Observing the birth of crystals using machine-learning assisted simulations

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While crystals 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 would allow for a rational control of material engineering and possibly the development of novel functional materials and technological applications. From the fundamental point of view, numerous works have been dedicated to elucidating the emergence of the nucleation core and its role in controlling the final crystal structure. For instance, it is now possible to observe the crystal birth with electron microscopy, and colloidal science has also provided numerous experimental results on nucleation. Yet, while numerical simulations should have been a pivotal instrument to investigate crystallization at the atomistic level, studying nucleation require large scale simulations in order to observe the phase transition. 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 focused on zinc oxide crystallization for which we developed a linear-based machine-learning interaction potential that can surpass all of the current classical models. Then, we combined large scale simulations and data-driven structure analysis to study the crystal nucleation. One key aspect of our work was to demonstrate that predictions of non-classical nucleation that were obtained with model materials including Lennard-Jones and hard spheres systems are still valid. Altogether, our results seems to demonstrate a universality of the crystallization processes ranging from soft to condensed matter.

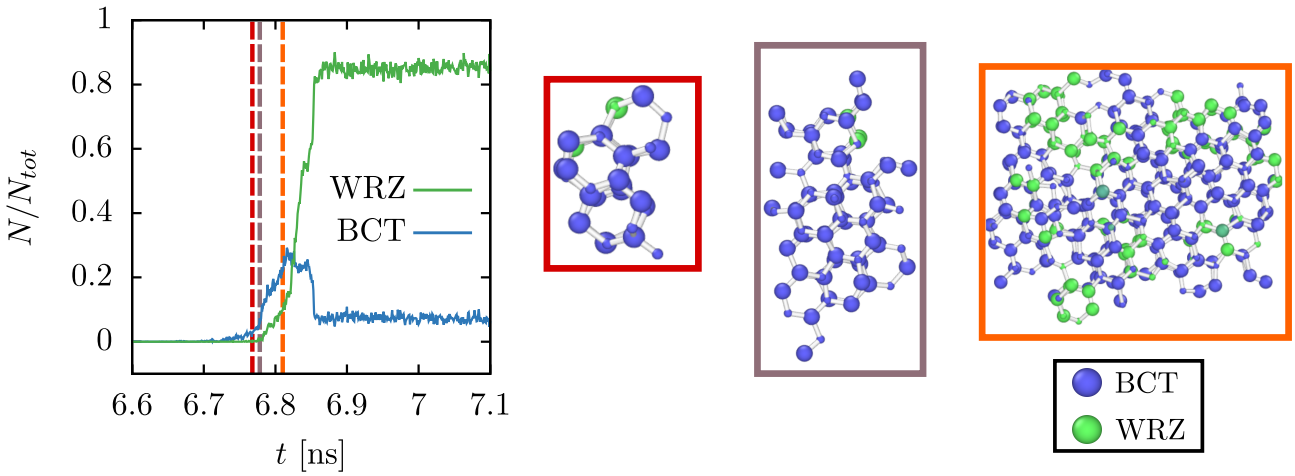

Figure: Nucleation and growth of zinc oxide crystals