Computer simulation study of nematic nanodroplets

J. M. Romero-Enrique, L. F. Rull
Departamento de Física Atómica, Molecular y Nuclear, Area de Física Teórica, Universidad de Sevilla, Spain.
A. Fernandez-Nieves
School of Physics, Georgia Institute of Technology, Atlanta, GA, USA

We perform Monte Carlo computer simulation of nematic nanodroplets in the vapour phase of a Gay-Berne fluid. We consider temperatures both above and below the vapour-isotropic-nematic triple point for different elongations. In all the cases we first run NPT simulations close to the coexistence region, allow for the system to equilibrate and induce a sudden volume expansion, which we follow with an NVT simulation. We observe the formation of nematic nanodroplets inside the vapour phase; these have an approximately ellipsoidal shape, have the molecules aligned parallel to the interface and have their main axis oriented along the nematic director. We conclude these are bipolar nanodroplets with the two surface defects located along the larger axis of the ellipsoid. We characterize the eccentricity of the droplet by evaluating its inertial tensor and find that the larger the value of molecular elongation is, the more elongated the droplet is. For the largest value of molecular elongation considered in our simulations,some evidence of the formation of singularities in the nanodroplet shape is observed in the vicinity of the topological defects.