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Supplementary Information for

Conservation of the Stokes-Einstein Relation in Supercooled Water

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1. Simulation details for the Jagla model

The initial configuration for the Jagla fluid model[1-3] consists of 1728 molecules with a constant box size determined under a constant pressure $P = 153.33$ bar at each temperature. Although the reduced unit is usually adopted when using the Jagla fluid model, we use the SI unit instead by assigning the unit of hardcore diameter $d = 0.3$ nm, that of potential $U_0 = 100k_\mathrm{B}$, and that of pressure $P_0 = U_0 / d^3$. All our molecular dynamics (MD) simulations were performed with the GROMACS MD simulation package[4, 5] and the periodic boundary conditions were applied in all three directions of the Cartesian space. The van der Waals interactions were calculated directly with a truncated spherical cutoff of 1.0 nm. Twenty-four temperatures simulated with the Jagla model are in the range of 30–140 K. The system temperature was kept a constant by the Nosé-Hoover thermostat[6, 7] and the pressure was controlled by the Parrinello-Rahman barostat.[8, 9] The simulation time step is 1 fs and the total simulated time for each case ranges from 0.1 to 10 ns depending on the temperature. The *k* values within 2.5–14.5 nm^{-1} with an interval of 1 nm^{-1} for the Jagla fluid model are adopted to investigate the *k* dependences of $D : \tau^{-1}$ and $D : T/\tau$. The viscosity $\eta = A\rho / Vq^2$ of Jagla is evaluated by *A/Vl* because the box size *l* is different at different temperatures.

2. Supplementary Figures

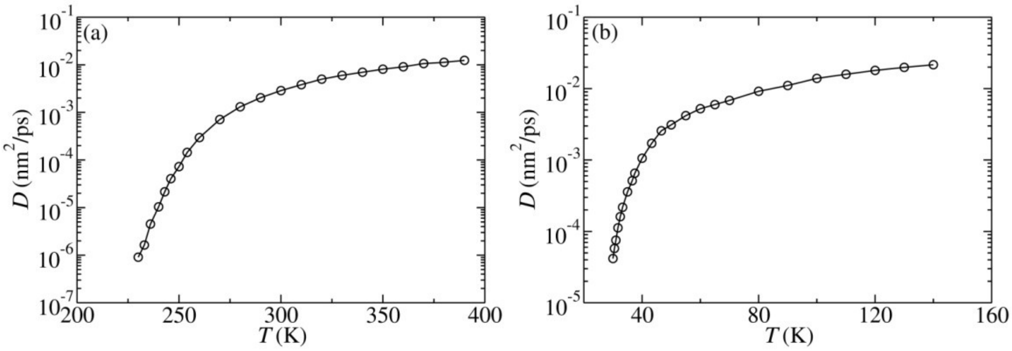

Fig. S1 The diffusion constant *D* as a function of temperature *T* within 240-390 K for TIP5P (a) and within 30-140 K for Jagla (b).

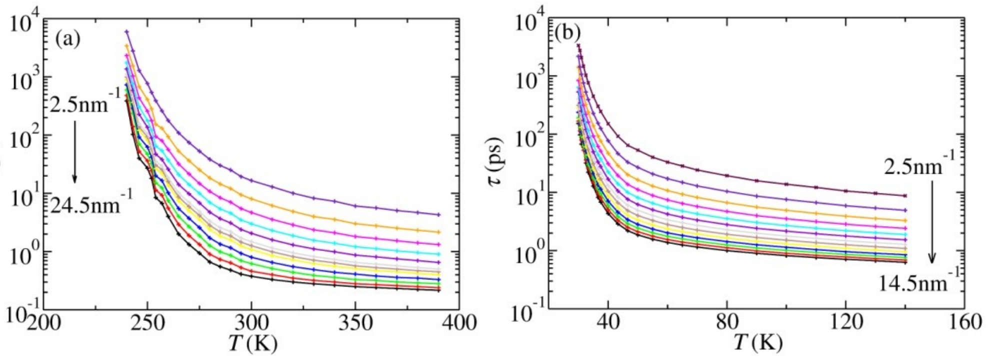

Fig. S2 The structural relaxation time τ for various *k* values as a function of temperature *T* for TIP5P (a) and for Jagla (b). The interval between two adjacent *k* values is 2 nm^{-1} for TIP5P and 1nm^{-1} for Jagla.

