The Effects of Surface Charge on Ice Melting: A Molecular Dynamics Study

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According to a recent report by Ehre *et al.* (Science **327**, 672-675, 2010), the freezing behavior of supercooled water in contact with a charged surface is profoundly influenced by the nature of the surface charge. The experiments show that the freezing of supercooled water is facilitated on a positively charged surface, while the water freezing is suppressed on a negatively charged surface. It is an intriguing phenomenon from a fundamental science perspective as well as from an aspect of various potential applications. The mechanism underlying the phenomenon is still not clear, although it is speculated that the dipole alignment of water molecules in the electric field plays a central role. Inspired by the experiments, we studied the effects of surface charge on ice melting by using molecular dynamics simulation. In our simulations, the prismatic and basal planes of hexagonal ice crystals have been set in contact with positively and negatively charged surfaces, and the melting behavior of the ice crystal at supercooled temperatures has been monitored. The negatively-charged surface has been found to facilitate the ice melting at the surface-ice interface, while the positively-charged surface to suppress the melting. The kinetics of the ice melting upon contact with negatively-charged surface has been compared for different magnitudes of the charge. The degree of melting in terms of the thickness of melted ice layer near the charged surfaces has been determined as a function of the surface charge. The molecular mechanism of the charge-induced ice melting will be explored, and possible connections on the charge-induced freezing/defreezing of supercooled water will be discussed.