

Supplementary Information

Effect of Counterions on the Structure and Dynamics of Water near a Negatively Charged Surfactant: A Theoretical Vibrational Sum Frequency Generation Study

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Table S1: Surface area per sodium dodecyl sulfate molecule (SDS) for each system. The experimental value of the surface area has been reported as 47.4 \AA^2 .¹

System	Calculated Surface Area (\AA^2)
No salt	44.83
MgCl ₂	46.01
LiCl	45.98
CsCl	46.86

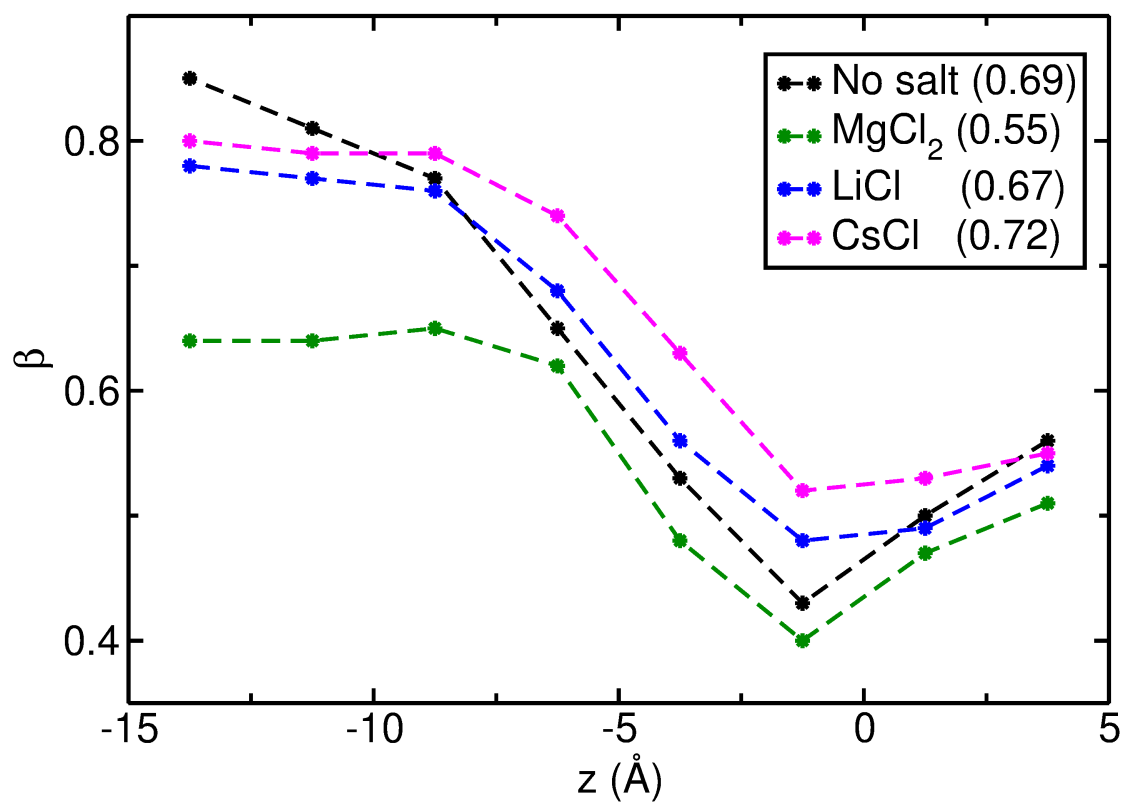


Figure S1: Heterogeneity parameter (β) for water molecules in each layer of width 2.5 Å. The numbers in the x-axis represent the distance from the reference Gibbs dividing surface (labeled as 0 in the x-axis). The values of β when the correlation functions are averaged over all water molecules for a given system are also shown in the legend for reference.

