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Self-Diffusion Coefficient of Bulk and Confined Water: A Critical Review of Classical Molecular Simulation Studies

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ABSTRACT

We present a detailed overview of classical molecular simulation studies examining the self-diffusion coefficient of water. The self-diffusion coefficient is directly associated with the calculations of tracer or mutual diffusion coefficient of mixtures and, therefore, is a fundamental transport property, essential for an accurate description of mass transfer processes in biological, geological (i.e., energy or environmentally related), and chemical systems. In the current review we explore two distinct research areas. Namely, we discuss the self-diffusion of water in the bulk phase and under confinement. Different aspects that affect the diffusion process, including the molecular models, the system-size effects, the temperature and pressure conditions and the type of confinement are discussed. Finally, possible directions for future research are outlined.

KEYWORDS: Self-diffusion coefficient; Water; Molecular simulations; Review; Bulk phase, Confinement

1. Introduction

Water is probably the most ubiquitous substance on earth and is directly involved in various aspects of biological processes in nature. It participates in the structure, stability, dynamics, and functions of proteins and other biomolecules [1]. It plays an important role in the development and sustainability of life and is also accounted in numerous aspects that are closely associated with everyday life (e.g., weather and atmospheric phenomena, the environment [2], industrial production [3], food science and technology). From a chemical point of view, water is a relatively non-complex substance that is composed by one oxygen and two hydrogen atoms. Yet, it is a highly associating dense fluid with long ranged interactions. Consequently, water has a very complex behaviour with the largest number of counterintuitive anomalies in its physical properties [4][5][6]. Currently, there are 73 anomalies listed (see for example [7]) and despite the immense research effort a number of them still remain unresolved. Numerous studies have appeared in the literature examining the various properties of interest of water.

Traditionally, these studies utilize an approach that typically can fall within one of the following four general groups of methods: (i) *ab initio*-based simulations, (ii) molecular simulations (e.g., molecular dynamics, MD and Monte Carlo, MC) based on empirical/semi-empirical force fields, (iii) effective continuum-scale theoretical methods, and (iv) experimental methods. Experiments are valuable tools for uncovering the fundamentals behind various phenomena. While experimental methods are also essential for testing the accuracy of computational methods, significant effort is also made to reduce the amount of experimental work required for the confirmation of theoretical models or the validation of molecular-scale computational studies. Performing experimental measurements for all the possible water containing systems, at all possible state points, is rather impractical. To address the issue, two characteristic approaches can be followed. First, an effective-continuum theory can be developed and tested using the available experimental data. Such theoretical or semi-empirical models can be utilized for performing accurate and detailed studies at conditions within the range of development of the theoretical models. Nevertheless, care should be taken for applications at conditions outside the range of development of the models. A second, attractive alternative would be to use a limited amount of experimental measurements to design and validate appropriate interaction potentials (empirical/semi-empirical or *ab initio*), which can be subsequently used for extensive molecular-scale computational studies. This latter approach is gaining significant momentum as a result of the increase of available computational power and the development of more efficient computational methods [8]–[10].

Providing a detailed review of studies related to water would be a daunting task, even if we focused only at the relevant review papers. Consequently, the different review studies are topic-specific and traditionally focus on a limited amount of aspects related to water. The following studies are typical such reviews, among numerous reported in the literature: Debenedetti and Stillinger [11] discussed the complex interplay between dynamics and thermodynamics encountered in supercooled liquids, and particularly in water. Stanley et al. ([12],[13],[14]) discussed in detail the hypothesis of liquid polyamorphism, as a possible explanation for the anomalous behaviour of water. Bartels-Rausch et al. [15] reviewed the science behind ice structures and patterns. Wallqvist and Mountain [16] presented a detailed discussion on the derivation and description of molecular models for water. Vega and Abascal [4] proposed a quantitative test that can be used to evaluate the performance of various computational water force fields. The test was based on 17 properties of water considering the vapour, liquid and solid phases of water. Subsequently, the test was utilized to examine five rigid non-polarizable water force fields. Striolo et al. [17] discussed the challenges involved in the modelling of the carbon-water interface. Gillan et al. [18] presented a detailed discussion on the quality of the Density Functional Theory (DFT) for water.

