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Enhancement of Hydrophobic Solvation by Hydrophilic Functional Groups: Trehalose and Kojibiose in Water[1] R. KRAMER CAMPEN, ANA VILA VERDE[2], FOM Institute for Atomic and Molecular Physics [AMOLF] — The structure and dynamics of water around biomacromolecules differs significantly from that of water in bulk in ways critical for biological function. The manner in which water structure differs is a function of both chemical and topological heterogeneity. Attempts to disentangle these effects have generally focussed on solvation of large molecules at either particular locations or in an averaged sense. In either case, understanding how chemical and topological heterogeneity combine can be difficult. Here we circumvent this problem by examining, in all atom simulations, water structure around the disaccharides Trehalose and Kojibiose. Taken together water structure around these molecules provides a series of internal control experiments for disentangling topological and chemical effects and allows us to conclude that, in the case of Trehalose, topological effects can lead to slow down of water reorientation by a factor of 2 relative to a chemically equivalent system.

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