MD Simulations of Clathrate Growth Near the Surface of Ice

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Clathrate hydrates are hydrogen-bonded crystalline cages of water around small nonpolar molecules, such as methane. They typically form at low temperatures and high pressures in the presence of liquid/solid water and dissolved gas. In view of their potential in the fields of energy, carbon sequestration, industrial separations, and natural gas transportation, a better understanding of the nucleation and growth of Clathrates is of great interest.[1] Molecular dynamic simulations with a coarse grained model for both water and methane are used to investigate the structural characteristics of the clathrate, the ice, and the interface between the two phases (shown below). The rate of growth of both clathrate and ice are measured at several different temperatures ranging between 250 K and 270 K. Depending on the size and position of the clathrate, the clathrate can actually prevent the growth of ice during the length of our simulations. At the interface between the ice and clathrate phases, we observe a ~10 Å layer of disordered liquid. The structure and thickness of the water at the interface is characterized as a function of temperature and compared to previous simulations without a clathrate.

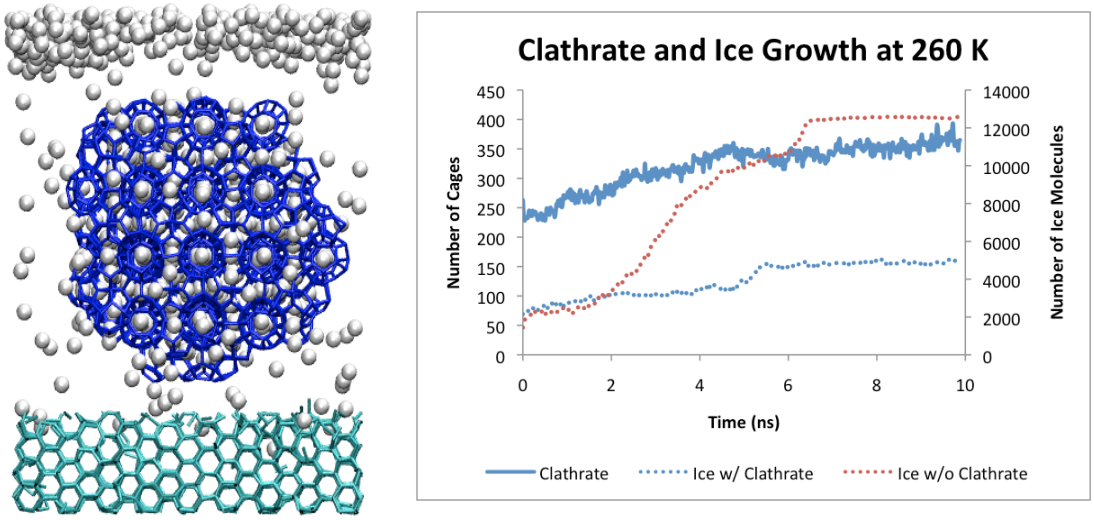

Figure 1 – A comparison of clathrate growth (blue solid) and ice growth (dotted). The growth of ice (as represented by the number of ice molecules) in the presence of a clathrate (blue dotted) is compared to that of the growth of ice without a clathrate present (red dotted).

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1 A. K. Sum, C. A. Koh, and E. D. Sloan, Industrial & Engineering Chemistry Research **48** (16), 7457 (2009).