Title

Does the topology of polymer brushes determine their sorption characteristics in vapors?

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Abstract

Previous studies have shown that a pure architecture change of polymer brushes from linear to un-concatenated cyclic chains without a change of effective grafting density, can only lead to trivial changes of swelling properties of brushes in solutions. But it remains unknown whether this conclusion is valid for the swelling characteristics of brushes in vapor phase, because vapors often introduce additional surface-tension effects comparing with solutions. Thus, we have done well-defined molecular dynamics simulation study on the vapor sorption characteristics of brushes with different topological structures (linear and cyclic brushes). Our results showed that a topological variation of brushes can drastically influence the vapor sorption characteristics of brushes, in agreement with recent experimental investigations. The simulation results clearly showed that cyclic brushes swell much less comparing with their topological counterparts (linear brushes) and adsorbs much more solvent in the interface between brush and vapor phases. Our results also indicated that the different vapor sorption characteristics between linear and un-concatenated cyclic topological brushes, is not due to the change of polymer architecture but due to the change of effective grafting density.