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Abstract for an Invited Paper  
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**Unravelling the structure and dynamics of concentrated aqueous proton defects using simulations incorporating both nuclear and electronic quantum effects.**

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Aqueous proton defects give rise to a range of structural and dynamical environments that vary with concentration. These manifest as a continuum of infra-red and Raman spectral features. However, assigning spectral features to the underlying structures formed in solution and their dynamical interconversion remains an area of significant debate. In this talk I will show how path integral ab initio molecular dynamics simulations, where the electronic structure is computed on the fly using density functional theory and nuclear quantum effects are included explicitly via path integral molecular dynamics, can be used to accurately describe the spectroscopic properties of liquid water and systems with aqueous proton defects. These simulations, which have previously been computationally intractable for such large condensed phase systems, are now possible due to our recent path integral developments. I will discuss how these simulations can be used to elucidate the linear and multidimensional spectroscopy of concentrated acid systems and the dynamics and structures that give rise to them.