

Modulated phases in two-dimensional systems of bent-core particles

We study the role of excluded-volume effects for the stabilization of different phases in systems composed of hard bent-core particles placed on a planar surface. In particular, we analyze molecular systems, in which modulated phases can appear. By the use of combined theoretical and simulational approaches, such as Onsager's Density Functional Theory and Monte Carlo simulations, we investigate how the details of bent-core particles composed of needles, polygons and disks can affect stability of surface order. We start by analyzing bent-core particles with two arms, for which we identified the nematic splay-bend phase, which turned out to be more stable than two-dimensional smectic ordering for particles with large opening angles and thin arms. Then, we present results for particles with three arms, for which we also identified modulated phases for wide range of molecular parameters. Lastly, we discuss the possibility of existence of nematic splay-bend in systems of banana-shaped molecules composed of connected disks.

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