Abstract Submitted for the MAR14 Meeting of The American Physical Society

Adsorption

of Polymers on Rough Surfaces ABISHEK VENKATAKRISHNAN, Univ of Cincinnati, VIKRAM KUPPA, University of Cincinnati — Most of the surfaces encountered in nature display irregularity and self-similarity at certain length scales. Such real surfaces can be mimicked via fractal surfaces using an algorithm that produces random surfaces. The problem of polymer chains adsorbed on smooth surfaces has been well understood whereas adsorption on rough surfaces still remains unclear due to the complexity involved in equilibration and sampling of molecules in such systems. The enthalpic interactions between the monomers and the entropic penalty arising due to adsorption on rough surfaces are significantly different from smooth surfaces. In this study, we investigate the adsorption of freely rotating polymer chains on fractal surfaces by Monte-Carlo molecular simulations. Random fractal surfaces are generated using the diamond-square algorithm for different values of the Hurst parameter. Properties like monomer-surface interaction, density profiles, chain orientation profiles and distribution of adsorbed chain fractions are investigated. We also demonstrate the significant effect of fractal dimension on adsorption of polymers on rough surfaces.

> Abishek Venkatakrishnan Univ of Cincinnati

Date submitted: 15 Nov 2013

Electronic form version 1.4