanocrystals.

Main tasks The student will have the opportunity to pursue numerous research avenues depending on their preferences. Indeed, further numerical developments based on machine-learning approaches can be envisaged for statistically sampling free energy barriers associated to nucleation or for better modelling the interactions between atoms fitted on electronic structure calculations. Meanwhile, it will also be possible to focus on a specific material and study different approaches leading to the nanocrystal formation including gas phase condensation, solvent mediated synthesis or deposition mechanisms.



Supervision and teaching The student will benefit from the supervision of Dr. Julien Lam who is currently *"Chargé de Recherche"* appointed at the Unité Matériaux Et Transformations (Université de Lille). His research is focused on the study of material modeling using many types of computational techniques. The selected student will gain experience in a large number of research domains, especially nanophysics, atomistic simulations, machine-learning and computer programming. The internship can lead to a PhD thesis with funding already obtained, subject to mutual agreement.

References

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