Self-diffusion and shear viscosity for the TIP4P/Ice water model

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With an ever-increasing interest in water properties, many intermolecular force fields have been proposed to describe the behavior of water. Unfortunately, good models for liquid water usually cannot provide simultaneously an accurate melting point for ice. For this reason, the TIP4P/Ice model was developed at targeting the melting point, and has become the preferred choice for simulating ice at coexistence. Unfortunately, available data for its dynamic properties in the liquid state are scarce. Therefore, we demonstrate a series of simulations aimed at the calculation of transport coefficients for the TIP4P/Ice model over a large range of thermodynamic conditions, ranging from \( T = 245 \) K to \( T = 350 \) K for the temperature and from \( p = 0 \) to \( p = 500 \) MPa for the pressure. We have found that the self-diffusion (shear viscosity) exhibits smaller (increased) values than TIP4P/2005 and experiments. However, rescaling the temperature with respect to the triple point temperature as in a corresponding states plot we find TIP4P/Ice compares very well with TIP4P/2005 and to experiment. Such observations allow us to infer that despite the different original purposes of these two models examined here, one can benefit from a vast number of reports regarding the behavior of transport coefficients for the TIP4P/2005 model and utilize them following the routine described in this paper.

I. INTRODUCTION

Water is one of the most ubiquitous substances on earth. Hence, it is not surprising that great experimental and computational efforts have been devoted to investigate its properties. Such measurements are of great practical significance, but they have showed also that water exhibits a large number of interesting anomalies. These range from the well known negative expansion coefficient below 4° C, to the sharp increase of response functions such as the compressibility upon cooling.

This anomalous behavior also extends to dynamic properties and transport coefficients. Since the end of the 19th century it is known that viscosity of water decreases with the increase of pressure.\(^2\) On the other hand, the diffusion coefficient increases as a function of pressure for both translation and rotation. This unusual behavior of transport properties is related to the breakage of the bond hydrogen network upon compression.\(^3\) Indeed, the conversion between highly ordered tetrahedral water arrangements and disordered domains of high density are in the origin of most of water’s anomalies.\(^4\) This equilibrium, which persists in room temperature water, can be traced back to thermodynamic anomalies of metastable supercooled water.\(^5\) Therefore, the properties of supercooled water have been extensively studied, including the fragile-to-strong transition\(^6\) or the preservation of the Stokes-Einstein relation.\(^7\)

The signature of bulk water’s anomalies is also relevant to the study of interfaces. Particularly, the interface of supercooled liquid water at carbon nanotubes\(^8\) and slit pores\(^9\) exhibits giant slip lengths which increase upon cooling and appear to be related with the failure of low temperature bulk water to follow the Stokes-Einstein relation. Similarly, the understanding of surface premelting\(^10\) and interfacial premelting\(^11\) as well as the related properties of the resulting quasi-liquid layer (QLL), have been the matter of intense debate.\(^12\)\(^13\) For ice premelting, for example, computer simulation studies show enhanced diffusivity of molecules at the water/vapor surface,\(^14\)\(^15\)\(^16\) but intriguingly, some experiments claim a strong increase of viscosity of the premelting films relative to bulk values.\(^17\)\(^18\)

In this regard, in silico studies of water properties provide very useful complementary information to experiments. Of course, such effort largely relies on the availability of intermolecular force fields, which are parameterized in such a way to be able to reflect behavior of water as close as possible. Among the most popular point charge models, one can mention TIP4P\(^19\) and its extended version TIP4P/2005\(^20\), SPC/E\(^21\), TIP5P\(^22\) and many other.\(^23\) Unfortunately, it appears that point charge models which are very good at predicting liquid water properties cannot simultaneously provide an accurate melting point for ice.\(^24\) In order to study the ice and ice-vapor equilibrium properties, which are of great importance for the determination of growth rates and shapes of snowflakes\(^25\) friction and lubrication of surfaces,\(^26\) and many other important phenomena,\(^27\) the TIP4P/Ice model has been developed.\(^28\) This force field exhibits a melting temperature of \( T \approx 270 \) K\(^29\) in ambient conditions which is very close to the experimental result and also reproduces the melting line. Therefore, it is pivotal to have a comprehensive outlook into the bulk water properties of the TIP4P/Ice model for studies of ice and water coexistence. However, it is worth emphasizing that while it is easy to find values of transport coefficients for different water models in a variety of system’s conditions,\(^30\)\(^31\) the literature data for TIP4P/Ice model has hardly been explored, except for a limited number of thermodynamic states.\(^15\)\(^16\)

In view of this, the aim of this paper is to calculate both...
diffusion coefficients and shear viscosities of the TIP4P/Ice model over a large range of thermodynamic conditions, from ambient temperature to the undercooled regime, as well as for a large range of pressures spanning atmospheric conditions to the hundreds of MPa.

