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What Can Interfacial Water Molecules Tell Us About Solute Structure? ADAM WILLARD, MIT — The molecular structure of bulk liquid water reflects a molecular tendency to engage in tetrahedrally coordinated hydrogen bonding. At a solute interface waters preferred three-dimensional hydrogen bonding network must conform to a locally anisotropy interfacial environment. Interfacial water molecules adopt configurations that balance water-solute and water-water interactions. Thearrangementsof interfacial water molecules, thereforeencode information about the effective solute-water interactions.This solute-specific information is difficult to extract, however,because interfacial structure also reflects waters collective response to an anisotropic hydrogen bonding environment. Here I present amethodology for characterizing the molecular-level structure of liquid water interface from simulation data. This method can be used toexplore waters static and/or dynamic response to a wide range of chemically and topologically heterogeneous solutes such as proteins.

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