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Evaluation and comparison of scattering data driven molecular dynamics simulations of water models

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Molecular dynamics simulations are an important tool in evaluating scattering data. They have a high potential, which is even further increasing with the ever increasing computation power and isn't yet fully exploited. For some systems, reliable simulations are already available that are compatible with measured data. For other systems, however, the agreement between simulation and experiment is not satisfactory yet. In this work, we compare measured and simulated data as well as mathematical models on the example of different liquid water models in order to later optimize the underlying forcefields in the simulation as well as the hitherto used mathematical models of the evaluation.
The water molecular dynamics simulations were performed with the program LAMMPS and the program SASSENA was used to calculate the corresponding scattering signals. The outcomes were compared to already existing experimental data and changes in the underlying force fields where evaluated in terms of their impact on the behaviour of the simulation. The long-term aim is to create a new evaluation tool, adapting the parameters of molecular dynamics simulations to match the scattering experiments.

Primary authors: REICH, Veronika (German Engineering Materials Science Center (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Hereon); BUSCH, Sebastian (German Engineering Materials Science Center (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Hereon); MÜLLER, Martin (Helmholtz-Zentrum Geesthacht)

Presenter: REICH, Veronika (German Engineering Materials Science Center (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Hereon)

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