

Abstract Submitted
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Microsecond MD Simulations of Nano-patterned Polymer Brushes on Self-Assembled Monolayers CREIGHTON BUIE, LIMING QIU, KWAN CHENG, SOYEUN PARK, Texas Tech University — Nano-patterned polymer brushes end-grafted onto self-assembled monolayers have gained increasing research interests due to their unique thermodynamic properties and their chemical and biomedical applications in colloids, biosensing and tissue engineering. So far, the interactions between the polymer brushes with the surrounding environments such as the floor and solvent at the nanometer length scale and microsecond time scale are still difficult to be obtained experimentally and computationally. Using a Coarse-Grained MD approach, polymer brushes of different monomeric lengths, grafting density and hydrophobicity of the monomers grafted on self-assembled monolayers and in explicit solvent were studied. Molecular level information, such as lateral diffusion, transverse height and volume contour of the brushes, were calculated from our microsecond-MD simulations. Our results demonstrated the significance of the hydration of the polymer in controlling the conformational arrangement of the polymer brushes.

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