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Adsorption and Pattern Recognition of Polymer at Complex Heterogeneous Surfaces LEILA RAJABIBONAB, Victoria University of Wellington, SHAUN HENDY, University of Auckland, SHAUN HENDY TEAM, LEILA RAJABI TEAM — The statistical mechanics of polymer adsorption on a substrate has been well studied. However, there has been recent interest in the conformational behaviour of polymer chains on patterned heterogeneous surfaces, where absorption strength varies. Here we report on Monte Carlo simulations of the adsorption of homo-polymer chains on patterned surfaces. One difficulty in studying polymer self-assembly on a patterned surface is the fluctuation of polymer conformations, which can make calculating the free energy a challenge. To overcome this we apply an expanded ensemble method to compute free energy differences. Applying this approach enables us to identify different adsorbed phases at a range of temperatures. The simplest case of heterogeneous surface is striped pattern, but we consider heterogeneous surfaces with four other that are structured on different length scales. At low temperatures we find that the polymer chain will recognise the pattern, by conformationally adapting as it adsorbs before eventually becoming fully relaxed on the surface. Polymers are found to adsorb on simple patterns at higher temperatures than on complex patterns.

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