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NONCOVALENT INTERACTIONS OF HYDRATED DNA AND RNA MAPPED BY 2D-IR SPECTROSCOPY

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Biomolecules couple to their aqueous environment through a variety of noncovalent interactions. Local hydration structures at the surface of DNA and RNA are frequently determined by directed hydrogen bonds with water molecules, complemented by non-specific electrostatic and many-body interactions. I will present recent results from 2D-IR spectroscopy of sugar-phosphate backbone vibrations of native and artificial DNA and RNA, together with theoretical calculations of molecular couplings and molecular dynamics simulations. The results reveal the femtosecond fluctuation dynamics of the water shell, a short-range character of Coulomb interactions, and the strength and fluctuation amplitudes of interfacial electric fields [1,2]. Recent applications of phosphate vibrations [3,4,5] as probes for local hydration patterns and contact ion pair configurations hold strong potential for quantifying folding-induced changes of the ion distribution around DNA and RNA on a multitude of time scales.

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