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Surface diffusion of adsorbed polymers studied by molecular dynamics simulation WONKI ROH, ERIK LUIJTEN, University of Illinois at Urbana-Champaign — We study the diffusion of adsorbed polymers near a flat surface by means of molecular dynamics simulations, as a function of chain length N, adsorption energy, and surface coverage ϕ. We find that the two-dimensional diffusion coefficient scales as $D \sim N^{-1.017\pm0.011}$, in agreement with other experimental and simulation results. The relation between lateral diffusion coefficient and surface coverage shows an exponential decay. We also investigate the conformation of the adsorbed chains. The number of "trains," "loops," and "tails" per chain, as well as the number of monomers in tails and loops increase as surface density increases and adsorption energy decreases, whereas the number of monomers in trains decreases. The parallel radius of gyration increases as a power law of the chain length, $\langle R_{g\parallel}^2 \rangle \sim N^{2\nu}$, with a power that is in good agreement with the Flory exponent $\nu = 3/4$ for two-dimensional chains. $\langle R_{g\parallel}^2 \rangle$ decreases with increasing surface density and decreasing adsorption energy, whereas $\langle R_{g\perp}^2 \rangle$ remains almost constant with increasing surface density and increases with decreasing surface energy.

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