

MAR08-2007-030079

Abstract for an Invited Paper
for the MAR08 Meeting of
the American Physical Society

Effects of lengthscales and attractions on the collapse of hydrophobic polymers in water

SHEKHAR GARDE, Rensselaer Polytechnic Institute

Hydrophobic and hydrophilic hydration and interactions play important roles in biological and colloidal self assembly processes. More recently, lengthscale dependences and manybody effects in these interactions have received renewed attention. We will present results from theory and molecular dynamics simulations on hydration of and interactions between solutes and interfaces of varying chemistries (from hydrophobic to hydrophilic) and lengthscales. These simulations combined with those of folding-unfolding of hydrophobic polymers in water and mixed aqueous solutions provide insights relevant to biological assembly.