Researchers conduct first quantitative study of liquid water combining dielectric relaxation and neutron scattering

October 25 2016, by Bob Yirka

Credit: George Hodan/public domain

(Phys.org)—A team of researchers from several institutions in Spain and France has conducted the first quantitative study of liquid water

combining dielectric relaxation and neutron scattering, and in so doing, has revealed three processes at frequencies below 3 THz. In their paper published in the journal *Physical Review Letters*, the team describes how they combined two water analysis techniques to gain a better understanding of the mechanisms that control the dielectric constant.

As many researchers have found, water is far more complex than it appears at first glance—it is made of H_2O molecules that are connected via hydrogen bonds that form and break over time as the water is subjected to other external objects, processes and forces. In this new effort, the researchers note that many spectroscopic techniques have been used to study the underlying mechanisms involved in water action, revealing such things as dielectric relaxation (amount of time it takes for electrons to return to an equilibrium state after being excited), amounts of infrared absorption, Ramen and neutron scattering and the absorption of x-rays. Researchers have combined techniques that involved neutron scattering and dielectric relaxation in the past, but they involved only qualitative observations. In this new effort, the researchers have done so quantitatively.

By conducting a variety of experiments on dielectric relaxation, the team found that they were able to depict the relaxation of dipoles in liquid water—the part of the process that is responsible for determining its overall dielectric response. And by conducting other experiments involving neutron scattering, they were able to better understand the connection between molecular dynamics and dielectric behavior. By looking at the results together, the researchers were able to confirm the existence of two processes related to the way molecules are diffused and the associations that are involved when hydrogen bonds are forged and broken. Also, they note their work revealed three processes at frequencies below 3 THz—local, relaxational and vibrational and diffusive. The team notes also that their findings are similar in some respects to experimental observations of molecular actions in polymers.

More information: A. Arbe et al. Dielectric Susceptibility of Liquid Water: Microscopic Insights from Coherent and Incoherent Neutron Scattering, *Physical Review Letters* (2016). DOI: 10.1103/PhysRevLett.117.185501

ABSTRACT

The analysis of neutron scattering results on H dynamics (H2O) and the dynamic structure factor (D2O) around the intermolecular peak and at intermediate length scales in terms of the susceptibilities reveals three processes (diffusive, local relaxational and vibrational) at frequencies below 3 THz, to which the contributions commonly invoked in dielectric studies can be directly mapped. We achieve a unified description of the results from both techniques, clarifying the nature of the molecular motions involved in the dielectric spectra and their impact on the structural relaxation.