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Refining Molecular Dynamics Simulations to Neutron and X-ray Diffraction and Spectroscopy Data

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The structure and dynamics of materials can be studied on the atomic level with neutron and X-ray scattering experiments as well as molecular dynamics (MD) simulations. We connect experimental data with MD simulations to further enhance the simulations and obtain forcefields that are able to reproduce the measured structure and dynamics.

On the example of water, we establish a workflow of running MD simulations in the program LAMMPS, calculating X-ray and neutron scattering data with the program Sassena, and comparing the diffractograms and incoherent intermediate scattering functions to already published experimental data.

The agreement between computed scattering curves and experimental data was optimized and the parameter distributions characterized with a Bayesian approach to obtain a set of parameters that can simultaneously reproduce the real nanoscopic structure and dynamics of water probed by the neutron and X-ray scattering experiments.

This scheme is highly adaptable to different MD simulations and will be adapted to crystalline materials in the future, in particular hydrogen storage materials.

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