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Dielectric Spectroscopy of Water: From Collective Relaxation to Quantum Effects[1]

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Despite many decades of studies, understanding and modelling dynamics of bulk and confined water still remains a great challenge. We present an overview of dielectric spectroscopy studies of water in a broad temperature range, from ambient T down to Tg˜136K. We demonstrate [1] that the main dielectric relaxation process of water at ambient T is a collective relaxation similar to the so-called Debye process known for many mono-alcohols. The structural relaxation of water actually appears at much higher frequency. Combining neutron scattering and dielectric relaxation spectroscopy we show that quantum fluctuations play a critical role in dynamics of deeply supercooled bulk water [2,3]. Water is the lightest molecule existing in a liquid state at ambient conditions. This strongly increases probability of quantum effects and we suggest that quantum tunneling might be the origin of water's unusual low temperature behavior [2,3]. The discovered anomalously large isotope effect in Tg of water [2] is consistent with the quantum tunneling dominating structural relaxation of water at these temperatures. Based on these results we suggest that the apparent Fragile-to-Strong Crossover in water dynamics can be ascribed to crossover from classical over-barrier relaxation to tunneling [3]. At the end we emphasize that neglecting quantum effects in simulations might be the main reason of their failure in the case of water.

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[1]NSF DMR