Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for: The Effect of Surface Polarity on the Structure and Collective Dynamics of Liquid Ethanol

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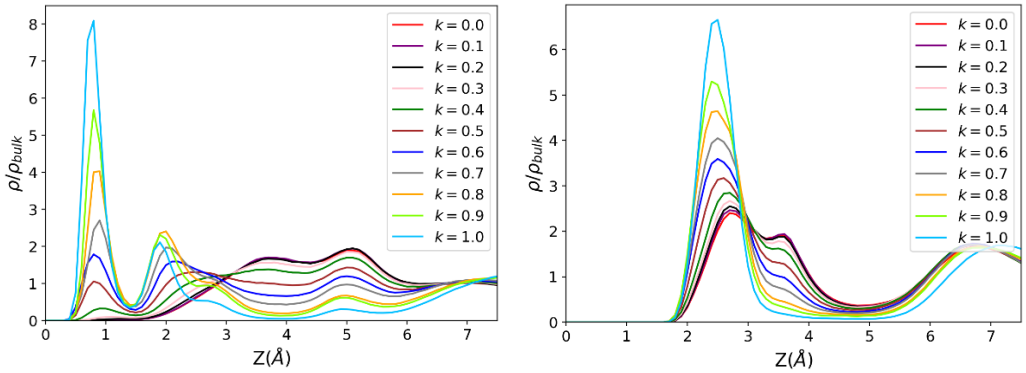
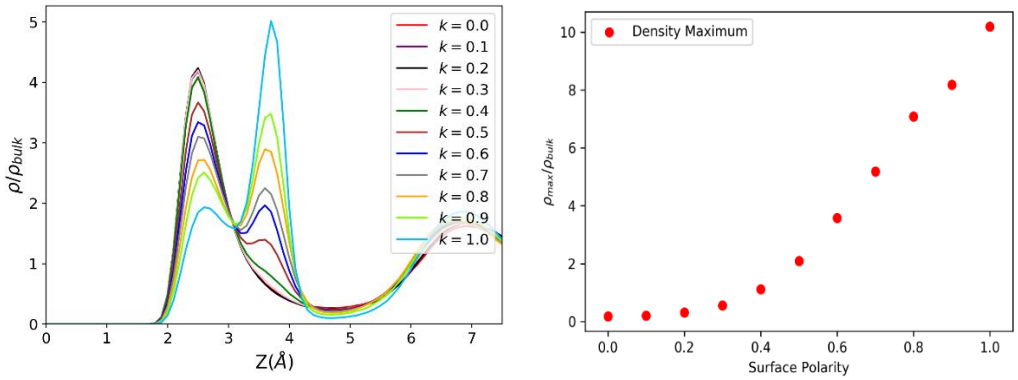


(a) (b)



(c) (d)

Fig. S1 (a) Density profile of ethanol hydroxyl hydrogen at different polarities (b) Density profile of ethanol methylene carbon at different polarities (c) Density profile of ethanol methyl carbon at different polarities (d) Peak value of the ethanol oxygen density profile's first peak at different polarities

