Molecular dynamics driven by X-ray diffraction and its application in the study of nucleation of crystalline materials

A talk by

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DATE / TIME: Thursday, 26th of September 2019, 02:00 p.m. (CET)

LOCATION: Seminaraum, Ground floor, Sensengasse 8, 1090 Vienna

Understanding the nucleation process of crystalline materials is of great relevance in physics, chemistry, technology, and environmental sciences. Yet in spite of remarkable progress, atomistic simulations of the nucleation process of crystalline materials remains a topic of intense challenge.

Here by introducing X-ray diffraction into advanced enhanced sampling method, we proposed a new approach on how to simulate the nucleation process. We have applied this approach to two systems that are notoriously difficult.

One is the simulation of silica crystallisation and the other is the freezing of water. These applications would not have been possible without the use of advanced enhanced sampling methods capable of lifting the time scale barrier. In the talk I will also show how machine-learning techniques can help in solving difficult problems encountered in atomistic simulations.