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Breakdown of the Stokes-Einstein Relation in Supercooled Water: The Jump-diffusion Perspective

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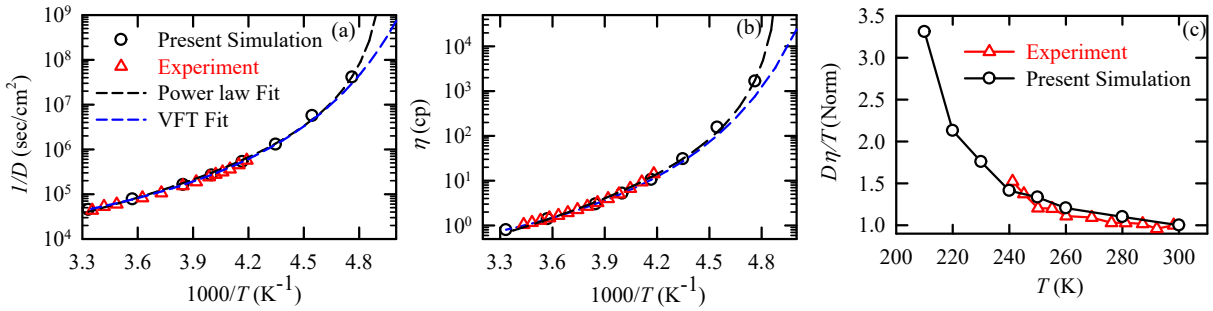

Figure 6. Simulated[1-5] and experimental[6, 7] transport properties. The Arrhenius plot of diffusion coefficient D (a) and viscosity coefficient η (b). (c) The temperature-dependent normalized $D\eta/T$ values where the normalization is done at T=300 K. The red triangles represent the experimental values, while the simulated values are represented by black circles in all three panels. The simulated diffusion and viscosity values are fitted with the power-law (black dashed line) and VFT equation (blue dashed line) in both (a,b). The fitting parameters of the power-law equation for the diffusion coefficient $D = D_0\left[\frac{T-T_s}{T_s}\right]^{-\gamma}$ are: $\gamma = -2.82, D_0 = 1.87 \times 10^{-4}\ cm^2/s,$ and $T_s = 201.64\ K$ and for the viscosity coefficient are: $\eta = \eta_0\left[\frac{T-T_s}{T_s}\right]^{-\gamma}$ are: $\gamma = 2.97, \eta_0 = 0.076\ cp$ and $T_s = 203.11\ K.$ The simulated singular temperature T_s for both the diffusion and viscosity coefficients are approximately 15 K less than T_s obtained by fitting the experimental data. The fitting parameters of the VFT equation for the diffusion coefficient $D = D_0 e^{\left[\frac{-B}{T-T_0}\right]}$ are: $D_0 = 3.69 \times 10^{-4}\ cm^2/s,$ $B = 364.05\ K,$ and $T_0 = 170.9\ K$ and for the viscosity coefficient $\eta = \eta_0 e^{\left[\frac{-B}{T-T_0}\right]}$ the fitting parameters are: $\eta_0 = 4.21 \times 10^{-2}\ cp,\ B = -378.4\ K, and\ T_0 = 171.4\ K$. The fittings is done using the Marquardt-Levenberg algorithm,[8, 9] which is a least square method, to find the fitting parameters. Adopted with permission from Ref. 1. Copyright (2019) American Chemical Society.

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