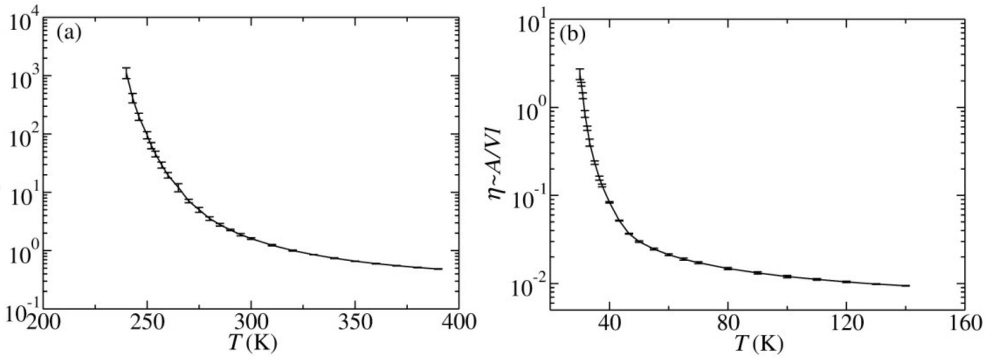

Fig. S3 The viscosity η as a function of temperature *T* for TIP5P (a) and Jagla (b).

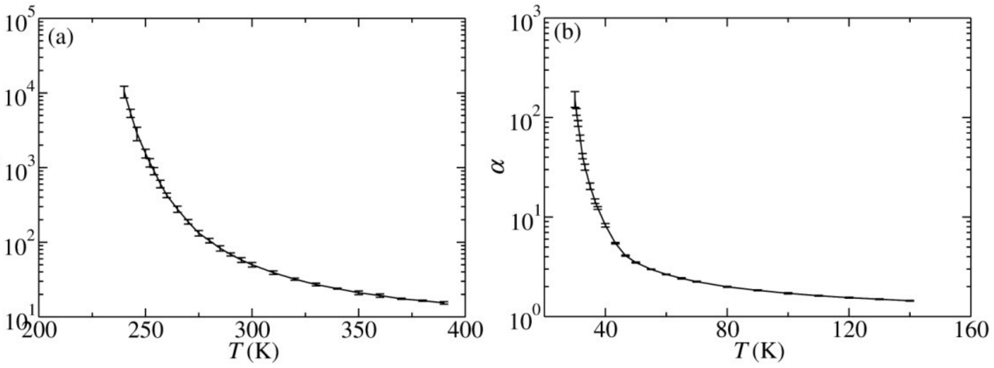

Fig. S4 The frictional coefficient α as a function of temperature *T* for TIP5P (a) and Jagla (b).

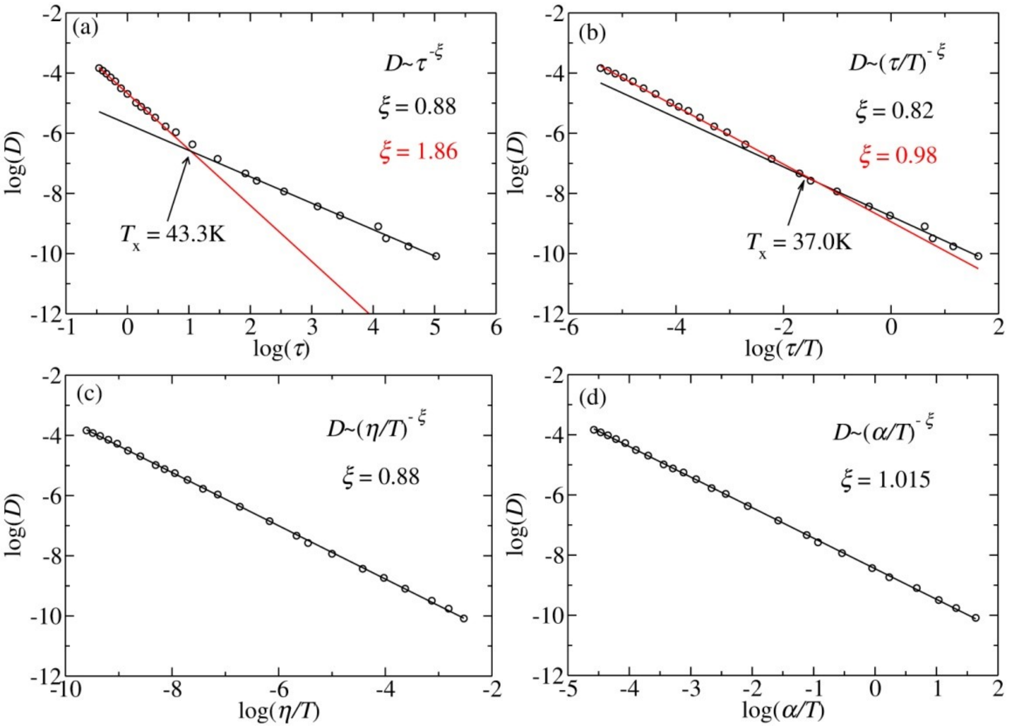

Fig. S5 Verification of the validities of the original SE relation $D : \tau^{-1}$ (a) and its three variants $D : T/\tau$ (b), $D : T/\eta$ (c), and $D : T/\alpha$ (d) for the Jagla fluid model. τ is calculated with the first maximum of static structure factor *k* = 12.5 nm^{-1}. The calculated data are represented by circles and fitted by $D : \tau^{-\xi_1}$, $D : (\tau/T)^{-\xi_2}$, $D : (\eta/T)^{-\xi_3}$, and $D : (\alpha/T)^{-\xi_4}$, respectively. The fitted exponent ξ is written in the same color as the corresponding solid fitting line.

