Thesis project: **Can vapor bubbles induce crystal nucleation?**

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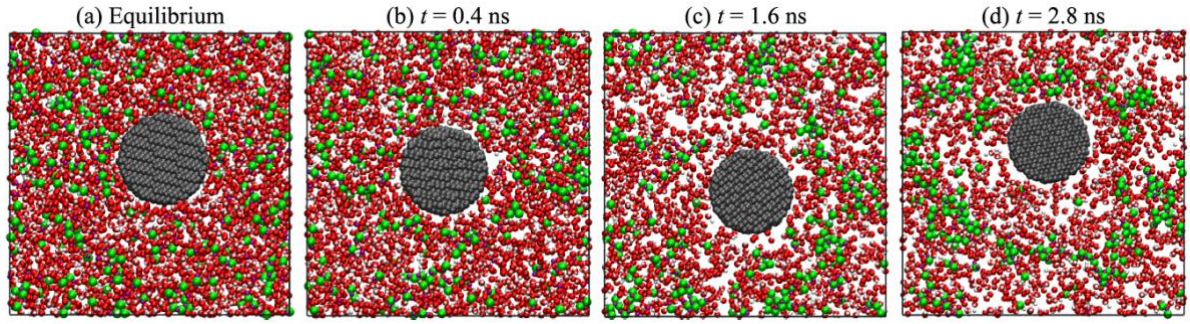
- Department: Process & Energy, 3mE
- Theme: Process Technology
- Is an external organization involved? No
- The thesis involves: Modeling (molecular dynamics)
- Prerequisite: programming skills (preferably Python),
  ideally also ME45211 Introduction to molecular simulation

Non-photochemical laser induced nucleation (NPLIN) uses short laser pulses to induce crystal nucleation in supersaturated solutions. This technique can be used for example to produce medicine in a controlled manner. The way in which the laser interacts with the solution to form nuclei is not understood yet, but one of the theories suggests that this happens when the laser light is absorbed by small inherent contaminants in the solution. The resulting high temperature of the contaminant is expected to lead to the formation of a vapor bubble surrounding it, with high concentration of salt at the vapor-liquid interface - potentially favorable conditions for nucleation during a short period of time. In our team, we managed to model the growth and collapse of a laser-induced vapor bubble in agreement with our experiments. However, neither the macroscopic model nor the experiments can resolve the molecular-level length and time scales over which the variations in local conditions occur near the vapor-liquid interface.

In this project, you will perform molecular dynamics simulations of a spherical solid particle in a supersaturated solution. You will calculate how the concentration and temperature, and with that also the local supersaturation, vary in space and time after applying the energy from the laser. This information will then be used as an input for the macroscopic model.



Reference:

[1] J.O. Sindt, A.J. Alexander, and P.J. Camp, Effects of nanoparticle heating on the structure of a concentrated aqueous salt solution, *J. Chem. Phys.* **147**, 214506 (2017)