The ACS journal *Chemical Reviews* dedicated recently an entire issue to water, entitled "*Water – The Most Anomalous Liquid*", where a number of topical reviews were presented. In the particular issue, Gallo et al. [6] provided a detailed review and explored several theoretical scenarios for the behaviour of water in the anomalous regime from ambient conditions all the way to the deeply supercooled region (i.e., 150 – 230 K at ambient pressure). Cisneros et al. [19] presented a review of the recent progress in the development of analytical potential energy functions that aim to represent correctly the many-body effects. Ceriotti et al. [20] presented the latest developments in the experimental, theoretical, and simulations studies of nuclear quantum effects in water. Fransson et al. [21] explored the use of X-ray and electron spectroscopy to probe water at different temperatures. Amann-Winkel et al. [22] discussed the use of X-ray and neutron scattering methods to study water structure at conditions ranging from ambient to deeply supercooled and amorphous states, while Perakis et al. [23] reported on the use of static and time-resolved vibrational spectroscopy of liquid water for the same conditions. Cerveny et al. [24] considered the study of water under geometrical confinement as a proxy of studying water in the deeply supercooled region (i.e., 150 – 230 K at ambient pressure). Such conditions are difficult to attain for bulk water since immediate crystallization to ice occurs.

The same pattern of approaching water is followed here as well. The current study focuses on the self-diffusion coefficient of water calculated with molecular simulations. Self-diffusion coefficient is a fundamental transport property that is essential for the accurate description of mass transfer processes and is involved in the design of various industrial separation processes [25]. Self-diffusion coefficient is also directly associated with the calculations of tracer or mutual diffusion coefficient of mixtures [26].

Furthermore, the self-diffusion coefficient is an important parameter because it is one of the few time-dependent properties that can be measured directly, using both experiments and simulations. Given that transport properties are intimately related to the short- and long ranged intermolecular potentials, the self-diffusion coefficient provides a fundamental test for a solvent model.

The objectives of the current study are the following: (i) to perform an exhaustive review of the available literature and collect the studies that report self-diffusion coefficient of water obtained from molecular simulations (using empirical/semi-empirical force fields). An extended list of water-related studies, along with reported values and comments on the studies are provided in the Supporting Information. Emphasis is placed in two distinct research areas. The first considers studies of water in the bulk phase [27]–[197], while the second explores studies of water under confinement [198]–[286]. (ii) To present comparisons of the most reliable calculations with available experimental data [287]–[298]. (iii) To discuss issues that could affect the accuracy of the self-diffusion coefficient calculated using molecular simulations. Such issues include: the system size effects (SSE) [i.e., the common practice of using a few hundred molecules, leads to a significant deviation between the simulated (i.e., finite system size) and real (i.e., thermodynamic limit) self-diffusivity]; the use of rigid classical water force fields and the effect of polarizability on the self-diffusion coefficient; the effect of internal degrees of freedom; the effect of temperature and pressure including the supercooled and near- or supercritical regions; and the use of coarse-grained models.

Water under confinement is currently a very active research area. It is encountered in diverse environments such as in biological systems, industrial processes and geological settings associated with energy (e.g., oil and gas production, hydrate deposits in oceanic and permafrost regions) or environmental related applications (e.g., pollutant migration, carbon dioxide sequestration). Water under confinement has also been an alternative approach to study water at supercooled conditions, without the problem of ice formation. Confinement results in shifting the temperature where ice formation occurs to lower values [24].

Developing intermolecular potentials for simulations of liquids has been, so far, a compromise between computational efficiency and accuracy of the developed models [299]. Empirical or semi-empirical potentials, once they are developed, they are subsequently used extensively in common molecular simulation packages [8]–[10]. On the other hand, quantum chemical methods allow for the calculation of intermolecular forces during each time step of the simulation (a process known as “on-the-fly” calculations). Such an approach is also known as the Car-Parrinello *ab initio* (CPAIMD) MD simulation. Due to the significantly high computational cost, only small systems (16 – 128 molecules) have been studied over short periods. Water has been examined extensively (i.e., typical examples of such studies include refs. [300] – [337]) by such *ab initio* methods since the pioneering work of Laasonen et al. [300] who used 32 D_2O molecules for their simulations and reported a value for the self-diffusivity, $D_o = (2.2 \pm 1) \times 10^{-9}$ m^2s^{-1}, in good agreement with the experimental value. Note, however, that no system size effects were considered (see also the discussion in Section 2.1). The self-diffusivity is usually among the parameters examined in order to evaluate the performance of the *ab initio* models. However, in the current study we have focused primarily on self-diffusivities obtained from empirical/semi-empirical models and no systematic study was undertaken for the self-diffusivities obtained from *ab initio* models. Given the amount of studies available, this issue is probably worth a separate review.

Similarly, in this review paper we do not provide an in-depth discussion regarding the calculation of self-diffusivities using reactive force fields in order to keep the number of references manageable for this study. Nevertheless, important advances in the use of reactive force fields for calculating transport properties of bulk and confined water have been reported during the recent years. Such is the case of the recent study by Manzano et al. [338] that found that ReaxFF [339] is able to simulate water properties in sub- and super-critical states in good quantitative agreement with experimental data. For further reading on this subject the reader is referred to ([340]–[343]) and references therein.

