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Comparison of experimental and computational estimation of non-freezing interfacial molecules[1] RAHMI OZISIK, NIHAT BAYSAL, DENIZ RENDE, Rensselaer Polytechnic Institute, SAMUEL AMANUEL, Union College — Recently, we have estimated that about 2.14 +/- 0.14 nm of interfacial cyclohexane molecules do not participate in phase transition. This estimation was determined from calorimetric measurements of physically confined cyclohexane in silica nanopores. In agreement with previous work, melting and freezing temperatures of the confined cyclohexane were lower than that of the bulk cyclohexane, and the apparent heat of fusion changed with silica pore size. Correcting for the layers of molecules at the interface that do not participate in the phase transition keeps the heat of fusion independent of the confined size scale. In the current study, we used molecular dynamics simulations to investigate the behavior of the cyclohexane molecules at the interface and compared their behavior to those in the bulk (away from the interface).

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