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Hydration Dynamics of Biomolecules from Co-solvents to Crowding

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Biomolecules self-assemble into complex functional structures with high fidelity largely due to interactions between the macromolecules and water. Once folded, the dynamics of water molecules in the vicinity of extended macromolecular interfaces can be altered relative to the bulk, leading to complex, heterogeneous and distance-dependent transport properties near these surfaces. Using a strategy based on transition metal carbonyl vibrational probes covalently conjugated to the protein surface, we have been able to use ultrafast two-dimensional infrared (2D-IR) spectroscopy to probe the dynamics from this most important perspective. In a series of studies, we have found these probes to be primarily sensitive to the orientational dynamics of the hydrating water molecules, and have studied both protein/water and membrane/water interfaces. Several key finding have emerged, including a modest 2-3-fold slowdown of hydration water's reorientational dynamics relative to the bulk, and a dynamical transition that occurs due to collective hydration induced by macromolecular crowding. We will summarize our progress to-date, as well as present our newest results on the effects of ions and the dynamical signatures of preferential solvation.