Theoretical Spectroscopy: From Proton Transfer to Hydrophobic Hydration

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Water is a fascinating liquid with naturally abundant extended hydrogen bond network. The presence of external solutes perturbs the length scale and the time scale of the hydrogen bond network that makes the systems even more interesting. As the vibrational frequencies of water are highly sensitive to the local microscopic solvation structure, ultrafast IR spectroscopy is an appealing method for investigating these systems. Despite its extensive use, meaningful interpretation of IR spectroscopy faces the formidable challenge of establishing the connection among the experimental spectra to the molecular structures in the bulk phase. On the contrary, the microscopic resolution of computer simulation assisted spectroscopy modelling enables us to study these systems at the molecular level. We use several theoretical spectroscopy methodologies to decipher the experimental data in a reasonably quantitative way. In this talk, I shall briefly discuss the theoretical spectroscopy method to investigate the isotope dilute aqueous solutions. Afterward, I shall be extending the discussion to show the application of this technique in the case of two important systems: (1) excess proton in water and (2) water in the presence of the small hydrophobic solute. A detailed structure-spectrum analysis will be demonstrated to exhibit the powerful efficiency of theoretical spectroscopy for understanding the microscopic features in a rather quantitative way.

Reference:

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