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Nanoscale Investigation of Frost Formation on Cold Plates

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Abstract **–** We investigated the atomic scale mechanism of frost formation on a cold plate with molecular dynamics (MD) simulations. The frost formation is a special type of heterogeneous nucleation process, where supersaturated vapor becomes condensed on the sufficiently cold surface without passing through liquid state (desublimation). Thus we expect this only for a narrow range of conditions (temperature and vapor density) and it may take substantially long time on the atomic scale. We conducted a series of MD simulations with two different types of water model, i.e., TIP4P full-atom model and mW coarse-grained one. For very long simulations with the mW, we successfully observed the formation of bilayer hexagonal ice on plates of 100-200 K.

Keywords**:** *water, frost formation, desublimation, molecular dynamics simulation*