A fundamental study of the conformational phase behavior of chain molecules at interfaces

W. P. Krekelberg and V. K. Shen

Chemical and Biochemical Reference Data Division
National Institute of Standards and Technology
Gaithersburg, Maryland 20899

Chain molecules tethered or adsorbed to solid surfaces are at the heart of a wide range of technologies. Examples include colloidal particle stabilization, chromatographic materials, and drug delivery methods. Unfortunately, despite significant computational and theoretical efforts, important fundamental questions remain. In particular, a basic understanding of how the conformational phase behavior of tethered and adsorbed chain molecules depends on thermodynamic constraints and surface chemistry is still lacking. In this talk, we comprehensively study the conformational phase behavior of model homopolymers at solid surfaces using advanced Monte Carlo simulation techniques that provide the free energy of the system of interest to within an additive constant. We systematically determine how factors such as chain length, chain density, and polymer-surface interactions impact the resulting structure of adsorbed and tethered polymers. The properties of adsorbed and tethered polymers are compared and contrasted to those of bulk polymer solutions.