II. METHODS

To determine the diffusion coefficient we have used the Einstein relation, which involves the calculation of mean squared displacement (MSD) of individual water molecules:

\[ \langle \Delta r^2(t) \rangle = \langle (\mathbf{r}(t) - \mathbf{r}(0))^2 \rangle \]  

(1)

where \( \mathbf{r}(t) \) is the position of a water molecule at time \( t \), and the triangular brackets denote a thermal average over all time origins and individual particles. For an \( n \)-dimensional system, the MSD is linear with time and the slope is related to the diffusion coefficient \( D \) as \( \langle \Delta r^2(t) \rangle = 2nDt \).

In order to calculate the viscosity, we have employed the Green-Kubo relation that involves the calculation of autocorrelation functions of components of the stress tensor, as:

\[ G_{\alpha\beta} = \frac{V}{k_B T} \langle \sigma_{\alpha\beta}(t) \sigma_{\alpha\beta}(0) \rangle \]  

(2)

where \( V \) is the volume of the system, \( \sigma_{\alpha\beta} \) represents the \( \alpha, \beta = x, y, z \) component of the stress tensor, and \( k_B \) is the Boltzmann constant.

To improve the statistics, we do not restrict to the off-diagonal components of the stress tensor. Daivis and Evans have shown that the diagonal components of the stress tensor are larger by the factor of 2 than the off-diagonal elements, where \( n \) is the dimensionality of the system. Therefore, one can use all of the six components of the stress tensor in the calculation of the shear viscosity, just given the fact that they are scaled by the adequate factor.

Knowing that, the shear viscosity is then calculated as

\[ \eta = \int_0^\infty G_\eta(t) dt \]  

(3)

where \( G_\eta(t) = \frac{1}{6} [G_{xy} + G_{yz} + G_{zx} + \frac{3}{2} (G_{xx} + G_{yy} + G_{zz})] \).

Water was modeled with the use of TIP4P/Ice force field. The number of water molecules was equal to 1280 for all systems studied. We decided to use such system size to avoid system size effects due to insufficient number of molecules and yet being able to perform simulations in a reasonable time which is particularly important in the case of the shear viscosity as these calculations are computationally expensive. Molecular dynamics simulations of bulk water were performed using the LAMMPS package. Trajectories were evolved using the velocity-Verlet algorithm with a 2 fs time step. Bonds and bond angles were constrained by the use of the SHAKE algorithm. Both the temperature and pressure was set using Nose-Hoover chains algorithm with damping factor equal \( \tau = 2 \) ps and the number of chains \( M = 3 \). To remain consistent with the definition of TIP4P/Ice, all dispersion interactions were truncated at 8.5 Å. Long-range coulombic interactions were computed using the particle-particle particle-mesh method. The charge structure factors were evaluated with the fourth-order interpolation scheme and a grid spacing of 1 Å, resulting in 36, 32 and 36 vectors in the \( x, y, z \) directions in reciprocal space, respectively.

The simulation scheme involved two steps. In the first one, simulations for bulk water have been performed for 15 ns in the \( NpT \) ensemble, in order to obtain an accurate average density. Then, the system was accordingly rescaled to the given average density, and further 40 ns runs in \( NVT \) ensemble were performed in which the relevant trajectories for the calculation of transport coefficients have been gathered over the last 30 ns, every 15 ps. For the calculation of shear viscosities, the stress tensor components have been printed every 10 fs. Simultaneous evaluation of the diffusion coefficients and shear viscosity has a particular advantage that one can test their coupling right away using a single molecular dynamics simulation.

