# Atomistic modeling of 5CB phase transition and diffusion

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The diffusion of molecular motors in liquid crystals in the experiment [1] is used as a parameter in a continuous model, that can be refined with MD methods. For that reason, the model of LC reproducing general properties should be developed. The phase transition from isotropic to nematic phase at temperature T = 300 K is observed in a long 1.8 $\mu s$ MD simulation in the GAFF force field [2]. The order parameter gradually grows from 0.11 to 0.57 via simulation for 1 $\mu s$ and remains stable afterwards. Order parameter and density values correspond to the experimental values [3, 4]. With anisotropic radial distribution function it is checked that observed nematic phase is indeed nematic, not smectic, for instance. By the annealing procedure (from T = 300 K to T = 380 K) it is checked that the temperature order parameter dependence is not influenced by the annealing speed. Thermodynamic stability at several temperatures is checked for two different initial phases, nematic and isotropic. Temperature dependence of diffusion coefficients is calculated and comparison with other experimental and computational works is done [5, 6].

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