Dielectric Spectroscopy of Water: From Collective Relaxation to Quantum Effects

ALEXEI SOKOLOV, University of Tennessee and Oak Ridge National Laboratory

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.


1NSF DMR