

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Phase behavior of disk-coil molecules YONGJOO KIM, ALFREDO ALEXANDER-KATZ, MIT — Using Monte Carlo simulations, we investigate the self-assembly of disk-coil molecules in the NPT ensemble. By changing the interaction parameters between the disk and the coil portion of the molecules, a full phase diagram of these four phases is constructed. Furthermore, we study the ordering of disks within the crystal phase and we find that the confinement imposed by the mesophase segregation induces stronger order compared to the pure disk case, which was also explicitly simulated. Our results show that by reducing the dimensionality of a system it is possible to induce higher order of the molecules and help orient the disks in the crystal phase. Furthermore, we simulated molecules with additional interaction and obtained interesting additional phases. Our results are relevant for organic photoactive (typically planar) molecules that are functionalized with tails to improve their processability and long-range order in the solid phase.

YongJoo Kim
MIT

Date submitted: 18 Nov 2010

Electronic form version 1.4