

Phase behaviour of monolayers composed of flexible, trimer-like molecules

Using Onsager-type of Density Functional Theory and constant pressure MC simulations we study the effect of conformational degrees of freedom on orientational and positional ordering of trimer-like molecules confined to monolayers.

The molecules are composed of three linked line segments. Each of the terminal segments is allowed to occupy one of the two internal states: α and $-\alpha$, where α is an angle between the central and the terminal segment. Depending on the internal state of its terminal segments this flexible hard-needle can dynamically adopt either a chiral zigzag or achiral bow-shaped conformation. A system composed of such molecules has a rich spectrum of stable, liquid-crystalline structures. The Density Functional Theory admits the existence of nematic and lamellar nonchiral and chiral phases, while Monte Carlo simulation also suggest existence of more complex, modulated structures, with splay-bend signature. The model is a generalization of recent studies [1-3], where separately zigzag and/or bow-shaped hard-needles were considered.

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[1] J. Peón, J. Saucedo-Zugazagoitia, F. Pucheta-Mendez, R. A. Perusquía, G. Sutmann, and J. Quintana-H, *J. Chem. Phys.* **125**, 104908 (2006).

[2] J. Martínez-González, J. C. Armas-Pérez, and J. Quintana-H, *J. Stat. Phys.* **150**, 559 (2012).

[3] R. Tavarone, P. Charbonneau, and H. Stark, *J. Chem. Phys.* **143**, 114505 (2015).

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