Hydrogen bond networks in water

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Extended networks of hydrogen bonds characterize liquid and solid forms of water, but it is often difficult to extract from experiment detailed microscopic information on the structural changes that underlie mutated thermodynamic conditions. In this context, computer simulations provide invaluable insight, as they allow us to construct molecular models with average properties that can be directly compared to experiment. In this talk the following topics will be emphasized: (i) how specific molecular interactions affect the structure, (ii) the signatures of quantized nuclear motion, (iii) the effects of network changes on the electronic structure. Current limitations of *ab-initio* modeling will be stressed throughout.