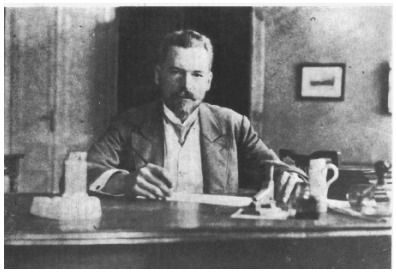

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Crystalline phases with splay modulation in a system of hard wedges composed of balls

Monday, 19 September 2022 12:35 (25 minutes)

Computer simulation studies of equilibrium phases of matter play a crucial role in many fields, including biophysics, nanotechnology and soft matter science. They can be used as a guidance for synthesis of materials with desired properties. Of especially high interest are simple interaction models, which are easy to implement, but capture the most important characteristics of modelled molecules. Hard-core resuplsion is one of them. It was already proven years ago by Onsager, that a simple model of hard spherocylinders can capture isotropic-nematic phase transition. Since then, many types of hard molecules were studied and numerous purely entropic phase transitions were observed. In this study, we focus on hard wedges composed of tangent balls with linearly increasing radii. The molecule model possesses axial symmetry, but the up-down symmetry is broken ($C_{\infty v}$ symmetry group). The system is studied using Monte Carlo integration. Liquid phases in this model undergo Iso-N-SmA phase transition sequence, typical for elongated molecules. For a solid state, however, non-standard phases emerge. Apart from a non-polar hcp-like structure, two types of polar phases can be observed, where hexagonal clusters with a non-zero net polarization form periodic metastructures with splay modulation in the director field.

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