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Structure of the Ice-Clathrate Interface¹ ANDREW NGUYEN, The University of Utah, MATTHEW KOC, TRICIA SHEPHERD, Westminster College, VALERIA MOLINERO, The University of Utah — In the laboratory, clathrates are customarily synthesized from ice and gas guest. It is not clear how and whether ice assists in the nucleation of clathrate hydrates. The structure of the ice-clathrate interface can help assess the role of ice in clathrate nucleation. However, only few studies have addressed the structure of the ice-clathrate interface. Here, we use molecular dynamic simulations to study the structure of the ice-clathrate interface. There is no lattice matching between any plane of ice and clathrate hydrates, therefore an interfacial transition layer has to form to connect the two crystals. We investigate the structure of the ice-clathrate interface produced by alignment and equilibration of the crystals, competitive growth of the two crystals from a common solution, and nucleation of hydrate in the presence of a growing ice front. We find that the interfacial transition layer between ice and clathrate has a width of two to three water layers and it is disordered in all cases. Water in the interfacial transition layer has tetrahedral order lower than either ice or clathrate and higher than liquid water under the same thermodynamic conditions.

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