Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

What can simulations of hydrophobic polymers teach us about cold denaturation? THOMAS TRUSKETT, The University of Texas at Austin, GAURAV GOEL, Case Western Reserve University, SHEKHAR GARDE, Rensselaer Polytechnic Institute, MANOJ ATHAWALE, Intel Corporation — Interactions between hydrophobic solutes in aqueous solution depend not only on their size and shape, but also on their van der Waals attractions with water. Molecular theories can explain these differences for idealized cases, e.g, small (high curvature) solutes versus extended (low curvature) surfaces. But do these idealized limits provide meaningful information for the hydrophobic interactions that drive the conformational transformations of proteins or polymers? In this talk, we discuss recent results that take a step toward addressing this question. Specifically, we discuss molecular simulations of hydrophobic polymers with collapse transitions that display some protein-like behavior (e.g., cold denaturation). We first show that the collapse thermodynamics reflect a competition between polymer-water attractions and a contribution due to the effect that "shape" of the polymer has on water, the latter of which can be described by a simple surface tension model. We also discuss the importance of attractive interactions for cold denaturation.

Thomas Truskett
The University of Texas at Austin

Date submitted: 02 Nov 2009 Electronic form version 1.4