

MOLECULAR DYNAMICS SIMULATION OF LIQUID WATER: PRESSURE EFFECT ON MOLECULAR DIFFUSION

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Many Molecular Dynamics simulations of liquid water have explored the temperature and pressure or density dependence of the translational diffusion coefficient and of the rotational diffusion via the computation of reorientational correlation times of molecular vectors.

By contrast, much less works have considered the direct calculation of rotational diffusion coefficients. An extensive study have been devoted to the *TIP4P-2005* model [1]. For the popular *SPC/E* model [2], values of the principal components of the rotational diffusion tensor $D_{\text{rot,xx}}$, $D_{\text{rot,yy}}$, $D_{\text{rot,zz}}$, of liquid water at 25°C obtained by different groups differ significantly [3,4]. In this talk, I will first discuss results of a systematic study of the translational and rotational diffusion of the *SPC/E* water model at moderate pressure (up to 3000 bar at 300-700 K and up to 6000 bar at 277K) [5,6].

In a second part, I will focus on water at very high pressure. At 400K up to 3 GPa, experiments on liquid water as well as simulations with the *TIP4P-2005* model [7] have shown the existence of thermodynamic states with quenching translation but easy rotation remaining insensitive to pressure. NMR experiments [8,9] have also obtained rotational diffusion coefficients nearly insensitive to pressure up to 1 GPa in the temperature range 268-363 K when infrared measurements [10] predict a maximum around 0.5 GPa at 298 K and 363 K. To investigate such an issue by Molecular Dynamics simulations, we have chosen the polarizable BK3 model [11]. This model has been found to be quite promising in predicting structural, thermodynamic and dynamical properties of water in a relatively large range of thermodynamic states [11,12]. In this talk, I will show our results about the structural and dynamical (up to pressure larger than the experimental crystallization pressure) of water at 298, 400 and 550 K and make a comparison with the experimental results at 400 K [7].

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