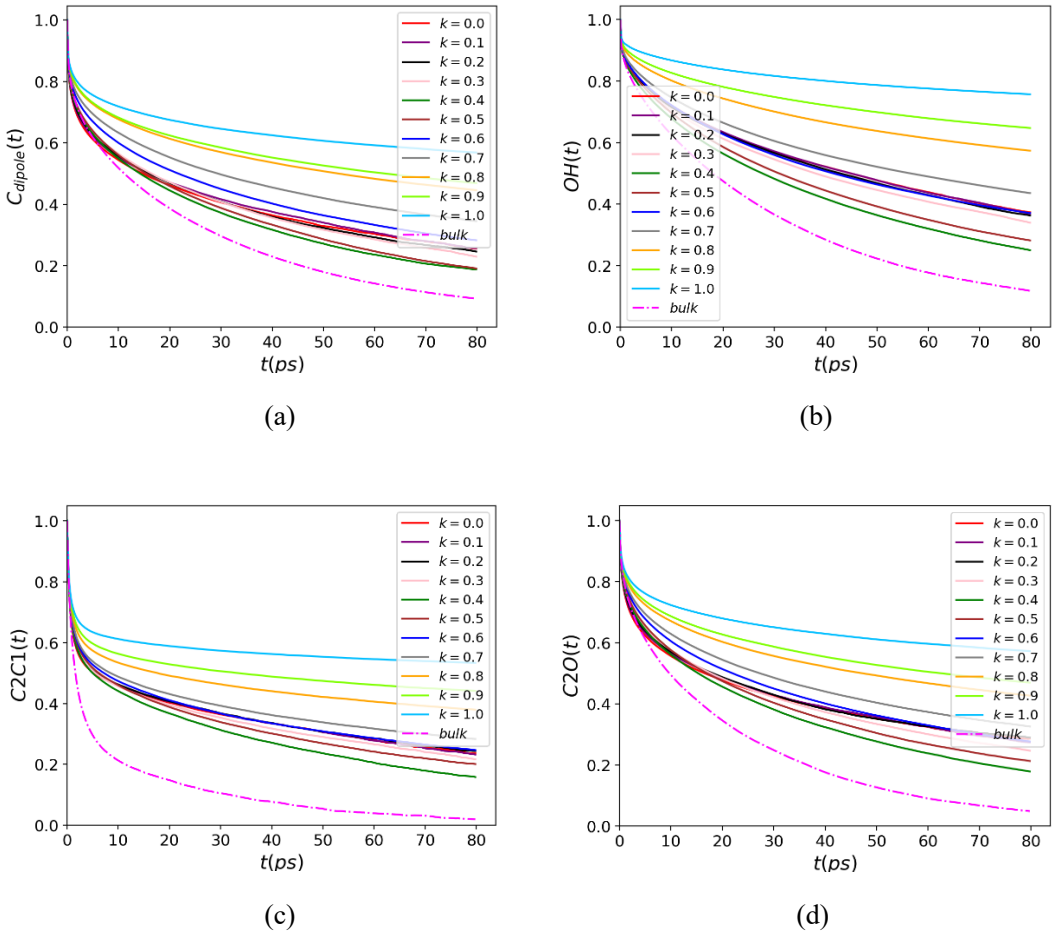


Fig. S2 Rotational time correlation functions (TCFs) of ethanol (a) dipole, (b) OH vector (c) C_1-C_2 vector (d) C_2-O vector in the LS region with different polarities

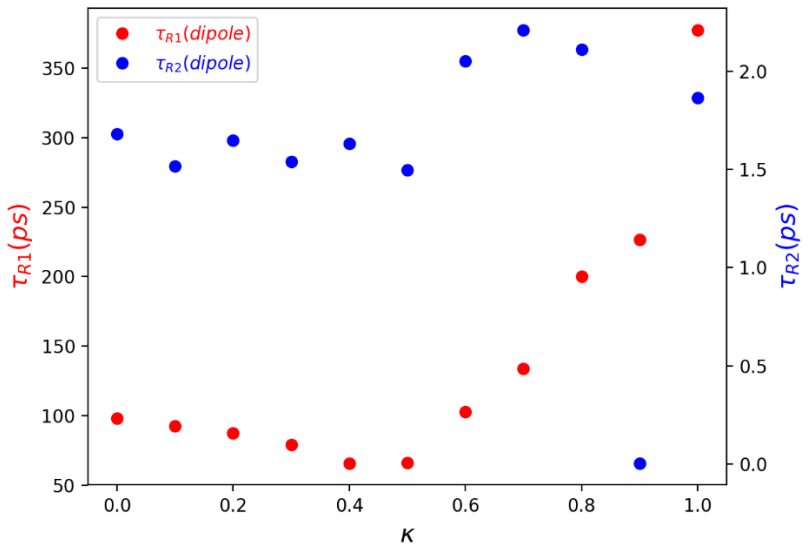


Fig. S3 The τ_1 and τ_2 from bi-exponential fit of ethanol dipole rotational time correlation

