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How does the presence of foreign surfaces impact the rates of ice nucleation?

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Atmospheric aerosols can promote heterogeneous nucleation of ice, impacting the radiative properties of clouds and Earth's climate. The experimental investigation of heterogeneous freezing of water droplets reveal a wide spread of ice freezing temperatures. It is not known which structural and chemical characteristics of the surfaces could account for the variability in ice nucleation efficiency. Here we use molecular dynamics simulations to investigate the nucleation of ice from liquid water in contact with both rigid and soft surfaces. We find that atomically flat graphitic surfaces promote heterogeneous nucleation of ice while molecularly rough surfaces do not, independently on their hydrophobic/hydrophilic character. Our analysis of ice nucleation on monolayers of long-chain alcohols indicates that the significant structural fluctuations of the surface strongly depresses its ice nucleation ability. By using importance sampling techniques, we find that the presence of both rigid and flexible surfaces changes the free energy of nucleation but does not impact the reaction coordinate of the transformation. While ordered domains are the birthplace of ice nuclei, the variable that drives the transformation is the size of the crystalline cluster, same as for homogeneous crystallization. The results could have important implications in the prediction of ice nucleation ability of different surfaces.