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Ordering transitions in confined melts of semiflexible polymers: A Monte Carlo simulation WOLFGANG PAUL, Martin Luther University, Halle, Germany, VIKTOR IVANOV, Lomonossov University, Moscow, Russian Federation, MARCUS MUELLER, Georg August University, Goettingen, Germany, KURT BINDER, Johannes Gutenberg University, Mainz, Germany — Using grand-canonical Monte Carlo simulations of the bond-fluctuation model confined between two hard walls we study the effect of confinement on the isotropic-nematic transition of a melt of semi-flexible chains. The walls have a stiffening effect on the chains in their vicinity leading to an ordering transition at the walls preempting the one in the bulk (surface-induced ordering). For a semi-infinite system the thickness of the ordered nematic layer increases with a complete wetting transition upon approaching bulk coexistence. For a finite extension, D, between the walls, the ordered surfaces induce a shift of the first order isotropic-nematic transition in the bulk of the film (capillary nematization). When D becomes comparable to the extension of a chain, the first order isotropic-nematic transition line ends in a critical point.

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