Friction contribution to water-bond breakage kinetics

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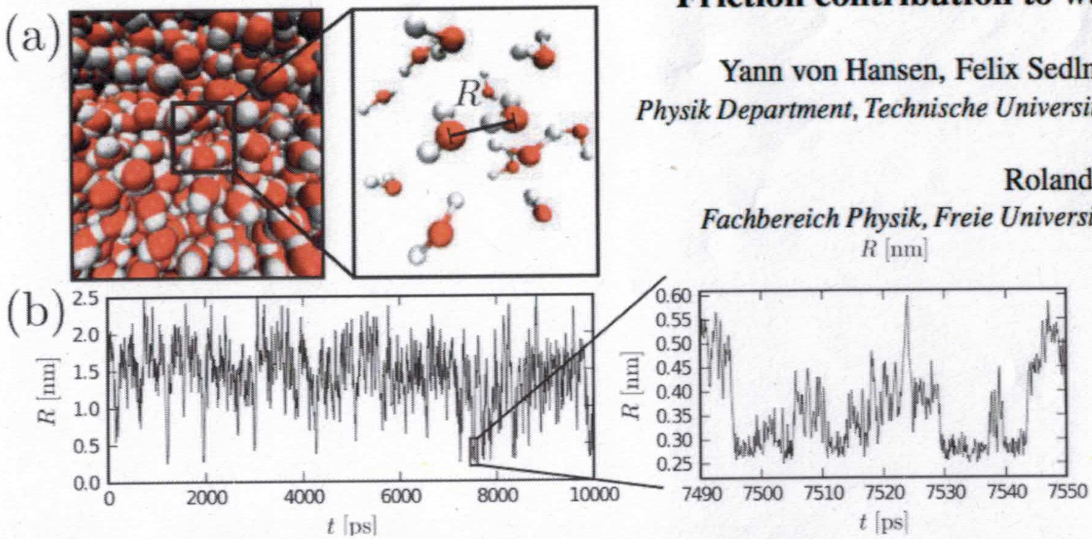

FIG. 1. (Color online) (a) Simulation snapshot visualized using VMD [15]: the coordinate R in the enlarged section is defined as the radial separation between the oxygen atoms. (b) Typical time series of R, the magnification reveals fluctuations on the subpicosecond scale. A simulation *movie* is provided as supplementary material [16].

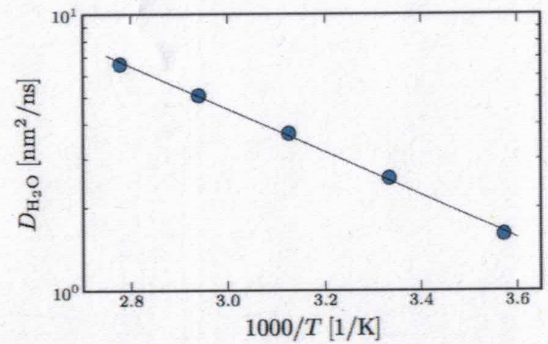

FIG. 7. (Color online) Arrhenius plot of the temperature dependence of the SPC/E diffusion coefficient: *Symbols* denote results obtained through fits (see text) to the MSD data shown in Fig. 6; the *line* shows that within the studied range of temperatures, this dependence is well approximated by $D_{H_2O}(T) \approx 956 \exp(-1783.6\,\mathrm{K}/T)\ \mathrm{nm}^2/\mathrm{ns}$.

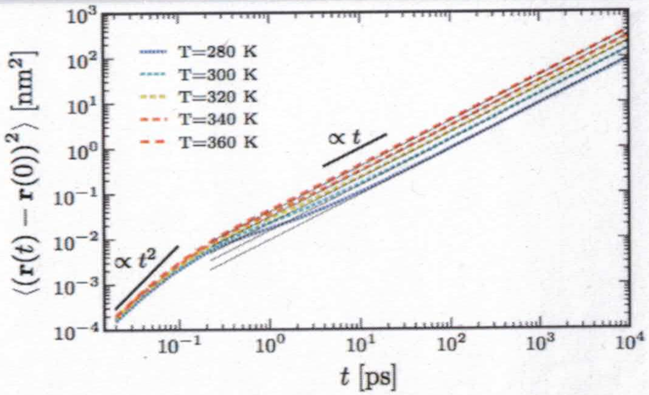

FIG. 6. (Color online) Single SPC/E water molecule MSDs for various temperatures (*dashed color lines*) and best linear fits to the data (*solid black lines*).

TABLE I. Temperature dependence of the diffusion coefficient D_{H_2O} of a single water molecule in bulk water. Simulation results for the SPC/E water model obtained by evaluation of the long-time MSD (cf. Appendix A) are compared to results from previous simulation studies and to experimental findings (both with references).

	D_{H_2O} [nm²/ns]	
T [K]	Simulations (SPC/E)	Experiments
278	–	1.313 [34]
280	1.60 ± 0.02	1.44 [35]
298	2.75 [36], 2.70 [37]	2.22 – 2.61 [34,35,38]
300	2.55 ± 0.05	–
318	–	3.575 [34]
320	3.70 ± 0.05	–
340	5.08 ± 0.05	–
360	6.60 ± 0.05	–