MD Simulations of the Quasi-Liquid Layer at the Methane/Ice Interface

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The presence of a liquid-like layer at the surface of ice can be found below the bulk melting temperature. Molecular dynamic simulations with a coarse grained model for both water and methane are used to investigate the properties of this quasi-liquid layer (QLL). Two types of systems were studied: 1) a slab of ice exposed to a vacuum and 2) ice in the presence of methane (shown below). The structure and thickness of the QLL is characterized as a function of temperature. In the presence of a hydrophobic methane-like guest at the same temperature, we found the thickness of the QLL increases dramatically, from ~5 Å to ~21 Å at 271 K. Because of this, the QLL has shown promise for the nucleation of natural gas hydrates, solid water cages that containing small, hydrophobic guest molecules. These results will be useful in future studies of clathrate formation from ice.

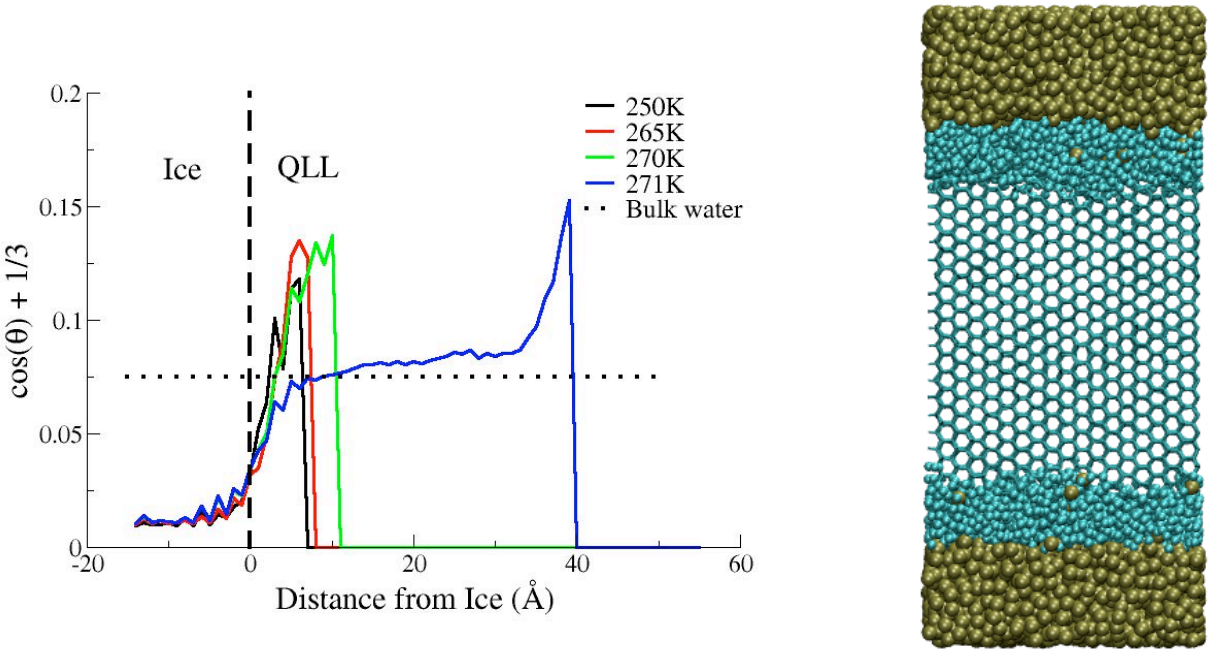

Figure 1: Measure of the tetrahedrality of the QLL based on distance from the ice/QLL interface. A perfectly tetrahedral shape would result in a value of 0.0. The angles are only measured from water molecules within 3.5 Å of the central molecule.