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X-ray Studies of Hydrogen Bonding of Water; the Liquid Phase and on Surfaces

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Many of the unique properties of water have been interpreted as due either to a continuum of distorted mainly near-tetrahedral hydrogen bond or a mixture of differently coordinated distinct species. Here we report high-resolution measurements of small-angle x-ray scattering and x-ray emission spectroscopy from liquid water at ambient conditions. A model based on 10-20 Å diameter size density fluctuations with energetically strongly tetrahedral bonded water in a soup of disordered entropic structures with large hydrogen bond distortion can explain the spectroscopy and scattering data. I will also address fundamental questions regarding geometric structure, electronic structure, nature of surface chemical and hydrogen bonding and reactivity of water on surfaces. The connection between studies performed at both UHV and ambient conditions will be emphasized. Several examples of different water adsorption system will be illustrated such as Pt(111), Ru(001), Cu(110), Cu(111), TiO₂, Fe₂O₃ and MgO.