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Surface Induced Crystallization In Tetrahedral Liquids[1]

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Freezing is a fundamental physical phenomenon that has been studied over many decades; yet the role played by surfaces in determining nucleation has remained elusive. While common wisdom regards surfaces as unfavorable nucleation sites, both atmospheric data and laboratory measurements on droplets of water support the hypothesis of surface-induced crystallization in some systems. In this talk I will discuss our recent work on employing accelerated molecular dynamics simulations to investigate nucleation in the presence of free surfaces in tetrahedral liquids with a negative slope of their melting line ($dP/dT < 0$). Through conducting extensive study on nucleation rates and nucleation pathways in a few systems, *e.g.*, Si and Ge, we provide direct computational evidence of surface induced crystallization in supercooled systems with $dP/dT < 0$. We show that the possibility of observing preferential nucleation in close proximity of free surfaces is related to the density decrease occurring upon freezing, and surface tension facilitating the initial nucleus formation. Furthermore, in contrast to the common assumption that regards surfaces as heterogeneous center, we identify the *homogeneous* nature of surface induced nucleation. This is related to both the local static and dynamical properties of liquid surface.

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