The manuscript is organized as follows: Initially, in Section 2 we present the related discussion of the self-diffusion coefficient of water in the bulk phase. Subsequently, in Section 3 we discuss the effect of confinement on the self-diffusion coefficient of water. We examine here the confinement in carbon compounds, minerals, biomolecules, and other materials. Finally, we end with future outlook and conclusions.

2. Bulk phase water self-diffusion coefficient

2.1 Finite size effects

As shown in a series of papers by Teleman and co-workers ([41], [55], [344], [345]), the self-diffusion coefficient of water obtained from molecular simulations depends on the number of the molecules used (i.e., the system size) due to the long-range interactions and the imposed periodic boundary conditions. A systematic study on this subject was presented by Dünweg and Kremer [346], who performed MD simulations of a polymer chain in a good solvent and showed that hydrodynamic interactions in a finite system are expected to have strong effects on the dynamical properties of the system. The authors showed that solvent particle mobility scales linearly with $1/L$ (which is proportional to $1/N^{1/3}$), where L is the length of the simulation box (and N the number of molecules). Thus, $1/L=0$ corresponds to the self-diffusivity at the thermodynamic limit, which is the quantity measured experimentally.

A decade later, Yeh and Hummer [102] performed a thorough study of Lennard-Jones (LJ) systems and TIP3P [32] water and observed that the same scaling behaviour applies also for the self-diffusion coefficient of small molecules (see Figure 2 of ref. [102]). Based on the work of Dünweg and Kremer, Yeh and Hummer presented an analytic term, based on the hydrodynamic theory for a spherical particle in a Stokes flow with periodic boundary conditions, which can be added to the MD computed self-diffusivity value in order to correct for the finite size dependences. Accordingly, the self-diffusivity of water at the thermodynamic limit, D_∞, can be calculated from Eq. (1):

$$D_\infty = D_{MD} + \frac{k_B T \xi}{6\pi\eta L} \tag{1}$$

where D_{MD} is the self-diffusivity obtained from MD simulations, k_B is the Boltzmann constant, T is the absolute temperature, ξ is a dimensionless constant which is approximately equal to 2.837297 for cubic simulation boxes, η is the shear viscosity of water and L is the length of the simulation box. As Eq. (1) assumes, shear viscosity is independent of the system size ([346], [102], [347]). The second term of Eq. (1) is the analytic correction. It is important to note that since different water models yield different shear viscosity values, the shear viscosity for use in the correction should be also obtained from MD simulations. However, studies that used the experimental value in Eq. (1) can be found in literature ([189], [121], [140]). Alternatively, if the viscosity is unknown, D_∞ can be obtained from the y intercept of the linear fit to two or more D_{MD} values, corresponding to different system sizes, as in the studies by Bauer and co-workers ([125], [126]) and Troster et al. [172]. Very recently, Jamali et al. [348] showed that a similar correction to Eq. (1) should be used for correcting the Maxwell-Stefan diffusion coefficient. Although, originally Eq. (1) was derived by Dünweg and Kremer [346] and has been already mentioned in the work of Spångberg and Hermansson [99], Yeh and Hummer's study was, most probably, the first in which this term was actually applied to obtain the water self-diffusion coefficient at the thermodynamic limit.

Despite the fact that finite size dependences on the dynamic properties of water were already reported in the 80's, only a small fraction of the self-diffusivity values reported in the literature are corrected accordingly. This observation, combined with the fact that in most of the studies the number of water molecules used is rather low (below 1,000), makes the consistent evaluation of the numerous water force fields an arduous task. A characteristic example is the TIP4P/2005 [105], which is often characterized as the best condensed-phase water force field. The self-diffusivity at 298 K and 1 bar, reported in the original work by Abascal and Vega, was calculated from a system of 530 molecules (without correction) and was shown to underestimate the experimental value. However, after the appropriate correction, it ends up slightly (approx. by 1%) overestimating the experimental diffusivity. Similarly, the self-diffusion coefficient of TIP4P-Ew (Horn et al., [101]) at 298 K and 1 bar, in the original paper was calculated from a system of 512 molecules and shown to be 2.4 x 10^{-9} m^2/s, which is only 4% higher than the experimental value (2.3 x 10^{-9} m^2/s [289]). However, after the appropriate correction, the self-diffusivity value becomes 2.7 x 10^{-9} m^2/s, which overshoots the experiment by 18%.

