Understanding crystal growth on nucleation is crucial for controlling crystal properties. Nucleation however takes place on a time scale that exceeds our ability to simulate this phenomena by straightforward atomistic molecular dynamics simulation. To this effect, we have developed metadynamics as very successful enhanced sampling method.

We apply this approach to the study of nucleation from solution. We unveil the complex nature of this process and its deviation from standard theories.

Finally, by taking advantage of recent development we are able to compute nucleation rates.