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Unraveling the coherent dynamic structure factor of liquid water measured by neutron spectroscopy with polarization analysis: a molecular dynamics simulation study

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This work is focused on atomistic molecular dynamics (MD) simulations of water carried out at 300 K. The main goal was to better understand the experimental results of the coherent dynamic structure factor S(Q,ν) of D_2O that were obtained by means of neutron scattering with polarization analysis and previously reported by us [1]. First, the simulations were directly validated by direct comparison of both imaginary part of the susceptibility χ"(Q,ν) and S(Q) –calculated from the simulations– with the corresponding experimental results. After that, we have considered the time domain S(Q,t) as well as its self- and distinct-contributions. We have also calculated S(Q,t) corresponding to a H_2O sample. The main results obtained are: (i) The Q-independent relaxation process identified in S(Q,ν) in the mesoscopic range (Q^0-mode) is the responsible of the restructuring of the hydrogen bond (HB) network at times shorter than that corresponding to the molecular diffusion; (ii) the vibrational contribution identified at high frequency in S(Q,ν) corresponds to a hydrodynamic-like mode propagating in a medium with fixed HB bonding pattern; (iii) in the crossover range from mesoscopic to intermolecular scales, diffusion also progressively contributes to the decay of density fluctuations; (iv) MD-simulations suggest that it would be basically impossible to measure S(Q,ν) of H_2O in the mesoscopic range with the current neutron scattering capabilities.

References

[1] A. Arbe, G. Nilsen, J. R. Stewart, F. Alvarez, V. García-Sakai and J. Colmenero, Physical Review Research **2**, 022015 (2020).

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