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Title: Vibrational Strong Coupling of Water

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Abstract:

Water as a universal solvent is known to control reaction pathways of many common reactions. The key to understanding this chemical behavior of water lies in its molecular structure, specifically in the possibilities of multi-point H-bonding in bulk water. The high lability of the H-bonded network makes water as one of the complex systems for spectroscopic characterization. Here, vibrational strong coupling (VSC) is used as a new spectroscopic tool to understand the density, oscillator strength, and possibly the details of the hydrogen bonding in water molecules. VSC results in the formation of hybrid light-matter states, a.k.a vibro-polaritonic states, which provides unique insight into understanding the associated H-bonding behavior. The central focus of the thesis is on how inhomogeneously broad O-H stretching band of water can be affected by VSC. We performed VSC of H 2 O and D 2 O by coupling their O-H/O-D stretching bands to an infrared photon of a Fabry-Perot cavity. We also studied the effect of cavity mirror thickness (cavity dissipation) under ultra-strong coupling conditions. All the experimental data, including the dispersion plots, are fitted with TMM simulations, and the corresponding Hopfield coefficients are extracted. The mixing ratio is 1: 1 at the ON resonance condition for O-H stretching bands. However, our angle-dependent studies observe a shallow dispersion behavior and slow change in the mixing ratios. The above results shine some light on understanding the hybrid character of vibro-polaritonic states formed in water molecules.

molecules

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