Effective Pair Potentials and Structure of Water

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Classical Monte Carlo calculations have been performed in order to investigate the ability of the TIP4P, SPC, and SPCE water models to reproduce the structural features of liquid water. The simulations were carried out in the NPT ensemble at 4 thermodynamic conditions. The results are compared with recent neutron diffraction data. Essentially, the three models capture equally well the thermodynamic and structural features of water. Although they were parametrized to reproduce the water properties at ambient conditions, the agreement with the experimental pair correlation functions was even better at supercritical conditions. This is because the effective pair potentials have some difficulty to reproduce cooperative interactions, like hydrogen bonds. These interactions are less effective at supercritical conditions, where the liquid behaves roughly like a gas

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