Following the above simulation scheme, the translational mean square displacement and shear viscosities were calculated at eight different temperatures spanning from \( T = 245 \) K to \( T = 350 \) K in the pressure range of \( p = 0 - 500 \) MPa. In all the conditions studied, the linear regime of MSD has been established starting from the first saved configuration. However, in the case of the Green-Kubo autocorrelation functions, the numerical integration by trapezoidal rule had to be performed up to the upper limit, denoted as \( \tau_{\alpha} \). Its value has been estimated by the inspection of a characteristic timescale where the autocorrelation function smoothly decays to 0, so that the contributions from the long tail to the integral which are a subject to the random noise are omitted. Averaged Green-Kubo autocorrelation functions evaluated at different temperatures in ambient pressure can be found in Figure 1. One can see that there is a significant change in the characteristic timescale \( \tau_{\alpha} \), which increases upon cooling and reaches up to 200 ps for the lowest temperature (cf. Table I in Appendix A).
III. RESULTS

Isotherms for a given transport coefficient examined in the paper are presented in Figure 2 and also can be found in Table I shown in Appendix A. Let us now compare currently obtained results with the available experimental data. For instance, at ambient pressure with this model we obtain $D = 12.368 \cdot 10^{-10} \text{ (m}^2 \text{s}^{-1})$ and $D = 5.079 \cdot 10^{-10} \text{ (m}^2 \text{s}^{-1})$, compared to experimental values of $D_{\text{exp}} = 23 \cdot 10^{-10} \text{ (m}^2 \text{s}^{-1})$ and $D_{\text{exp}} = 10.9 \cdot 10^{-10} \text{ (m}^2 \text{s}^{-1})$ at $T = 298$ K and $T = 273$ K, respectively. One can see that the values of self-diffusion coefficients are lower than those reported experimentally. On the other hand, the viscosities of liquid water are higher than experimental values which is not surprising due to the Stokes-Einstein relation. Consequently, the aforementioned observations concern all other points studied. It is worth highlighting that the decreased (increased) value of diffusion coefficient (shear viscosity) has already been noted and is consistent with other papers.

In view of this fact, it is well-known that TIP4P/2005 is widely used due to its successful description of liquid water properties, consistent with experimental data. Therefore, it seems reasonable to validate our current simulation results with those obtained for TIP4P/2005 model. Figure 3 shows a comparison between our simulations and those performed by Montero de Hijes et al. Indeed, one can see the same behavior for the transport coefficients that, as stated before, TIP4P/Ice exhibits a decreased (increased) value of diffusion coefficient (shear viscosity) compared to TIP4P/2005 water model in the whole range of points studied. We conjecture that this behavior can be congruent with the shift in the melting point ($T_m$) of ice Ih and triple points ($T_t$) of these models. They were reported to be at $T_{2005,m} \approx 250$ K and $T_{2005,t} = 252.1$ K and $T_{\text{ice,m}} \approx 270$ K and $T_{\text{ice,t}} = 272.2$ K for TIP4P/2005 and TIP4P/Ice, respectively.

Therefore, a naturally arising questions is whether the origin of these differences is just due to the temperature shifts? Or as the models were parametrized to describe different features of water, exhibiting different transport properties is a natural consequence? Here, we aim to answer these questions. In order to do that, we assumed that the simulation points for different models should be presented in reduced units. We mapped the points by the law of corresponding states reduced by the triple points of TIP4P/2005 and TIP4P/Ice models, i.e.
FIG. 4. Relation of self-diffusion coefficient (A, B) and viscosity (C, D) with respect to density or pressure. Filled and open symbols depict currently obtained data for TIP4P/Ice and TIP4P/2005 from Ref. 33 (parts A, C) and Ref. 32 (parts B, D), respectively. Solid lines correspond to the experimental data taken from Ref. 41, Ref. 42, and Ref. 43.

FIG. 5. Relation of \( \frac{D\eta}{T} \) with temperature, normalized at \( T = 350 \) K for all pressures studied.

\[ T^* = T_X / T_{X,f} \] where \( X \) is either TIP4P/2005 or TIP4P/Ice. It has to be emphasized that the ratio \( T_m / T_c \) between melting to critical points of these two models is equal to 0.39 and 0.383 for TIP4P/2005 and TIP4P/Ice, respectively (see Table V of Ref. 32 for critical points estimation). In other words, there is no significant difference whether we choose to rescale the temperature by a triple or critical point (aside from the temperature scale) to preserve the universal features shown later on. The results can be found in Figure 4 and Table II, III in Appendix A.

