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Homopolymer Adsorption on Hexagonal Surfaces: A Replica-Exchange Monte Carlo Study BENJAMIN LIEWEHR, MICHAEL BACHMANN, The University of Georgia — The adsorption behavior and thermodynamic properties of a coarse-grained flexible homopolymer, grafted on a hexagonal patterned surface, are investigated by means of parallel-tempering replica-exchange Monte Carlo simulations. In this study, the strength of the polymer-surface interaction, which is based on a standard Lennard-Jones potential, is changed systematically, mimicking different hexagonally patterned substrate materials. Specific order parameters are introduced to discriminate structural phases, at different surface adsorption strengths and temperatures, into classes of expanded, globular, droplet, and compact conformations. Finally, we provide a complete structural hyperphase diagram for a polymer with 55 monomers and discuss representative polymer structures.

Benjamin Liewehr
The University of Georgia

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