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Amphiphile-Induced Reorganization of Nematic Liquid Crystals at Aqueous Interfaces AMIN RAHIMI, HADI RAMEZANI-DAKHEL, Univ of Chicago, JOEL PENDERY, NICHOLAS ABBOTT, university of wisconsin, JUAN DE PABLO, Univ of Chicago, PROF JUAN DE PABLO TEAM, PROF NICHOLAS ABBOTT COLLABORATION — Recent studies have shown that ordering transitions in 4-cyano-4'-pentylbiphenyl (5CB) molecules can be triggered by the self-assembly of specific amphiphiles near a flat aqueous-LC interface. In the absence of adsorbed amphiphiles, LC molecules adopt a parallel orientation at the aqueous interface. Self-assembly of amphiphile molecules at the LC-aqueous interface triggers a spontaneous reorientation of the LC at the aqueous interface. A number of observations indicate that the hydrophilic headgroup of the surfactant has marginal effect on the orientation of 5CB whereas the aliphatic tail structure, length, and conformation greatly affect the ordering of the LC. The structural reorganization of liquid crystals at aqueous interfaces has been primarily ascribed to a weakening of the surface anchoring strength induced by amphiphile molecules. Such explanations, however, have only been supported by *a posteriori* microscopic observations. The underlying mechanism of such an ordering transition and the effect of amphiphile structure remain poorly understood. Here, we study the nature of molecular interactions between amphiphiles, 5CB, and water to understand the mechanism of ordering transitions using atomistic molecular dynamics simulations.

Amin Rahimi
Univ of Chicago

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