One can now see an excellent agreement between the two models when expressed in reduced units. Such observation refers both to the self-diffusion and shear viscosities. Although one can easily notice that there is a mismatch in the comparison between current simulation results and the points extracted from Montero de Hijes et al.\textsuperscript{33} (Fig. 4 A, C) the trends are still preserved within the whole range of points studied. Differences in the examined densities result from different approaches between our and their paper. In other words, we wanted to examine the behavior in a wide pressure range for TIP4P/Ice model rather than explicitly match points from other papers. Nevertheless, we can observe nearly perfect agreement between two models and also experimental data. It has to be noted that while for viscosity it seems that the differences are quite large, they in fact differ by just about 10%, however still preserving the trend observed experimentally. It now seems to be clear that the answer to the origin of the differences in transport coefficients between TIP4P/2005 and TIP4P/Ice models can be attributed to the different absolute temperature scales. In practice, for comparison with experiments this means that transport properties obtained at temperature \( T \) from the TIP4P/Ice model are good estimates for liquid water properties at an effective temperature of \( T_{ef} = \frac{T_{m,05}}{T_{c,05}} T \).

According to the Stokes-Einstein relation, the self diffusion of a spherical particle can be related to the viscosity of the surrounding media as \( D = \frac{k_B T}{3\pi \eta a} \), where \( a \) is the molecular diameter. Surprisingly, there exists ample evidence that this hydrodynamic result also holds quite accurately down to molecular scales. In analogy to other water models and experimental systems we checked the Stokes-Einstein (SE) relation for the TIP4P/Ice model by plotting \( \frac{D\eta}{T} \) as a function of temperature. The results are presented in Figure 5. To show the temperature variation of \( \frac{D\eta}{T} \), it has been normalized by the reference temperature which usually is the highest temperature examined. In our case, it is taken to be \( T = 350 \) K at
all pressures studied. We can see that at pressures higher than $p = 200 \text{ MPa}$, the deviations start to occur already at $T = 320 \text{ K}$, and at a somewhat lower temperature of $T = 298 \text{ K}$ for all the remaining pressures. This is consistent with previous work reporting the violation of the SE relation for temperatures way higher than in regular supercooled liquids which usually is $1.3T_g$ where $T_g$ is the vitrification temperature (for water $T_g \approx 136 \text{ K}$). On the other hand, it has to be noted that aside from the lowest temperature studied $T = 245 \text{ K}$, the deviation is still moderate and does not exceed 30%. Importantly, the deviations are roughly independent on the pressure. Therefore, the SE relation does not serve as a quantitative theory, but it is still useful as an order of magnitude estimate of the viscosity for the TIP4P/Ice model down to $T = 245 \text{ K}$. Given that, one can obtain values of viscosity from the self-diffusion coefficients using Stokes-Einstein relation $\eta = \frac{k_B T}{\pi \sigma a}$ within an acceptable error margin with $a = 3.1 \text{ Å}$ being the molecular diameter of water.

Since the SE relation is violated, having calculated the values of self-diffusion coefficient and shear viscosity for a series of isotherms, it is also interesting to check what is the hydrodynamic diameter $\phi_h$ required to obey the SE relation exactly. It can be extracted as follows:

$$\phi_h = \frac{k_B T}{3 \pi \eta D} \quad (4)$$

Figure 6 shows $\phi_h$ calculated from the simulation data. Compared to the Lennard-Jones parameter for interaction between the oxygen sites of two molecules in TIP4P/Ice which is $\sigma_O = 3.1668 \text{ Å}$ it exhibits a smaller value at all temperatures studied. $\phi_h$ is independent on the pressure and decreases with temperature, however the deviations from $\sigma_O$ does not exceed 30% except for the outlier at $T = 245 \text{ K}$ at ambient pressure. This feature of decreasing $\phi_h$ upon cooling has been observed in many fragile glassformers.\[15]

