## Probing nucleation mechanisms in nanoparticles from nanoalloys to nanoxide

While nanocrystals in material science are ubiquitous, the mechanisms of their formation which spans from nucleation to crystal growth remain one of the most intriguing process in nature. Better understanding crystallization in general would allow for a rational control of material engineering and possibly the development of novel functional materials and technological applications. From the experimental viewpoint, numerous works have been dedicated to elucidating nucleation by observing the intricate relationship between experimental conditions and final structures. Yet, even if numerical simulations should have been a pivotal instrument to investigate crystallization in nanoparticles, studying nucleation require large scale simulations that were so far too computationally demanding to achieve. As such, most works based on simulations have only focused on simple model materials thus preventing from targeting specific technological applications.

In this presentation, we will introduce innovative numerical tools based on machine-learning approaches and show how they can be employed to probe the nucleation processes in more complex materials. In particular, we will present results obtained for gold/silver nanoalloys using machine-learning assisted simulations combined with gas-aggregation magnetron-sputter deposition. Next, we will focus on zinc oxide nano-crystallization for which we developed a data-driven approach for structural analysis and observed non-classical nucleation mechanisms.