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The role of latent heat in heterogeneous ice nucleation

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Understanding the way in which ice forms is of great importance to many fields of science. Pure water droplets in the atmosphere can remain in the liquid phase to nearly -40º C. Crystallization of ice in the atmosphere therefore typically occurs in the presence of ice nucleating particles (INPs), such as mineral dust or organic particles, which trigger heterogeneous ice nucleation at clearly higher temperatures. The growth of ice is accompanied by a significant release of latent heat of fusion, which causes supercooled liquid droplets to freeze in two stages [Pruppacher and Klett, 1997].

We are studying these topics by utilizing the monatomic water model [Molinero and Moore, 2009] for unbiased molecular dynamics (MD) simulations, where different surfaces immersed in water are cooled below the melting point over tens of nanoseconds of simulation time and crystallization is followed.

With a combination of finite difference calculations and novel moving-thermostat molecular dynamics simulations we show that the release of latent heat from ice growth has a noticeable effect on both the ice growth rate and the initial structure of the forming ice. However, latent heat is found not to be as critically important in controlling immersion nucleation as it is in vapor-to-liquid nucleation [Tanaka et al.2017].

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