The adsorption of fluorinated dopants at the surface of 5CB: A neutron reflection study

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SUPPLEMENTARY INFORMATION

The scattering length densities, $\rho$, of the materials used in the experiments were calculated using the number density, $N$ and scattering length, $b$ [1] of each element, $i$ in the molecule in the following equation.

$$\rho = \sum_i N_i b_i$$

The number densities were determined in the following ways: For 5CB the temperature dependent density data was used from the work of Deschamps et al. [2] and used with the molecular masses to define the number density. The density of F17 was estimated using the method of Girolami [3]. Owing to the similarity in the structure of F3 to F17, both being modified 11OCB, its scattering length density was estimated from the same number density. The bulk densities for the silanes, fluorinated and non-fluorinated silanes used, PFDS and OTS, were determined by the manufacturers Fluorochem and Sigma-Aldrich.

Figure S1 SANS intensity profile for both 0 and 2% F17 in 5CB with two theoretical curves for 100 and 60 Å spherical micelles.
Figure S2 Reflectivity curves with lines representing model fits to the data for 2% F17 in 5CB at its interface with air for three different temperatures, offset for clarity.

Figure S3 Reflectivity curves with lines representing model fits to the data for 0, 0.7 and 1% F17 in 5CB against a perfluorodecyl silyl (PFDS) coated surface, offset for clarity.
Figure S4 Reflectivity curves with lines representing model fits to the data for 0 and 9% F3 in 5CB against a perfluorodecyl silyl (PFDS) coated surface, offset for clarity. The model for the 9% is without an adsorbed layer.

Figure S5 Reflectivity divided by the Fresnel reflectivity of a clean interface for F3 in 5CB against a PFDS surface, the difference between the two is primarily caused by the difference in the scattering length densities of the two subphases.
Figure S6 Scattering length density profiles for from pure 5CB to 5CB containing 9% F3, both do not have an adsorbed layer however the 9% data required a slight change in the base layer scattering length density ($0.1 \times 10^{-6}$) and roughnesses (3 Å).

Figure S7 Reflectivity curves with lines representing model fits to the data for 0 and 2% F17 in 5CB against an OTS coated surface, offset for clarity.
Table S1 Parameters used for the thicknesses and roughnesses of the PFDS and OTS.

| Surface coating | Silicon oxide layer thickness, Å | Silyl layer thickness, Å | Roughness Si/oxide layer, Å | Roughness oxide layer/liquid crystal, Å |
|-----------------|---------------------------------|--------------------------|-----------------------------|----------------------------------------|
| PFDS            | 40                              | 8                        | 5                           |
| OTS             | 24                              | 32                       | 4                           | 3                                      |

References

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3. Girolami GS. A Simple Back of the Envelope Method for Estimating the Densities and Molecular Volumes of Liquids and Solids. J.Chem. Ed. 1994, 71, 962.