Due to the magnitude of the finite size dependences and the wide range of system sizes used in different studies (in the range of approx. 200 to 4,000 molecules), multiple values for the self-diffusivity of water are reported for each force field. In Figure 1, the self-diffusivity of water is shown as a function of the system sizes used in the MD simulations, for four of the most widely used force fields, namely the SPC [349], SPC/E [39], TIP4P [32], and TIP4P/2005 [105]. The values shown in Figure 1 are obtained from multiple sources. As it can be seen, for relatively high numbers of molecules (approx. 2,000) the distinction between the models is clear, with the exception of some outlying points. However, for the area of the plot showing the low numbers of molecules (i.e., below 500), the values calculated from different models overlap. Moreover, self-diffusivities obtained from small system sizes (approx. 100 to 300) are scattered, indicating that these calculations have much higher uncertainty. The latter is expected since self-diffusion coefficient is a single-molecule property (i.e., calculated from the mean square displacement (MSD) of every individual molecule in the system) and consequently the statistical uncertainty decreases by increasing the system size.

Attention also should be drawn to the fact that most of the studies do not report the exact methodology used to obtain the self-diffusivity and the respective statistical error. Pranami and Lamm [350] presented a rigorous approach for calculating accurate self-diffusion coefficient, highlighting the importance of running multiple independent and sufficiently long simulations as well as paying attention to the proper fitting to the mean squared displacement of the diffusing molecules. Wang et al. [351] and Casalegno et al. [352] have shown that long runs are needed in order for the molecules to get from the sub-diffusive regime into the (Gaussian) Fickian, from which accurate self-diffusivity values can be obtained in MD simulations. Although these studies focus on more viscous systems, the same principles apply to water and thus, particular attention should be paid in the actual displacement of the diffusing molecules, especially at low temperatures.

The self-diffusion coefficient, and transport properties in general, are not often taken into account in the parameterisation of water models, but calculated afterwards to validate their efficiency. However, if self-diffusivity is part of the parameterisation, it is crucial that the finite size effects are taken into account; otherwise the optimization procedure will be inaccurate. This is the case for the polarizable SWM4 model ([353] and [107]), for which Lamoureux and co-workers took into consideration self-diffusion coefficient as a target property, but the value used was not corrected for finite size effects, resulting in a model that in reality significantly overestimates self-diffusivity (by approx. 20%). In the parameterisation procedure of the polarizable models SWM6 [158] and POL4D [144], the three-body potential E3B3 [183], and the SSMP [189] model, the self-diffusivity at ambient conditions was also used. In these four studies, the extrapolated self-diffusivity value was taken into account (by applying the correction of Eq. (1)). However, in the case of SSMP the experimental value for viscosity was used instead of the MD-computed one. This is expected to have an effect on the corrected value if the MD obtained viscosity deviates from the experimentally measured. Finally, Izaldi et al. [174] used self-diffusivity as a target property, in the fitting procedure of the OPC model, but the authors do not report if the system size used was the extrapolated to the thermodynamic limit.

Except from the finite system sizes, quantum nuclear effects are expected to have some effect in the MD calculations of the self-diffusion coefficient [77]. However, this effect according to Habershon et al. [354] is small and thus ignored in most of the studies.

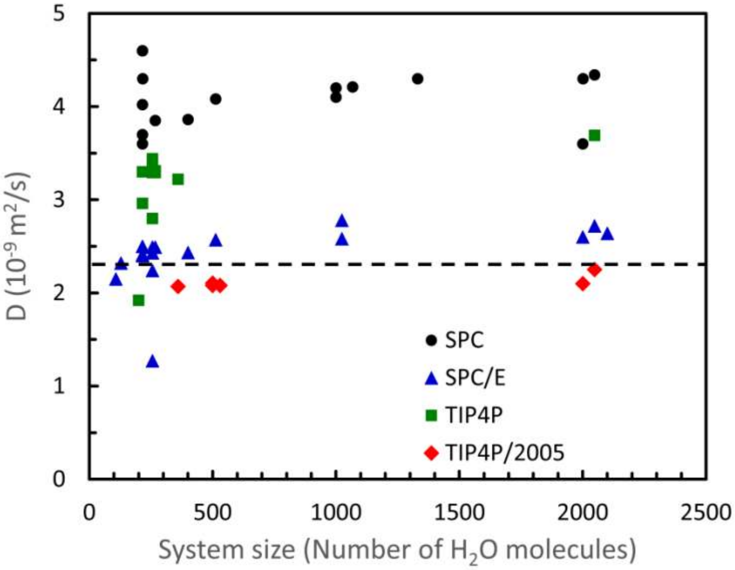


Figure 1. The diffusion coefficient of water at ambient conditions (i.e., 298/300 K and 1 bar) computed from widely used water force-fields as a function of the number of molecules used in the MD simulations. These values are not corrected for system size effects. The experimental data are collected from multiple studies: SPC ([39], [43], [56], [57], [83], [95], [99], [108], [137], [139], [148], [150], [170], [173], [177]); SPCE ([39], [43], [44], [61], [62], [83], [90], [99], [108], [121], [139], [148], [156], [157], [169], [173]); TIP4P ([36], [40], [43], [83], [91], [121], [123], [139], [157], [161]); and TIP4P/2005 ([105], [123], [139], [141], [171], [173]). The dashed line denotes the experimental value: 2.3 x 10^{-9} m^2/s [289].

