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Fitting Molecular Dynamics water model parameters to neutron scattering experiments

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Molecular dynamics (MD) simulations are a valuable tool to investigate structure and dynamics of samples on the same time- and lengthscales as probed by neutron scattering experiments. Force fields for water and bigger molecules have been established, but can they reproduce neutron scattering experiments?

Different parameter fits for MD water models were made and compared to neutron scattering experiments of water.
For the MD simulation the program LAMMPS was used, subsequently SASSENA to calculate the neutron scattering curves –wide-angle diffraction for structure determination and the incoherent intermediate scattering function to probe the dynamic behaviour of the sample, respectively.

The calculated curves show a satisfactory qualitative agreement with neutron scattering data from the literature but also great potential for improvement of the parameters used in the tested force fields. The ultimate goal is to transfer the findings presented here on the example of water to the investigation of hydrogen storage materials.

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