Abstract Submitted
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Nonequilibrium-molecular-dynamics measurement of the Leslie coefficients of a Gay-Berne nematic liquid crystal[1] TIEZHENG QIAN, Hong Kong University of Science and Technology — We carried out nonequilibrium molecular dynamics (MD) simulations to measure the six Leslie coefficients of a nematic liquid crystal composed of molecules interacting via the Gay-Berne potential. In the presence of a simple shear flow, an external field is applied to control the molecular orientation, and a uniform director is stabilized in the central region of the channel in which the liquid crystal is confined and sheared. With the director tuned by varying the applied field, a number of orientational states are stabilized in the presence of a shear flow, and various viscous stress components are measured in these states of different directors. The six Leslie coefficients α_i are determined by interpreting the MD measurement data for viscous stress according to the constitutive relations in the Ericksen-Leslie-Parodi (ELP) theory. The Parodi relation $\alpha_2 + \alpha_3 = \alpha_6 - \alpha_5$ is well satisfied. Given the values of the Leslie coefficients, liquid crystal orientations are evaluated for different field directions and shear rates. Comparison with those directly measured in MD simualtions demonstrates a quantitative agreement, showing that in the Gay-Berne nematic liquid crystal, the viscous stress and the coupling between orientation and flow are well described by the ELP theory.

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