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Anomalous Vibrational Signatures of Ions and Solvation

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Vibrational spectroscopy has long served as one of the key experimental windows into the inner workings of molecules. Developments in recent decades have continued to expand these techniques toward exotic ions and biologically relevant systems. Such developments have unearthed a wealth of anomalous vibrational signatures, many of which challenge canonical computational approaches to the simulation of vibrational spectra. In this presentation, the vibrational spectra of particularly challenging ionic systems will be explained via new computational simulations and theoretical frameworks. Examples include (a) strongly anharmonic—yet characteristic—vibrations in protonated, misfolded DNA base pairs, as well as (b) signatures of electronic motion in the vibrational spectra of water oxidation intermediates. Both cases demonstrate strong coupling of a unique electronic structure to quantum mechanical molecular motion. New methodology to enable the interface of these two requirements will also be briefly discussed.