functions

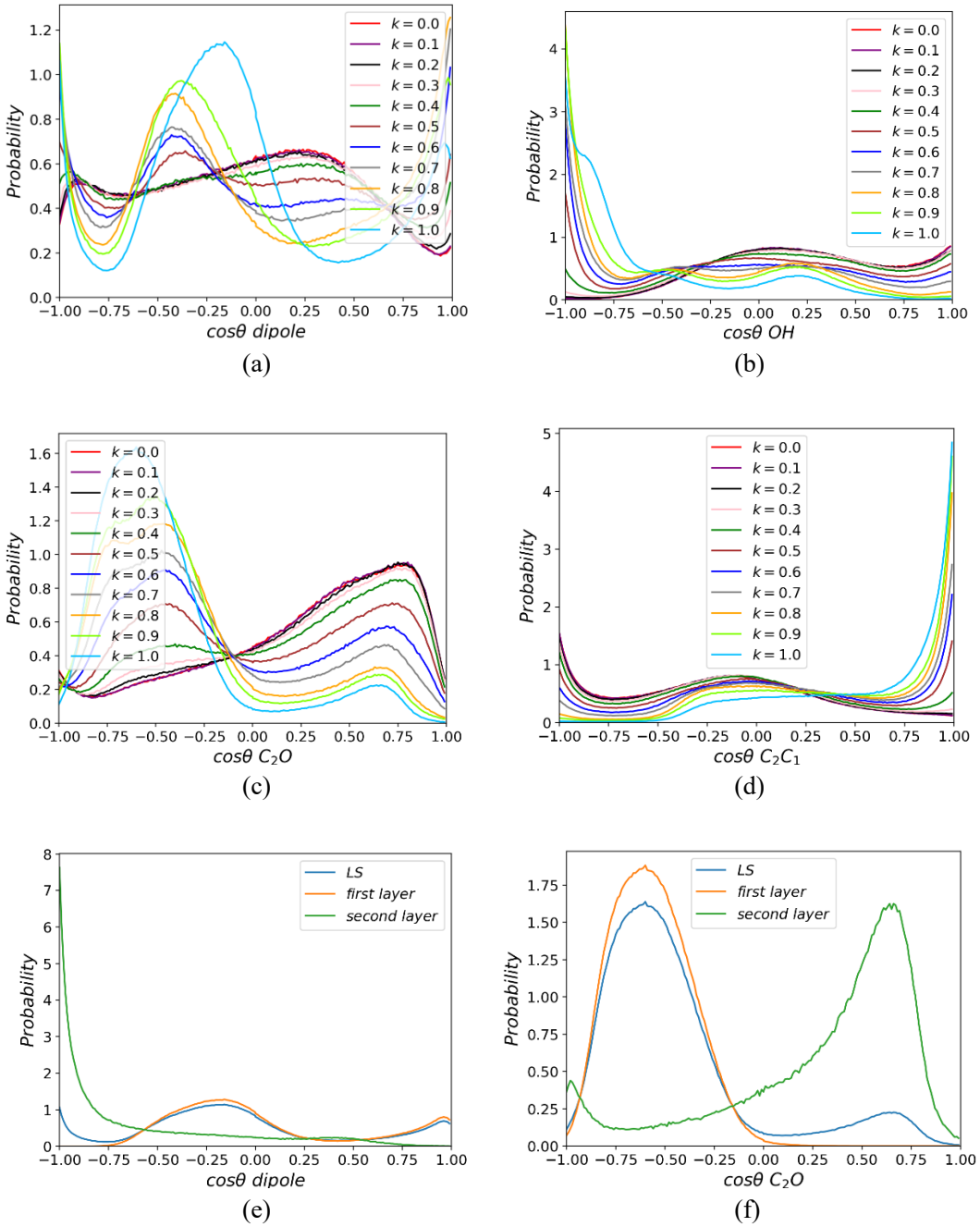


Fig. S4 The angular distribution of ethanol a) dipole vector b) O-H vector c) C_2-O vector d) C_2-C_1 vector in the LS region with different surface polarity k, where θ is the angle between the given vector and surface normal. (e), (f) the dipole vector, C_2-O vector with the same surface polarity k=1.0 in different region LS, first layer, second layer, respectively.

