Atomistic modelling of phase transition in liquid crystal

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Liquid crystals are widely used in science and technologies due to their self-assembly properties. We investigate the transport properties of nematic phase of liquid crystal 5CB in order to reproduce the experiment of light-driven molecular motors diffusion in liquid crystal [1]. The problem is currently being actively investigated. For example, the authors of [2, 3] have created their own QMD-FF potential for predicting the properties of a liquid crystals mixture. The molecular dynamics method with GAFF potential is used. An equilibrium computational cell with 1100 molecules with periodic boundary conditions is used. A phase transition from an isotropic phase to a nematic one is observed in NPT-ensemble over more than 1.4 μs. The experimental values for order parameter are reproduced for 300 K. The density, system size, dipole moment, energy and other properties changes during the phase transition are received.The diffusion coefficients for the nematic phase $D_{\perp}$ and $D_{||}$ are computed using the Einstein-Smolukhovsky relation.

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[1] Orlova T, Lancia F, Loussert C, Iamsaard S, Katsonis N and Brasselet E 2018 *Nature nanotechnology* **13** 304–308
[2] Vilhena J, Greff da Silveira L, Livotto P R, Cacelli I and Prampolini G 2021 *Journal of Chemical Theory and Computation* **17** 4449–4464
[3] Prampolini G, Greff da Silveira L, Vilhena J and Livotto P R 2021 *J. Phys. Chem. Lett.* **13** 243–250