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Semi-flexible polymer brush confined in a nanoslit: A high performance single chain in mean field simulation study JIUZHOU TANG, Institute of Chemistry,Chinese Academy of Sciences, XINGHUA ZHANG, Beijing Jiaotong University,Department of Physics, DADONG YAN, Beijing Normal University,Department of Physics — We develop a single chain in mean field simulation method based on worm-like chain model for investigating the compression effect of semi-flexible polymer brush. For the commonly used self-consistent field theory (SCFT) based on the Gaussian chain model, the compression of the polymer brush leads to an isotropic deformation of the chain. However, for the case of high grafting density, the nematic phase will be formed even in a flexible brush. SCFT with gaussian chain model cannot provide any prediction on this property. Therefore, all the effects from the compression of nematic phase were totally ignored in the previous theoretical studies. In present work, the response of nematic polymer brush to the compression along the nematic axis is studied by applying a high performance single chain in mean field simulation. Our results predict that for the semi-flexible polymer chain under compression, the nematic order director of polymer brush reorient, leading to a XY-model-like lateral rotational symmetry breaking. The quasistatic analysis of the compressing and the relaxing of the confinement indicates that this symmetry breaking corresponds to a first order phase transition.

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