2.2 Self-diffusion coefficient at ambient conditions

2.2.1 Rigid non-polarizable force fields

Since the pioneering work of Stillinger and co-workers ([27]–[30], [355], [356]) in the 1970's who presented the first "Computer Era Models" [16], numerous models have been developed, trying to reproduce the most important thermodynamic and transport properties of water. The models by Matsuoka et al. [357], Jorgensen et al. ([358] and [32]) and Berendsen et al. ([39] and [349]) developed in the 1980's, formed the foundation for numerous others in the decades that followed. Already 30 years ago, the number of water force fields was such that Watanabe and Klein [43] stated: "… *there are now probably more articles in the literature dealing with potential models for water than there are groups actually interested in using the potentials in molecular dynamics or Monte Carlo simulation studies* …".

The majority of these water force fields are designed based on the concept of pairwise additivity. In that fashion, the total potential energy of the system can be expressed as the sum of pair interactions. This class of models implicitly incorporating the induced polarization through optimized dipole moments and fixed point charges are called non-polarizable and are widely used due to their computational efficiency. Such interaction potentials are the well-known SPC- ([349], [39], [359], [108]] and TIP- ([32], [360], [101], [105]) families.

The accurate prediction of the self-diffusion coefficient at ambient conditions (i.e., 298 K and 1 bar) is a highly desirable characteristic of any water model due to the potential use of the model as a predictive tool for relevant applications. To that end, one should expect that self-diffusivity is a common target property in force-field parameterisation. However, as already discussed previously (Section 2.1) this is not the case. In fact, only very few models are designed this way, while the prediction of self-diffusivity is very often based on the accurate prediction of other properties, e.g., liquid density and pair correlation function.

In this section, a brief discussion on the performance of various non-polarizable models will be presented, but given the huge amount of work done in this field and the inconsistency between some reported values, not all of the relevant studies will be analysed in order to keep this manuscript in a logical size. Additionally, it should be noted that although there exist more than a hundred different self-diffusion coefficient values reported in the literature for water at ambient conditions, only a small fraction of those are corrected for system size effects (see discussion in Section 2.1) and thus, an accurate performance check of all water models in predicting self-diffusivity seems impossible to be achieved. Particularly, our search revealed that approximately 80% of the total available self-diffusivity values reported are computed from MD simulations of up to only 500 molecules. This directly leads us to the conclusion that the biggest part of the gathered data needs to be shifted upwards by 5–15%, to compensate for the finite size dependences. A collection of self-diffusion coefficient found in the open literature is gathered in Table SI–1 of the Supporting information, along with the original references. Detailed reviews on the various model types and their general performance can be found, in the works by Wallqvist and Mountain [16], Guillot [361] and Vega and Abascal [4].

In Figure 2, twelve different force fields are compared based on their ability to predict the self-diffusivity of water at ambient conditions. For the sake of a fair comparison, only results corrected for finite size effects are shown. The most accurate force filed is found to be the E3B ([121], [140]), which achieves “perfect” agreement with the experimental self-diffusion coefficient (2.3 x 10^{-9} m^2/s [289]). E3B model adopts the gas phase geometry of water and considers explicit three-body interactions, which were obtained from electronic structure calculations. The model is one of the few exceptions in which self-diffusivity at ambient conditions was used in the fitting procedure (corrected for system size effects according to Eq. (1), but with the experimental viscosity value). As can be seen from Figure 2, later versions of the E3B model, namely the E3B2 [362] and E3B3 [183], are also relatively accurate. At this point one should argue that a comparison of two-body potentials (i.e., all models in Figure 2 except from the E3B family) with the E3B family is unfair, exactly because the latter ones include three-body short ranged interactions. However, the incorporation of these additional interactions does not necessarily lead to better self-diffusivity predictions. Characteristic is the case of the three-body potential version of the MCY model [37], the diffusion and reorientation dynamics of which are much slower, compared to the original two-body MCY ([357], [31]) and the experimental value. For a general discussion on the effect of three-body interactions in water simulations the reader is referred to the work by Wojcik and Clementi [37].

