

## Sub-picosecond dynamics of water studied by neutron scattering and molecular dynamics simulations

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**Abstract:**

The dynamics and the structure of materials on the atomic scale can be measured by x-ray and neutron scattering. The structure on the Ångström scale is by now well established, as is the diffusive dynamics on time scales above roughly one picosecond as measured for example by the neutron time-of-flight spectrometer TOFTOF at MLZ. However, recent measurements of the dynamics in the femtosecond to picosecond range on the resonant neutron spin-echo spectrometer RESEDA at MLZ showed some surprising features at these very short time scales. These two measurements will be compared in this contribution to see if their results are compatible with each other to exclude any instrumental effects. The dynamics will also be modeled by a molecular dynamics simulation and the calculated scattering function will be compared to the data. The results can be used to improve the water model used in the simulation and in turn to identify how different motions leave their mark in the data.

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