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**Molecular Simulation studies of adsorption of polymers on non-planar surfaces: Influence of surface characteristics** ABISHEK VENKATAKRISHNAN, University of Cincinnati, ANNE SHIM, Ohio State University, AQUIL FROST, Central State University, JOHN LEWNARD, VIKRAM KUPPA, University of Cincinnati — Molecular simulations are employed to investigate the adsorption of freely rotating polymer chains adsorbing on to non-planar surfaces. Adsorption studies on planar surfaces have been studied extensively and fairly well understood. However, in reality, surfaces are non-planar and cannot be represented using smooth surface models. We investigate the effect of surface characteristics on adsorption via molecular dynamics and Monte Carlo molecular simulations in the NVT ensemble. Both regular (uniform) and irregular (self-affine) roughness parameters are studied. The adsorbed polymer chains are characterized by density and orientation profiles, adsorbed fraction and chain topologies. Our results elucidate the extent to which surface roughness influences adsorption, in competition with other factors such as chain length and monomer-surface interaction. We also demonstrate how both adsorption and desorption can be controlled solely by tuning surface inhomogeneities.

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