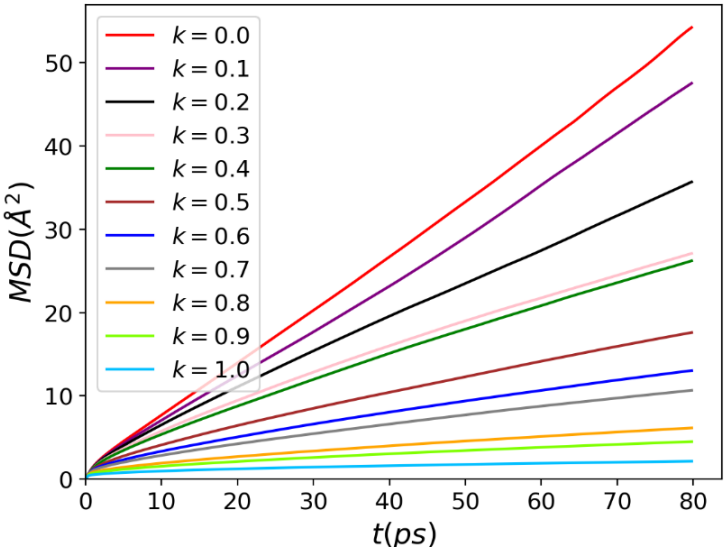


Fig. S5 the ethanol molecule in the solid-liquid region Mean Square Displacement (MSD) for the methylene carbon into hydroxyl oxygen atoms change over charge k in the 80ps.

