

Abstract Submitted
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Molecular nature of liquid crystal defects MOHAMMAD RAHIMI, Institute for Molecular Engineering, University of Chicago, NICHOLAS L. ABBOTT, Department of Chemical Engineering, University of Wisconsin - Madison, JUAN J DE PABLO, Institute for Molecular Engineering, University of Chicago, RUI ZHANG, University of Chicago — Distortion of liquid crystal (LC) director creates defects which can be easily observed and controlled experimentally. Liquid crystal defects, which are a consequence of symmetry breaking, have significant influence on the macroscopic properties of liquid crystals, and many of the features that make LCs particularly exciting for new applications can be traced back to the existence of liquid crystal defects. However, the molecular nature of liquid crystal defects remains largely unknown. In this work, we perform large-scale atomistic simulations of 5CB/8CB mixture with a cylinder with strong homeotropic anchoring. The presence of the cylinder distorts the nematic field around the cylinder surface and creates two line defects. The local order parameter and biaxiality are calculated to characterize these defects. The results of this study indicate that, the density and the order parameter are correlated, and at the defect both parameters are low.

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