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Structural organization of liquid crystals at liquid crystal-air interface: Synchrotron X-ray reflectivity and computational simulations

MONIROSADAT SADATI, HADI RAMEZANI-DAKHEL, IME, UChicago, WEI BU, CARS, UChicago, EMRE SEVGEN, IME, UChicago, ZHU LIANG, CEM EROL, Dept. Phys., UIC, NADER TAHERI QAZVINI, MOHAMMAD RAHIMI, IME, UChicago, BINHUA LIN, CARS, UChicago, BENOIT ROUX, Dept. Biochem. Molecular Biol., UChicago, MARK SCHLOSSMAN, Dept. Phys., UIC, JUAN J. DE PABLO, IME, UChicago — Numerous applications of liquid crystals (LC) rely on control of molecular orientation at an interface. However, little is known about the precise molecular structure of such interfaces. In this work, we have performed synchrotron X-ray reflectivity measurements accompanied by an advanced theoretical and computational analysis to study the structural organization of liquid crystals at the air-liquid crystal interface. The X-ray reflectivity was measured from two nematic (5CB) and smectic (8CB) liquid crystals at several temperatures, in the nematic phase and above the nematic-isotropic transition. Our computational simulations and X-ray reflectivity results indicate that in the case of 8CB nematic phase, incipient bulk smectic fluctuations are pinned at the interface to form temperature-dependent multilayers at the interface. Such layers can extend far from the interface. However, the interface of 5CB in the nematic phase exhibits a relatively small number of layers. These measurements will be extended to the study of the LC-aqueous electrolyte interfaces to understand the effects of electrostatic interactions and external stimuli on the interfacial anchoring energy and LC orientational ordering.

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