Title:	Hydrogen bond assisted anchoring transitions in nematic liquid crystals at the aqueous interface
Authors:	Nandi, Rajib (/jspui/browse?type=author&value=Nandi%2C+Rajib) Jain, Varsha (/jspui/browse?type=author&value=Jain%2C+Varsha) Devi, Manisha (/jspui/browse?type=author&value=Devi%2C+Manisha) Gupta, Tarang (/jspui/browse?type=author&value=Gupta%2C+Tarang) Pal, Santanu Kumar (/jspui/browse?type=author&value=Pal%2C+Santanu+Kumar)
Keywords:	DFT Liquid crystal-aqueous interface
Issue Date:	2021
Publisher:	Elsevier
Citation:	Colloids and Surfaces A: Physicochemical and Engineering Aspects, 625, 126952.
Abstract:	Homeotropic alignment of liquid crystals (LCs) at the aqueous interface and their fundamental understanding is still limited known, which is a prerequisite for the development of new kinds of LC-based sensors for the detection of biomolecules in the aqueous phase. Herein, we have investigated the orientational ordering of nematic LC at LC-aqueous interface in contact with the different hydrogen bonding strength of para-substituted phenol derivatives (X; functional group attached to phenol at para position = -NO2, -CN, -Cl, -F, -CHO, -H) intending to understand how the intermolecular hydrogen bonding interactions at LC-aqueous interface amplified into supramolecular ordering in LCs. The hydrogen bonding interactions between -CN group of 5CB and -OH group of phenol derivatives lead to a change in tilt angle from planar to homeotropic ordering of 5CB molecules at LC-aqueous interface. Raman measurement of different mixtures between 5CB and para-substituted phenol derivatives have been recorded to correlate the experimental observations at the LC-aqueous interface as well as direct evidence of hydrogen bonding at the LC-aqueous interface. Density functional theory (DFT) has been used to calculate hydrogen bonding strength and charge transfer mechanism between 5CB and phenol derivatives. The orientation of LC at the aqueous interface depends on the strength of the interfacial hydrogen bonding between phenol derivatives and LC, which varies on substitution of phenol and concentration of the phenol molecules.
Description:	Only IISER Mohali authors are available in the record.
URI:	https://www.sciencedirect.com/science/article/pii/S0927775721008219?via%3Dihub (https://www.sciencedirect.com/science/article/pii/S0927775721008219?via%3Dihub) http://hdl.handle.net/123456789/5036 (http://hdl.handle.net/123456789/5036)
Appears in Collections:	Research Articles (/jspui/handle/123456789/9)

Files in This Item:

File	Description	Size	Format	
Need To Add…Full Text_PDF (/jspui/bitstream/123456789/5036/1/Need%20To%20Add%e2%80%a6Full%20Text_PDF)		15.36 kB	Unknown	View/Open (/jspui/b

Show full item record (/jspui/handle/123456789/5036?mode=full)

(/jspui/handle/123456789/5036/statistics)