IV. CONCLUSIONS

In this paper we computed transport coefficient of bulk liquid water using TIP4P/Ice model at eight different temperatures ranging from $T = 245 \text{ K}$ to $T = 350 \text{ K}$ in a pressure range of $p = 0 - 500 \text{ MPa}$. We emphasize that to our knowledge, such a systematic study for this particular water model has not been performed to date. We have shown that the self-diffusion (shear viscosity) exhibits decreased (increased) values than experimental findings or those extracted from TIP4P/2005 water model. However, if one would switch to the reduced units formalism with respect to the model’s triple point (or critical point), the behavior changes dramatically. In such a case, models are now in excellent agreement with each other and also reflect experimental data nearly quantitatively. Such observations allow us to infer that in spite of different original purpose of considered models here, one can benefit from a vast number of reports regarding the behavior of transport coefficients for TIP4P/2005 model and utilize them following the routine described in this paper. It seems that the answer to the origin of the differences in transport coefficients between models is just because of different absolute temperature scales.

Despite that, we would like to emphasize that we did not study deeply supercooled regime and therefore, cannot guarantee that this is a universal feature so a special caution has to be paid. Moreover, in view of these findings, a naturally arising questions are: does the same behavior would regard other quantities such as dielectric constant\[46], surface tension\[47], densities of ices, and perhaps other\[58]? Is this the universal feature for all water models? Our results suggest the analogy could be exploited at least for the study of transport properties, so that accurate data for a model with unknown transport coefficients could be inferred from other models with known transport properties.

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DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Appendix A: Simulation data

All of the simulation points are presented in Table I with the uncertainties presented in the form of standard errors. The calculation of uncertainties for the viscosity was straightforward as we obtained six independent integrals of autocorrelation functions of the traceless stress tensor elements. In the case of self-diffusion coefficients, we have followed the same routine as in the reference.\[33] Briefly, the trajectory was divided into four blocks of the same duration equal to 7.5 ns and for each of them the self-diffusion coefficient was calculated as the slope of the mean-squared displacement as explained in Section II.

Tables II and III show the comparison of the transport properties of liquid water for TIP4P/2005 and TIP4P/Ice water models in the reduced temperatures. As described in the text, it shows an excellent agreement between the models as well as with experimental findings.
TABLE III. Comparison of simulation results for two water models for the shear-viscosity \( \eta \) in mPa-s. Experimental temperature is the same as for TIP4P/2005. Experimental values are taken from Ref.\(^{49}\) whereas TIP4P/2005 are extracted from Ref.\(^{42}\).
M. M. Conde, C. Vega, and A. Patrykiejew, “The thickness of a liquid layer of ice,” *Physical Chemistry C J. Phys. Chem. Lett.***transition in supercooled water,” *Acta Physica,* vol. 114, no. 17, pp. 4312–4317, 2017.

C. A. Cerdeiriña, “Water’s unusual thermodynamics in the realm of physical chemistry,” *J. Phys. Chem. B,* vol. 126, no. 35, pp. 6608–6613, 2022. PMID: 36001372.

G. Debenedetti, “Supercooled and glassy water,” *Journal of Physics: Condensed Matter,* vol. 15, pp. R1669–R1726, oct 2003.

K. Ito, C. T. M. Moynihan, and C. A. Angell, “Thermodynamic determination of fragility in liquids and a fragile-to-strong liquid transition in water,” *Nature,* vol. 398, pp. 492–495, Apr 1999.

R. Shi, J. Russo, and H. Tanaka, “Origin of the emergent fragile-to-strong transition in supercooled water,” *Proceedings of the National Academy of Sciences,* vol. 115, no. 38, pp. 9444–9449, 2018.

A. Dehoui, B. Issenmann, and F. Caupin, “Viscosity of deeply supercooled water and its coupling to molecular diffusion,” *Proceedings of the National Academy of Sciences,* vol. 112, no. 39, pp. 12020–12025, 2015.

T. Kawasaki and K. Kim, “Identifying time scales for violation/preservation of stokes-einstein relation in supercooled water,” *Science Advances,* vol. 3, no. 8, p. e1700399, 2017.

M. Majumder, N. Chopra, R. Andrews, and B. J. Hinds, “Enhanced flow in quasiliquid layers on ice crystal surfaces,” *Phys. Rev. Lett.* vol. 115, pp. 20396–20403, 2020.

P. J. Daivis and D. J. Evans, “Comparison of constant pressure and constant volume nonequilibrium simulations of sheared model decane,” *The Journal of Chemical Physics,* vol. 149, no. 9, p. 094503, 2018.

