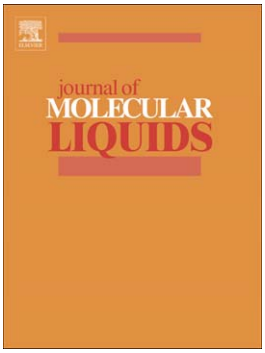

Comparison of 9 classical interaction potentials of liquid water: Simultaneous Reverse Monte Carlo modeling of X-ray and neutron diffraction results and partial radial distribution functions from computer simulations

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Comparison of 9 classical interaction potentials of liquid water: simultaneous Reverse Monte Carlo modeling of X-ray and neutron diffraction results and partial radial distribution functions from computer simulations

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Abstract

Following preliminary studies on a few interaction potentials and at most two sets of diffraction data of liquid water (L. Pusztai et al., J. Chem. Phys. 129 (2008) 184103; Z. Steinczinger et al., Cond. Matt. Phys. 16 (2013) 43604), here an extended collection of water potentials is considered, along with four experimental total scattering structure factors. The basis of comparing interatomic potentials was the compatibility with results of neutron and X-ray diffraction experiments on pure water, using the scheme applied by Pusztai et al. (2008). The scheme combines experimental total scattering structure factors (TSSF) and partial radial distribution functions (PRDF) from molecular dynamics simulations in a single structural model. Goodness-of-fit values to the O-O, O-H and H-H simulated PRDF-s and to the experimental neutron and X-ray TSSF provided a measure that can characterize the level of consistency between interaction potentials and diffraction experiments. As an addition to classical water potentials, PRDF-s from one 'ab initio' molecular dynamics simulation have also been investigated. Out of the sets of partial RDF-s investigated here, the ones corresponding to the BK3 polarizable, and—somewhat surprisingly—to the simple 3-site TIP3P potentials have proven to be the most consistent with various combinations of diffraction results taken for the present study.

Keywords: liquid water; inter-atomic potentials; X-ray diffraction; neutron diffraction; partial radial distribution functions; Reverse Monte Carlo modeling

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