Interfaces involving Water, Ice and Vapor

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We present a Molecular Dynamics simulations study of interfaces involving the three phase of water. Ice nano-columns in vapor are considered in order to understand the dependency of the melting temperature of small particles with curvature. The same ice rods in water provide the temperature dependency of the critical embryo needed for the system to crystalize. In both cases, our results are analyzed in terms of the Gibbs-Thomson effect. The melting of small water clusters in vapor follows a non-monotonic size dependency with temperature and we found that the cluster total dipole moment could be used as an indicator of the melting. Finally, the affinity of halide ions to for the water/vapor interface is study, using a fully polarizable force field, for the case of mixtures involving three different anions. The results show a pattern of enhancement directly correlated to the anion polarizability. This effect is explained in terms of the charge distribution across the interface resembling an electrical double layer. As a result, the anions with higher polarizablity lower the system's potential energy by enhancing their presence at the interface.

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