

Supplementary Information for: The Role of Solute Polarity on Methanol-silica Interfacial Solvation: a Molecular Dynamics Study

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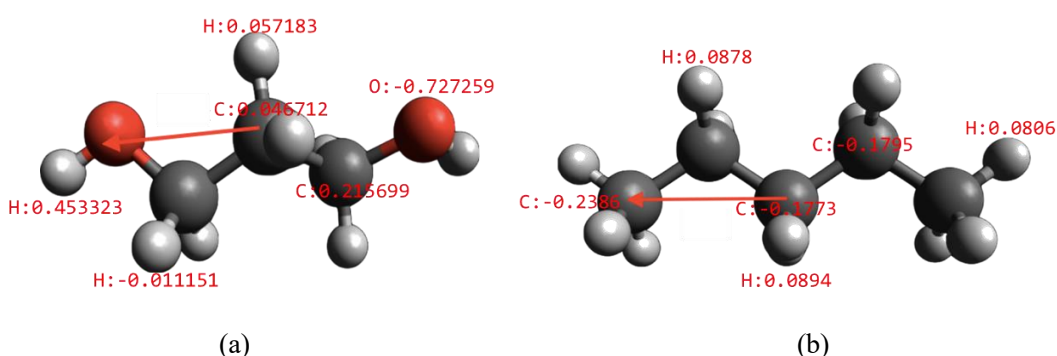


Fig. S1 (a) Configuration of 1,3-propanediol molecule with atomic charges (b) Configuration of n-pentane molecule with atomic charges. Arrows denote the intramolecular vectors that were used for calculating orientational distributions.

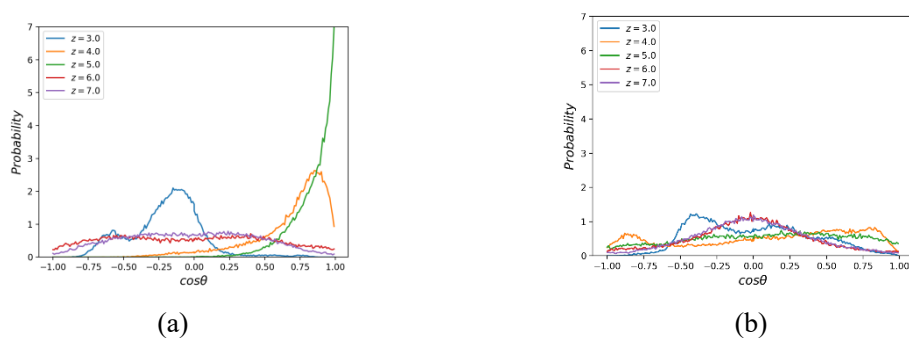


Fig. S2 (a) Orientational distribution profiles of 1,3-propanediol molecule in windows near the silica surface (b) Orientational distribution profiles of n-pentane molecule in windows near the silica surface.

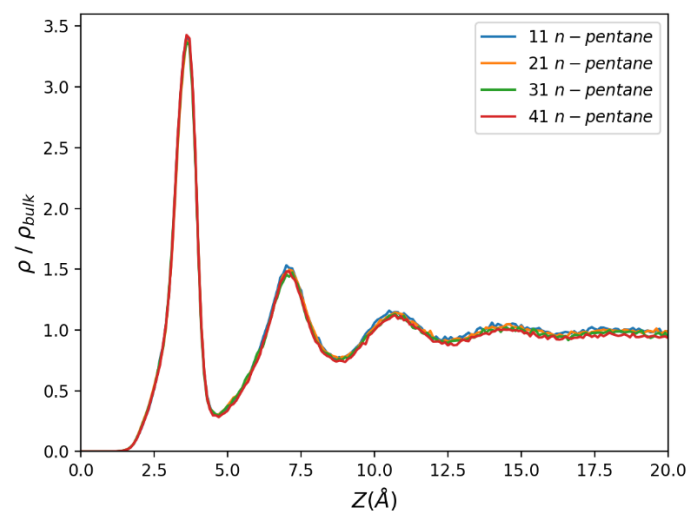


Fig. S3 Methanol carbon density profiles with different number of n-pentane molecules in the solution. All the density values has been scaled by the bulk density.