Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Molecular Weight Distribution Effects on the Structure of Strongly Adsorbed Polymers by Monte Carlo Simulation VIKRAM KUPPA, University of Cincinnati — Monte Carlo simulations are used to investigate the adsorption of polymers from solution onto strongly attractive, perfectly smooth substrates. Using a coarse-grained united atom model for freely rotating polymer chains, three systems with different polydispersities are studied. The structure of the adsorbed layers, exemplified by density profiles, bond orientation order parameters, radii of gyration, and distribution of the adsorbed chain fractions, is shown to be highly dependent on the molecular weight distribution of the polymer phase. The results for the more monodisperse polymer systems are qualitatively similar to experimental and theoretical investigations, but devolve from very different chain conformations and statistics. For the first time ever, equilibrium polymer adsorption on highly attractive surface is studied, with all molecules in the adsorbed layers demonstrated to be indistinguishable from each other. The ergodicity of states explored by the polymer chains is in contrast to the kinetically constrained viewpoint of irreversible adsorption, and the observed behavior is explained in the context of the competition between polymers to make contact with the surface.

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Date submitted: 11 Nov 2011 Electronic form version 1.4