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Order and phase behavior of diblock copolymers and nanoparticles mixture in confinement : A Molecular Dynamics study¹ LENIN S. SHAGOLSEM, JENS-UWE SOMMER, Leibniz Institute of Polymer Research Dresden — Diblock copolymers(DBC) and nano-particles(NP) composite show new structures apart from that of a pure DBC. Interesting effects are observed when such composite are in confined geometries. For example, morphology changes, inhomogeneous NP distribution and its effect on the formation of ordered structures. We study, via MD simulation, a coarse grained model of cylinder forming DBC and NP composite confined between walls (which can be neutral or selective) with a particular focus towards an understanding of its order and phase behavior in this restricted environment. In particular, we investigate the effect of temperature on the NP enrichment near the walls also orientation of cylinders for different wall separation. Further, we study how the variation of NP volume fraction affects segregation and morphology.

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