Calculation of dipolar flexoelectric coefficients in liquid crystal with hard pear-shaped molecules

Sadrallah Fathi, Maryam Abdipour, Abolghasem Avazpour *

Department of Physics, Yasouj University, Yasouj, Iran

Abstract

In liquid crystals, pear- and banana-shaped molecules form splay and bend arrangements due to their asymmetry. In these crystals, the director deviation from equilibrium produces pure polarization. This effect is called flexoelectricity. Flexoelectric coefficients in liquid crystals are derived from simulation and experimental methods. In density functional theory, these coefficients depend on the molecular direct correlation function and the angular distribution function. In this study, the shortest contact distance between hard pear-shaped molecules is calculated using the hard Gaussian overlap model. The approximate direct correlation function for pear-shaped molecules is obtained using the contact distance. Using this correlation function and the deduced proper orientation distribution function, we calculate the dipolar flexoelectric coefficients for liquid crystals formed by pear-shaped molecules with elongations k = 3 and 5. The results are consistent with the simulation results qualitatively.

Keywords: flexoelectric coefficients, nematic crystal, direct correlation function, orientation distribution function, Pear-shaped molecule

*Corresponding Author: avazpour@yu.ac.ir