M. A. González and J. L. F. Abascal, “The shear viscosity of rigid water models,” *The Journal of Chemical Physics,* vol. 132, no. 9, p. 096101, 2010.

P. Montero de Higes, E. Sanz, L. Joly, C. Valeriani, and F. Caupin, “Viscosity and self-diffusion of supercooled and stretched water from molecular dynamics simulations,” *The Journal of Chemical Physics,* vol. 149, no. 9, p. 094503, 2018.

I. de Almeida Ribeiro and M. de Koning, “Non-newtonian flow effects in supercooled water,” *Phys. Rev. Research,* vol. 2, p. 022004, Apr 2020.

D. A. McQuarrie, *Statistical Mechanics.* New York: Harper & Row, 1976.

P. J. Dai vis and D. J. Evans, “Comparison of constant pressure and constant volume nonequilibrium simulations of sheared model decane,” *The Journal of Chemical Physics,* vol. 100, no. 1, pp. 541–547, 1994.

A. P. Thompson, H. M. Aktulga, R. Berger, D. S. Bolintineanu, W. Brown, P. S. Crozier, P. J. in ’t Veld, A. Kohlmeyer, S. G. Moore, T. D. Nguyen, R. Shan, M. J. Stevens, J. Tranchida, C. Trott, and S. J. Plimpton, “LAMMPS - a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales,” *Comp. Phys. Comm.,* vol. 171, pp. 108171, 2022.

G. J. Martyna, M. L. Klein, and T. C. Weare, “Nosé–hoover chains: The canonical ensemble via continuous dynamics,” *The Journal of Chemical Physics,* vol. 97, no. 4, pp. 2635–2643, 1992.

G. J. Martyna, D. J. Tobias, and M. L. Klein, “Constant pressure molecular dynamics algorithms,” *The Journal of Chemical Physics,* vol. 101, no. 5, pp. 4177–4189, 1994.

R. Hockney and J. Eastwood, *Computer Simulation Using Particles.* CRC Press, 1988.

K. Krynicki, D. C. Green, and D. W. Sawyer, “Pressure and temperature dependence of self-diffusion in water,” *Faraday Discuss. Chem. Soc.,* vol. 66, pp. 199–208, 1980.

F. X. Prielmeier, E. W. Lang, R. J. Speedy, and H.-D. Lüdemann, “The pressure dependence of self-diffusion in supercooled light and heavy water,” *Berichte der Bunsengesellschaft für physikalische Chemie,* vol. 92, no. 10, pp. 1111–1117, 1988.

K. R. Harris and L. A. Woolf, “Temperature and volume dependence of the viscosity of water and heavy water at low temperatures,” *Journal of Chemical & Engineering Data,* vol. 49, no. 4, pp. 1064–1069, 2004.

C. Vega, J. L. F. Abascal, and I. N ezbeda, “Vapor-liquid equilibria from the triple point up to the critical point for the new generation of tip4p-like models: tip4p/ew, tip4p/2005, and tip4p/ice,” *The Journal of Chemical Physics,* vol. 125, no. 3, p. 034503, 2006.

A. Hodgdon and F. H. Stillinger, “Stokes-einstein violation in glass-
forming liquids,” Phys. Rev. E, vol. 48, pp. 207–213, Jul 1993.

46 J. L. Aragones, L. G. MacDowell, and C. Vega, “Dielectric constant of ices and water: A lesson about water interactions,” The Journal of Physical Chemistry A, vol. 115, no. 23, pp. 5745–5758, 2011. PMID: 20866096.

47 C. Vega and E. de Miguel, “Surface tension of the most popular models of water by using the test-area simulation method,” The Journal of Chemical Physics, vol. 126, no. 15, p. 154707, 2007.

48 C. Vega, J. L. F. Abascal, M. M. Conde, and J. L. Aragones, “What ice can teach us about water interactions: a critical comparison of the performance of different water models,” Faraday Discuss., vol. 141, pp. 251–276, 2009.

49 G. Guevara-Carrion, J. Vrabec, and H. Hasse, “Prediction of self-diffusion coefficient and shear viscosity of water and its binary mixtures with methanol and ethanol by molecular simulation,” The Journal of Chemical Physics, vol. 134, no. 7, p. 074508, 2011.