TIP4P/2005 [105] self-diffusivity predictions are shown to be very accurate, deviating less than 1% from the experimental value, making it by far the best performing among the TIP family. As Vega and Abascal [4] observed, models like TIP4P/2005 that overestimate the vaporization enthalpy of water by 10–15% tend to give quite reliable self-diffusion coefficient. In the same manner, models fitted to reproduce the vaporization enthalpies like TIP3P [32], TIP4P [363] and TIP5P [360] tend to significantly overestimate the self-diffusivity value (deviation of more than 30% from the experimental value). More particularly, TIP3P has the lowest predictive ability for the self-diffusion coefficient of water, deviating from the experimental value by almost a factor of 2. This failure can be partially attributed to the inability of TIP3P to properly reproduce the water structure. That was the reason which lead to the design of TIP4P, in which the introduction of a dummy site carrying the negative charge instead of the oxygen atom improved both the prediction of water structure and the self-diffusion coefficient. As it can be seen in Figure 2, is much closer to the experimental value compared to the TIP3P and TIP4P. TIP5P features positive charges placed on the hydrogen sites and two negative ones in the so called “lone pair electrons” positions, in an attempt to describe the water molecule in a more chemistry-accurate way.

In 2004, Rick [364] and Horn et al. [101] presented the TIP5P-Ew and TIP4P-Ew models, which are re-optimised versions of the TIP5P and TIP4P, respectively. In these models the long-ranged electrostatic interactions are treated with Ewald techniques, instead of simple spherical cut-offs. Both models give much improved self-diffusivity predictions (below 20% deviation from the experimental value), as shown by Yu et al. [159], who presented a series of self-diffusion coefficient calculations by taking into consideration the system size dependences.

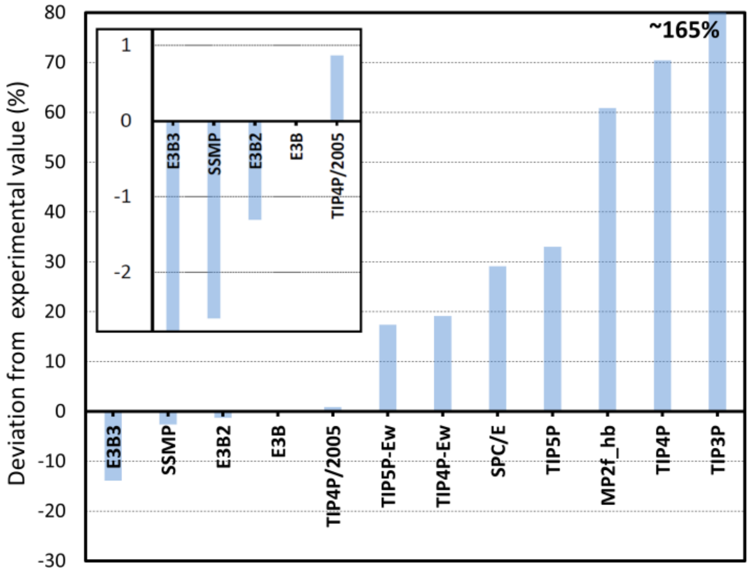


Figure 2. The relative deviation of self-diffusion coefficient from the experimental value at ambient conditions (2.3 x 10^{-9} m^2/s [289]), obtained by various force fields. MD obtained values are corrected for finite size effects (see Section 2.1). The actual values of the self-diffusivities can be found in Table SI–1 of the Supporting Information). The experimental data are collected from multiple studies: E3B3 [183]; SSMP [189]; E3B2 [183]; E3B [140]; TIP4P/2005 [183]; TIP4P-Ew [159]; TIP5P-Ew [159]; SPC/E [152]; TIP5P [159]; MP2f_hb [129]; TIP4P [159]; TIP3P [149].

