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

Electronic Supplementary Information

Contents

S1: Simulation cell parameters for liquid alcohols.

Table-S1: Simulation cell parameters for alcohols in liquid state

	Number of Molecules	Box dimension (Å)	Experimental density[1] (gcm^{-3})
Methanol	100	18.86	0.792
Ethanol	100	21.32	0.789
Propanol	100	23.16	0.803
Butanol	100	24.76	0.810
Pentanol	100	26.19	0.814

S2: DFT functional validation: comparison of experimental and calculated partial radial distribution functions, $\boldsymbol{g}_{OO}$ and $\boldsymbol{g}_{OH}$ for methanol using BLYP, HCTH and PBE functional.

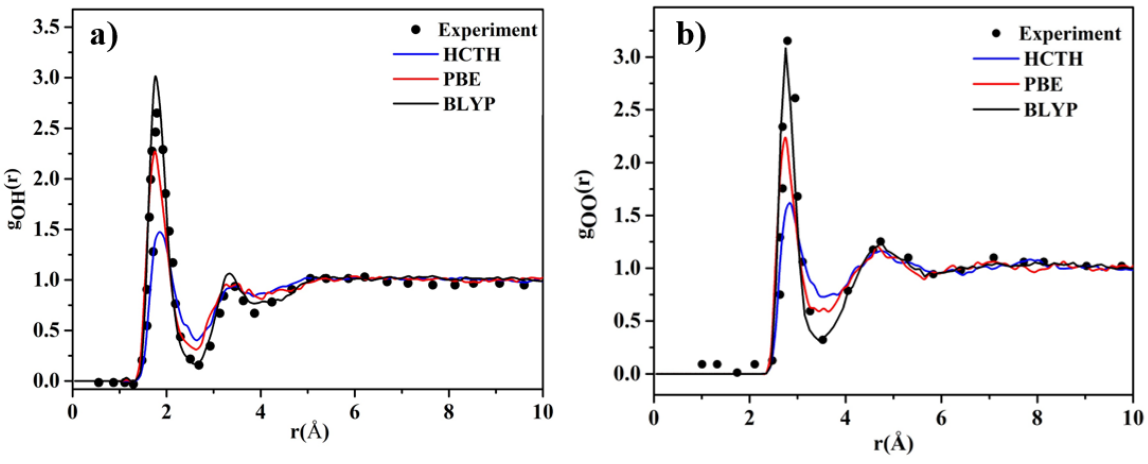

Figure S1: Comparison of prdfs calculated using different DFT functional for liquid methanol a) The non-bonded -O to hydroxyl proton -H, $\boldsymbol{g}_{OH}$ b) The non-bonded -O to -O rdf function, $\boldsymbol{g}_{OO}$.

S3: Simulation cell and comparison of calculated and experimental radial distribution function (rdf) and partial rdfs, $\boldsymbol{g}_{H1H1}$, $\boldsymbol{g}_{XH1}$ and $\boldsymbol{g}_{XX}$ of ethanol.

