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Abstract for an Invited Paper
for the MAR10 Meeting of
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Structure, Self-assembly, Solvation, and Phase Equilibria in Hydrogen-bonding Fluids[1]

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This talk will focus on applications of efficient particle-based simulation methods and accurate force fields to obtain molecular-level insights on structure and solvation in complex chemical systems. These simulations help to reconcile often conflicting views based on macroscopic measurements. In particular, the following applications will be discussed: (i) aggregation of alcohols in dilute solutions, (ii) influence of water saturation on structure and solvation in 1-octanol, and (iii) retention in reversed-phase liquid chromatography.

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