2.2.2 The effect of polarizability

As discussed previously, most water models up to date are pairwise additive and treat electrostatic interactions through fixed point charges. However, many important forces are of non-additive nature, with the most important of those being the electronic polarizability. Polarizability is the quantity measuring the relative tendency of the electron cloud of a molecule to be distorted from its normal arrangement in the presence of an electric field. In a homogeneous condensed system, like bulk water, the effect of polarization is almost isotropic. With this in mind, and given that liquid is the most common form of water in nature, the main targets of research groups developing force fields are usually bulk water properties (e.g., density, internal energy, dielectric constant, structural, and perhaps transport properties). Although non-polarizable force fields may perform reasonably well for liquid water at ambient conditions (see Figure 2), in which the instantaneous environment of each molecule is very similar to the average environment, it is expected that they are less accurate for inhomogeneous systems (e.g., close to surfaces, near ions or biomolecules, multiple phases in the same simulation, binary and multicomponent mixtures) or for predicting properties spanning the entire phase diagram. To overcome these inherent limitations, force fields that include a many-body polarizability term have been developed. These models are called polarizable, and based on the approach to treat polarization, can be divided in four groups, namely models with a) induced molecular point dipoles or multipoles, b) induced atomic dipoles, c) classical Drude oscillators (or Shell model), and d) fluctuating charges. For thorough discussions on polarizable models the reader is referred to the studies by Wallqvist and co-workers ([42], [16]), Soetens and Millot [66], Fanourgakis and Xantheas [110], Kolafa [118], Lopes et al. [365], Kiss and Baranyai [160], Yu et al. [159], Tröster et al. [166], and Jiang et al. [190].

As already mentioned, self-diffusivity is very rarely taken into account as a target property in the parameterisation of a water model. In contrast, being a very important transport property, it is often computed to assess the predictive ability of the force fields. Thus, a logical question is: "*how much and in what way the explicit description of water polarization affects the self-diffusion coefficient predictions at ambient conditions*?" As already discussed, for bulk water the effect of polarization is nearly isotropic and therefore, an average effective potential is expected to give quite satisfactory results. However, multiple polarizable force fields have been utilized for predicting the self-diffusivity of bulk water. In Figure 3 (a), the deviation from experimental data of self-diffusion coefficient computed from various polarizable force fields is shown. Although, more results do exist in the literature (for the same or other models), we show only the values that are reported to be corrected for finite size effects, either by using Eq. (1) or by fitting to multiple system sizes and extrapolating to the thermodynamic limit (see Section 2.1). Most of the models give rather satisfactory predictions (deviation approx. 15%), with the TIP4P-QDP-LJ [126] and TL6P [172] force fields being 100% accurate (0% deviation from the experimental value). This finding is quite interesting since self-diffusivity was not considered as a fitting parameter in the original development of these two models. TIP4P-QDP-LJ model is a modified version of TIP4P-QDP [125], which incorporates polarizability dependence in the repulsion and dispersion LJ terms. TIP4P-QDP-LJ model is able to predict density, self-diffusivity, enthalpy of vaporization, dielectric constant, and the liquid-vapour coexistence curve quite accurately. TL6P is a six-point model (belonging to the TL*v*P [166] family), which is developed by applying DFT/PMM hybrid techniques [366], and except for the excellent prediction of the diffusion coefficient, it is also able to reproduce very accurately a series of liquid-phase properties of water, including the temperature of the maximum density, T^{md}. Recent models like the BK3 [160] and HBP [190] are also in good agreement with the experimental diffusivity value (deviation approx. 1% and approx. 5%, respectively). These two models utilize Drude oscillators with Gaussian charges, to model polarizability, and the Buckingham potential for the dispersion interactions. In the case of HBP, a short-ranged directional hydrogen-bonding interaction term is part of the potential and therefore water structure is also captured accurately.

Particularly interesting is the case of the SWM6 model. Although it was originally parameterised with self-diffusion coefficient as one of the target properties, its prediction deviates approx. 7% from the experimental value. Another, interesting case is the MFP/TIP3P model by Leontyev and Stuchebrukhov [149], which performs equally poorly with TIP3P (deviation from experiment approx. 165%), regardless of the inclusion of polarization. These two examples show that by taking the electronic polarizability of water into account when designing a model is insufficient to guarantee an accurate prediction of the self-diffusion coefficient.

As shown in Figures 3 (a) and (b), relatively accurate values of self-diffusivity at ambient conditions can be obtained by various other polarizable models, belonging to diverse families and types. Some of those are the CC-pol-8s' [158], uAMOEBA [367] and TL6P^{sk} [172]. Although the diffusivity predictions of the models presented in Figure 3 (b) are not corrected for finite size effects, the use of at least 1,000 molecules is expected to yield a relatively good prediction (possibly within 10–15%, depending on the accuracy in the computed viscosity) and therefore some force fields of the IPOL- and COS/- families are expected to be close to the experimental value. For more information on these models, the reader is referred to the original papers ([170], [368], [118]). Other polarizable water force fields, not presented here (see Table SI–1 in the Supporting Information), which exhibit relatively good self-diffusion coefficient predictions are: (a) the TTM2-R [89], which employs Thole-Type polarizable dipoles, (b) the Gaussian charge GCPM (Paricaud et al., [369]), which yields accurate predictions of various water properties for a wide range of conditions, and (c) the HBB2-pol [151], a full-dimensional model based on first principles.