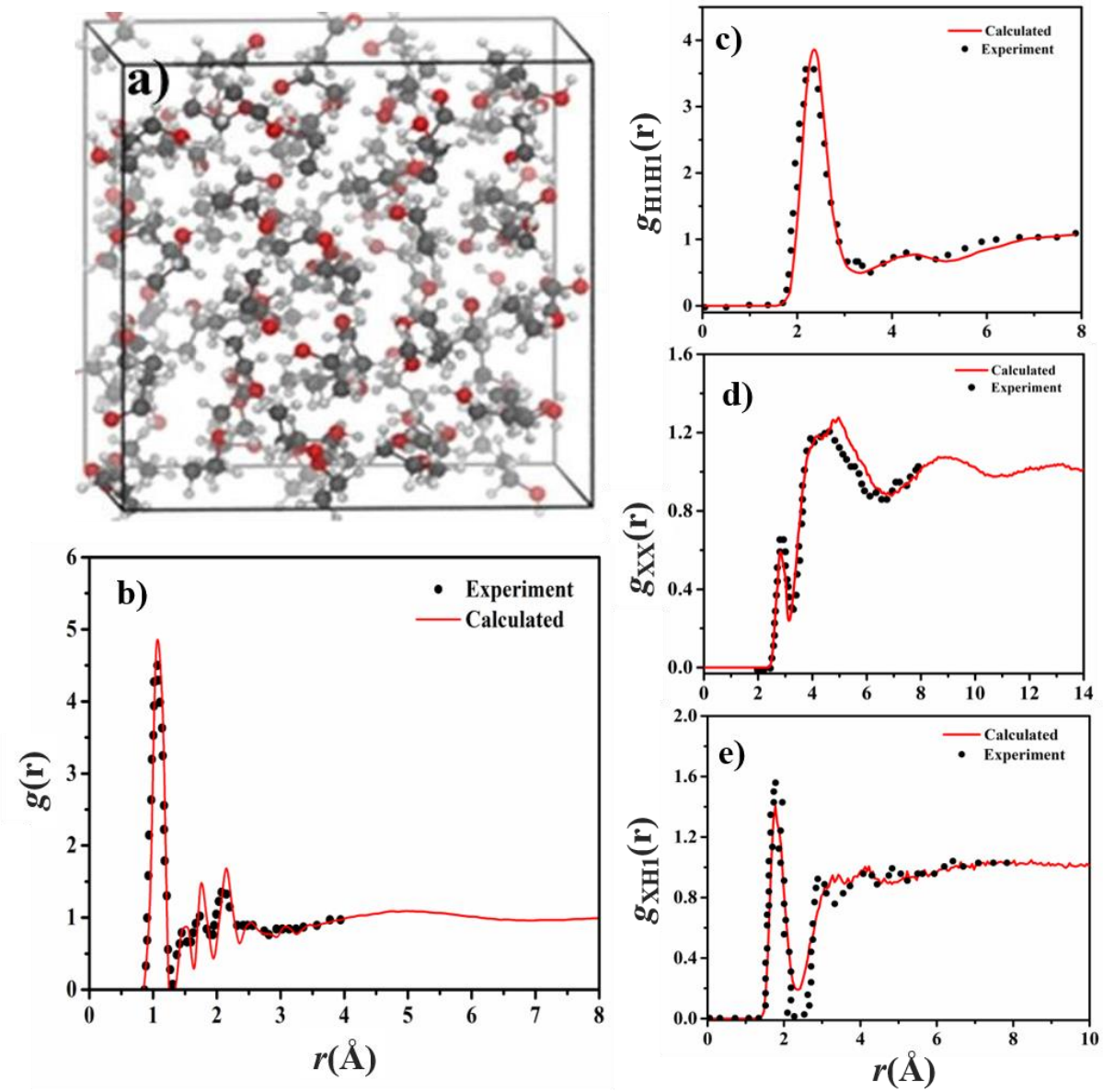

Figure S2: a) Snapshot of post-equilibration simulation cell for ethanol. Comparison of radial distribution function (rdf) b) *g*(r), and prdfs of ethanol in liquid state calculated using CPMD simulation with BLYP functional and neutron scattering data.[2,3] c) $\boldsymbol{g}_{H1H1}$ d) $\boldsymbol{g}_{XX}$ e) $\boldsymbol{g}_{XH1}$. Here X and H1 refers to non-hydrogen atoms (C & O) and hydroxyl protons, respectively.

References

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2 C. J. Benmore and Y. L. Loh, The structure of liquid ethanol: A neutron diffraction and molecular dynamics study, *J. Chem. Phys.*, 2000, **112**, 5877–5883.

3 D. G. Montague, I. P. Gibson and J. C. Dore, Structural studies of liquid alcohols by neutron diffraction, *Mol. Phys.*, 1982, **47**, 1405–1416.