The quest for real density-splay coupling constant

Jaka Sočan

jaka.socan@ki.si

Laboratory for Molecular Modeling, National Institute of Chemistry, Hajdrihova 19, SI-1001 Ljubljana, Slovenia

Our aim is to prove the existence of a finite density-splay coupling constant across various real-life polymers. To achieve this, we derive a multiscale continuum field model of a polymer in the isotropic phase [1], using sufficiently decorrelated simulation trajectories as the basis for analysis. By examining long-wavelength fluctuation amplitudes of monomer density and nematic tensor components, we gain quantitative insight into the coupling between density and order. To date, we have characterized density-splay coupling in double-stranded DNA and are currently extending this analysis to other polymer systems.

References:

[1] D. Svenšek, J. Sočan, M. Praprotnik, Macromol. Rapid Comm. 45 (2024) 2400382.