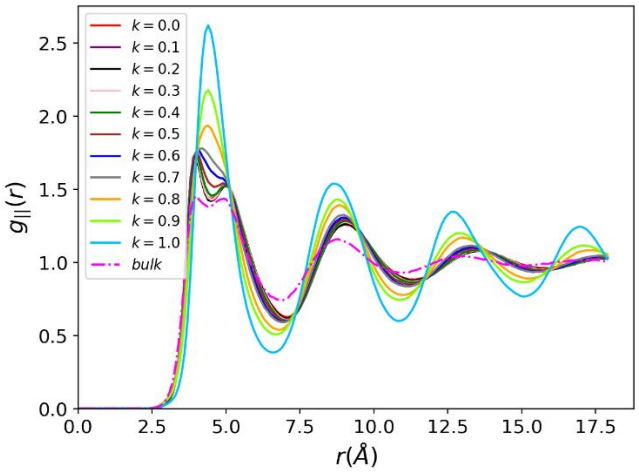
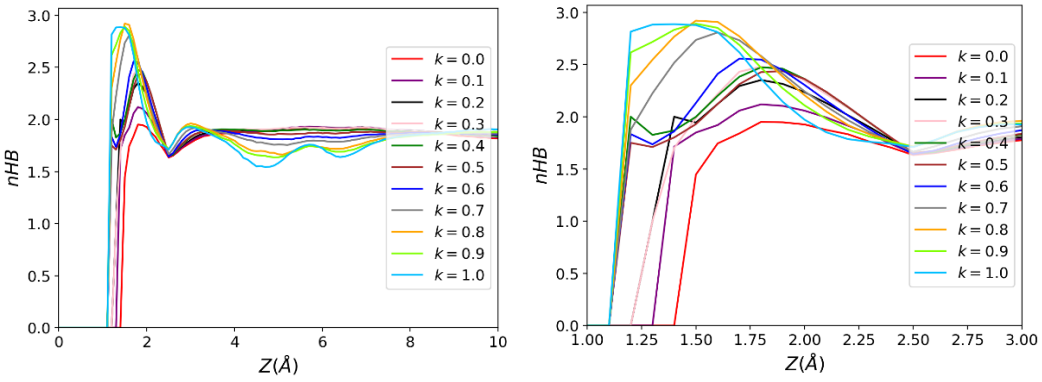
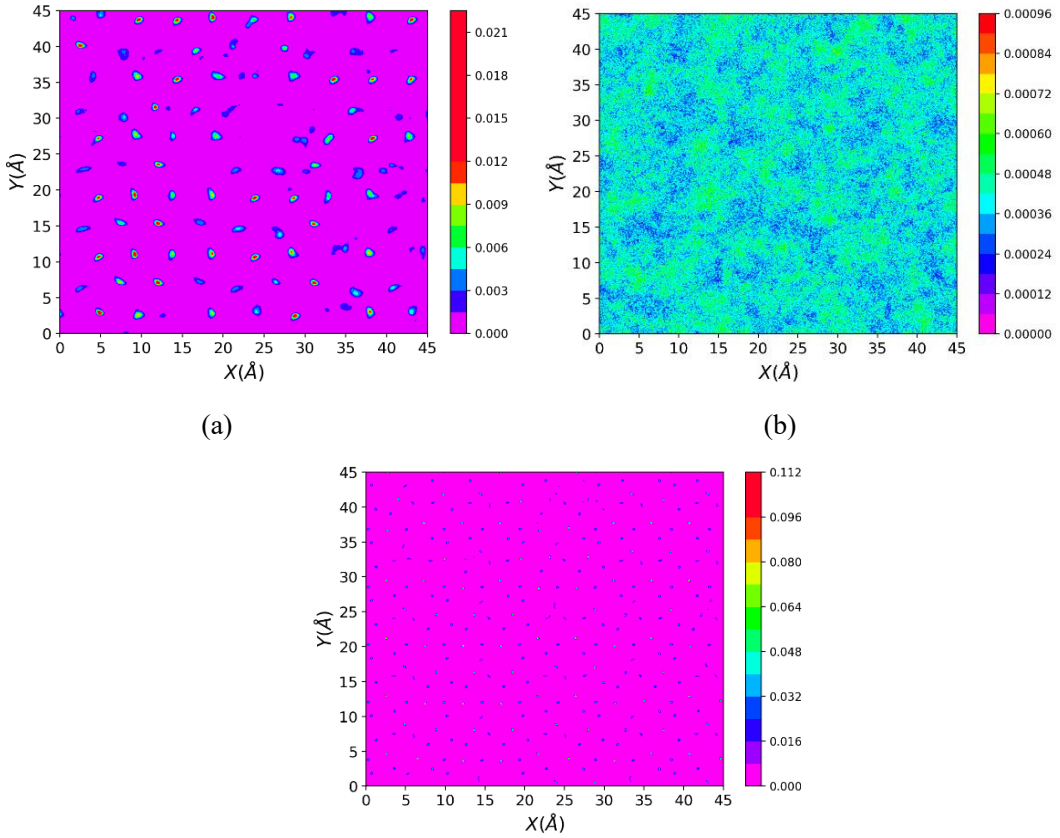


Fig. S6 In-plane radial distribution functions of ethanol molecules in the LS region at different surface polarities.(a) the range between the 0~10 Å, (b) zoom in the region of 1-3 Å.



(a) (b)

Fig. S7 (a) The number of hydrogen bonds per ethanol molecule as a function of z distance at different surface polarities. (b) Zoomed in figure showing the region of 1-3 Å of Fig. S7(a).



(a) (b)

(c)

Fig. S8 The in-plane probability density distribution for (a) ethanol oxygen atoms in the LS interface region at surface polarity k=1.0; (b) ethanol oxygen atoms in the LS interface region at surface polarity k=0.0; (c) hydroxyl groups on the alumina surface at surface polarity k=1.0.

	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
First layer	21.37	22.507	25.189	30.156	37.990	61.511	118.23	193.96	430.62	614.55	1252.8
Second layer	22.49	23.496	24.481	25.764	26.864	29.059	32.558	34.390	37.099	38.296	39.467

Table. S1 The residence time (in unit of ps) for ethanol molecules in the first layer and second layer at different surface polarities.