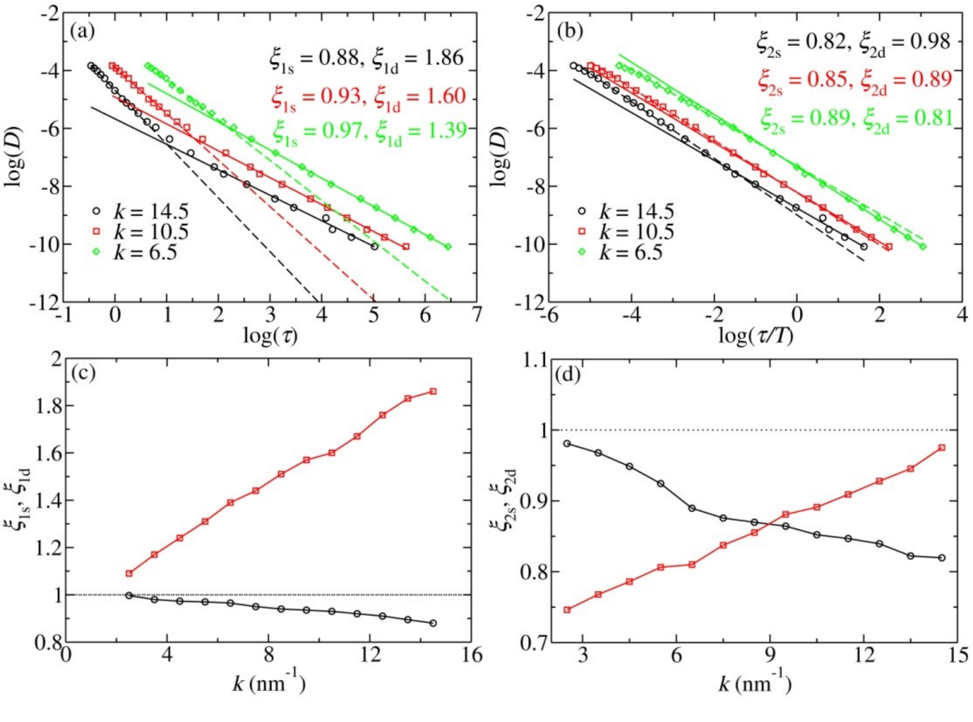

Fig. S6 Fitting of the *k*-dependent exponent ξ_1 by $D : \tau^{-\xi_1}$ (a) and ξ_2 by $D : (\tau/T)^{-\xi_2}$ for Jagla (b), as well as

ξ_1 vs. *k* (c) and ξ_2 vs. *k* (d). In (a) and (b), the calculated data are represented by different symbols and the fitted exponent is written in the same color as the corresponding fitting line; ξ_{1s} ,ξ_{2s} values correspond to solid lines and ξ_{1d} ,ξ_{2d} values correspond to dotted lines. In (c) and (d), black circles represent ξ_{1s} , ξ_{2s} and red squares are ξ_{1d} , ξ_{2d} .

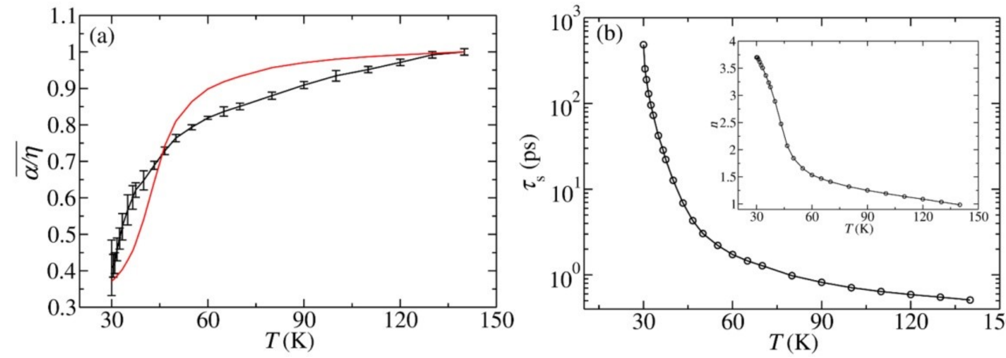

Fig. S7 (a) Effective hydrodynamic radius rescaled by the value at *T* = 140 K $\overline{\alpha/\eta}$ vs. *T* for the Jagla model. The black line is the simulated result and the red one is the fitted result with $\tau_0 = 19$ ps. (b) Residence correlation time τ_s and coordination number *n* (inset) of the first solvation shell vs. *T* for the Jagla fluid model.

References

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