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Monte Carlo Simulation of Polymer Adsorption on Rough Substrates[1] VIKRAM KUPPA, Univ of Dayton, ABISHEK VENKATAKRISHNAN, University of Cincinnati — Polymer films adsorbed on atomistically smooth substrates have been studied for decades, but little is known about adsorption on surfaces displaying both physical and chemical inhomogeneities. Such interfaces are more realistic, and exhibit rich behavior arising from intricate relaxation processes. Focusing on physical irregularities, we investigate the molecular mechanisms governing chain adsorption. Monte Carlo simulations are employed to study the freely rotating chains adjacent to self-affine substrates, exploring the influence of surface fractal dimension and amplitude. The adsorbed polymers are characterized by density and orientation profiles, adsorbed fraction and chain topologies. Our results reveal chain attachment and film structure can be controlled solely by manipulating entropic factors such as surface physical heterogeneities and adsorbate molecular weight distributions. The correlation between adsorbed chain fraction and surface topology is revealed, and shows a counter-intuitive and non-monotonic dependence on roughness.

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