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Conformational behavior of polymers adsorbed on nanotubes SIMCHA SREBNIK, INNA GUREVITZ, Technion - Israel Institute of Technology — We study the interaction of a dilute solution of semiflexible polymers with a weakly attractive infinitely long nanotube using Monte Carlo simulation. Apart for bending stiffness of the polymer chains, the only interactions considered in our model are weakly attractive short-ranged Lennard-Jones interactions between the monomers and with the surface. These nonspecific interactions are found to result in stable helical and multi-helical adsorbed conformations for semiflexible chains. Adsorption of these chains is found to occur in a sequential manner through tight wrapping of the polymer around the nanotube. Adsorption occurs quickly and is characterized by a sharp peak in the heat capacity. A second transition follows whereby opening and reorganization of the adsorbed chains into nearly perfect helices and multiple helices. Extension of the model to block and triblock copolymers reveals rich conformational behavior. These results are discussed on physical grounds and implications towards polymer-carbon nanotubes composites are offered.

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