Phase behavior of decorated soft disks in thin films

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We use molecular dynamics simulations to study the phase transitions of disks with attached ligands in two-dimensional systems. The ligands are assumed to be small disks. They can be tangent to the core or overlap partially the nanodisk. The ligands slide on the core. We investigate also disks with rigid geometry, in which ligands are permanently grafted on vertexes of a square. All entities interact via Lennard-Jones (12-6) potential.

We present phase diagrams for several model systems. The morphology of the different phases is analyzed using the calculated structure factors and radial distribution functions.

We discuss effects of the ligand mobility. We show also how the length of core-ligand bond and core- ligand interactions influence phase transitions.

In the studied systems we observe vapor-liquid coexistence, fluid-solid transitions and structural transitions in a solid phase. We show that the ligand mobility considerably affect fluid-solid transition. In the case of mobile ligands the transition always leads immediately to a hexagonal phase. On the contrary, for the decorated disks with rigid geometry there are a square phase that changes into an orthorhombic phase for highest densities. We discuss distribution of ligands on the core in different conditions. We present the analysis of clusters in a supercritical fluid.