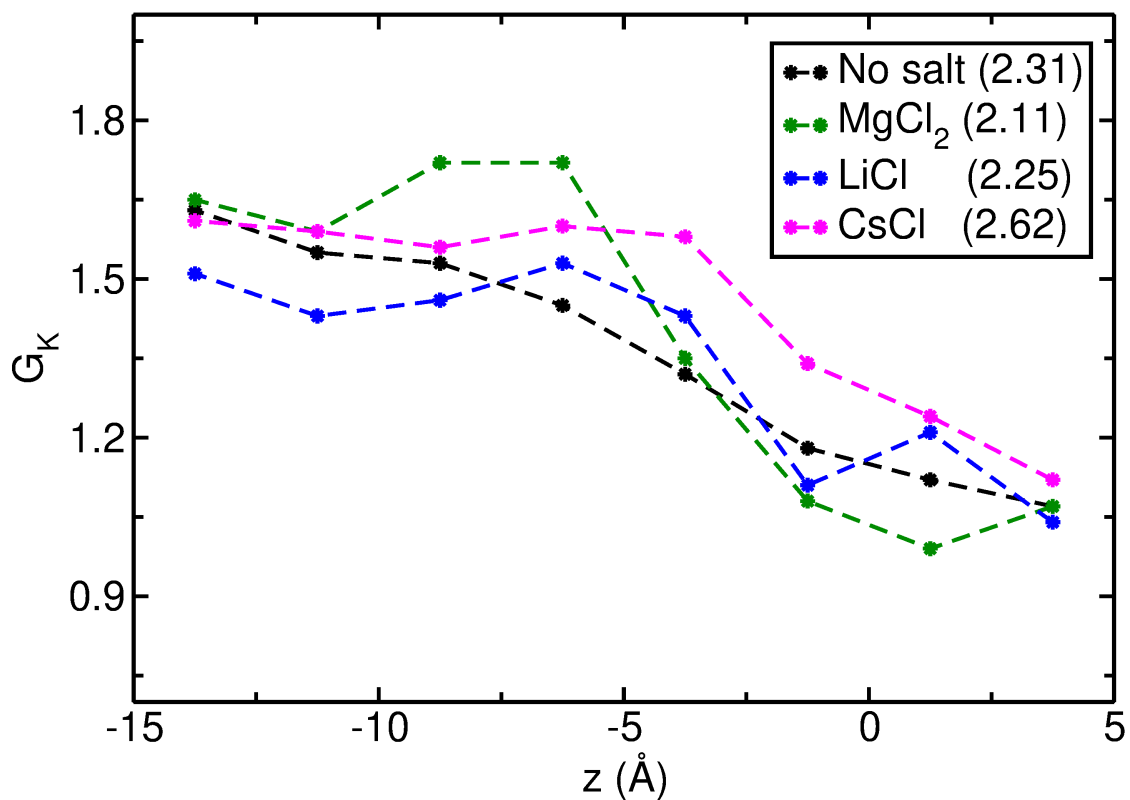


Figure S2: Kirkwood g-factor (G_K) for water molecules in each layer of width 2.5 Å. The numbers in the x-axis represent the distance from the reference Gibbs dividing surface (labeled as 0 on the x-axis). The values of G_K when obtained through averaging over all water molecules for a given system are also shown in the legend for reference.

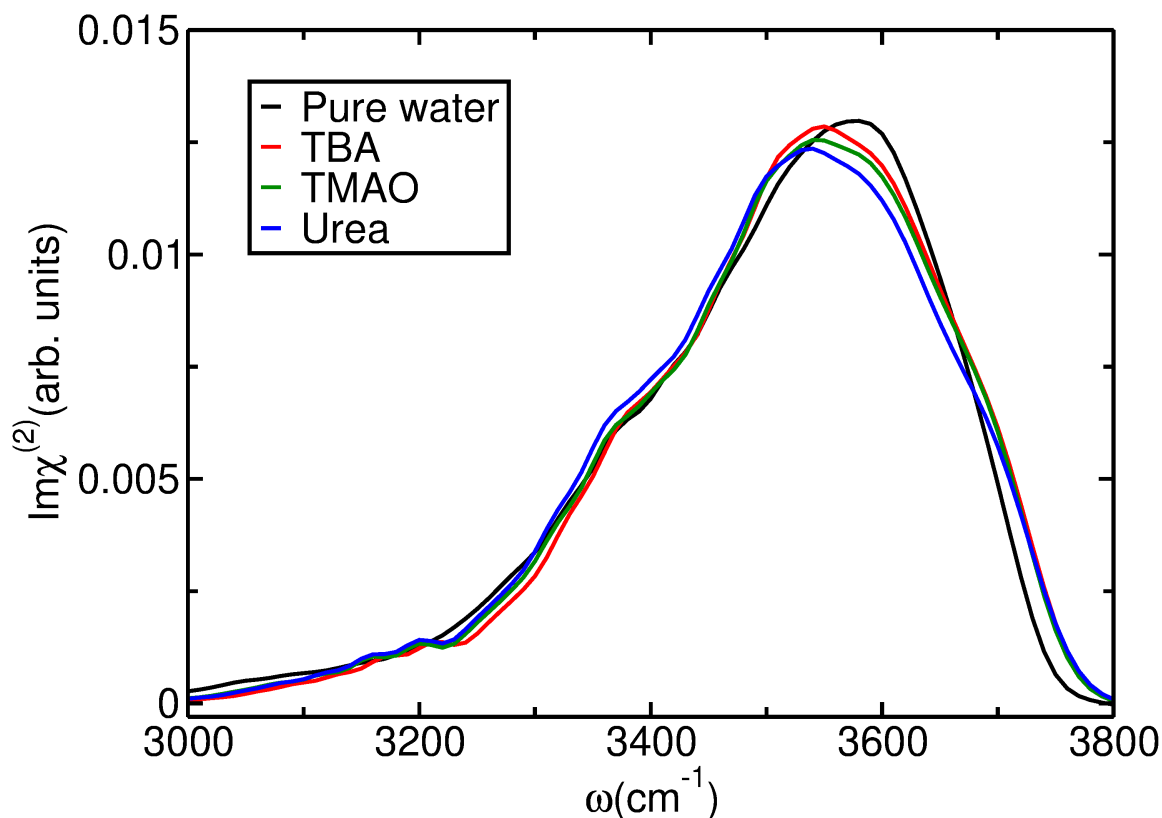


Figure S3: The VSFG spectrum calculated for water-surfactant system with the added salt MgCl_2 . The spectral maps derived for pure water² (black), aqueous solutions of *tert*-butyl alcohol³ (red), trimethylamine-N- oxide⁴ (green), and urea⁴ (blue) are used to calculate the VSFG spectrum.

References

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