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Improving a Molecular Dynamics Water Model by Comparing it to Neutron and X-ray Scattering Data

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The structure and dynamics of water in all its possible states has been investigated and simulated extensively in the past with multiple methods. Experiments have been conducted on a molecular level with neutron and X-ray scattering techniques; molecular dynamics (MD) computer simulations are also widely used for the study of water and solvated molecules. In our work we connect experimental data of water with MD simulations to further enhance the simulations and obtain forcefields that reproduce the data better.

MD simulations were run of two well established water models, TIP3P and TIP4P/2005. X-ray and neutron scattering data were calculated from it with the program Sassena, and these structure and dynamics curves were compared to published experimental data of water at ambient conditions.

The agreement between scattering curves and experimental data was improved by a multiple parameter fitting Monte Carlo scheme to obtain a set of parameters that reproduces the real nanoscopic structure and dynamics of water as probed by neutron and X-ray scattering experiments better. This scheme is highly adaptable to other substances.

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