The total average deviation between experimental data and calculations from the models listed in Figure 3 (a) is approx. 19%, while the corresponding total average deviation of non-polarizable models shown in Figure 2 is 34%. This difference, although is not by any means a rigorous physical comparison, indicates that on average models with explicit polarization do provide improved self-diffusivity predictions. Such differences are expected to be much more pronounced when surface phenomena or ionic systems are examined ([370], [371]). As the results presented in Figure 3 suggest, the vast majority of the polarizable water force fields tend to overestimate self-diffusion coefficient. This finding could be attributed to several facts. For instance, although density predictions are in most of the cases quite accurate, the degree of hydrogen bonding between water molecules may not be correctly captured. In addition, the actual intermolecular energy plays a significant role, as the attractive and repulsive interactions can affect vastly the dynamic behaviour of the liquid. Finally, the dipole moment of the water molecule in each force field hugely affects the dynamic behaviour, since it affects the actual intermolecular interactions.

From the computational point of view, although comparisons between models are difficult to make, due to the plethora of different characteristics (e.g., number of sites, treatment of polarization etc.), polarizable models, such as the ones presented above, are expected to require more computer time compared to the non-polarizable ones, with the same number of atomic sites. More specifically, as shown by Jiang et al. [372] the SWM4-NDP [107] model implemented in NAMD simulation package [373] has shown an increase in computational cost by approximately a factor of 2 compared to the TIP3P force field [32]. Similarly, the HBP polarizable force field by Jiang and co-workers [190] is 3 times slower compared to the nonpolarizable TIP4P/2005 [105]. Therefore, the additional computational demand justifies up to a point, the dominant use of non-polarizable models by the molecular simulation community.

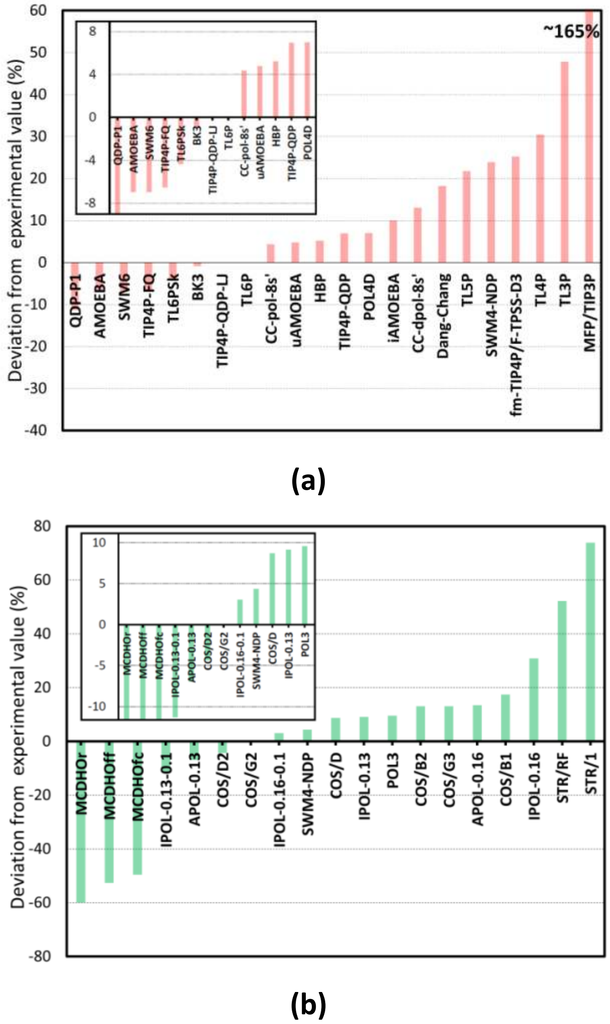


Figure 3. The relative deviation of self-diffusion coefficient from the experimental value at ambient conditions (2.3 x 10^{-9} m^2/s [289]), obtained by various polarizable force fields. **(a)** MD-obtained values are corrected for finite size effects (see Section 2.1), **(b)** MD simulations of 1,000 molecules or more without corrections for finite size effects. The actual values of the self-diffusivities can be found in Table SI–1 of the Supporting Information. *For AMOEBA we used the value reported by Yu et al. [159]. Wang et al. [167] reports *D* for AMOEBA to be equal to 2.0 x 10^{-9} m^2/s which has a relative deviation from the experimental value equal to -13%. The experimental data are collected from multiple studies: **(a):** QDP-P1 [125]; AMOEBA [159]; SWM6 [159]; TIP4P-QDP [125]; TL6P^{sk} [172]; BK3 [160]; TIP4P-QDP-LJ [126]; TL6P [172]; CC-pol-8s' [158]; uAMOEBA [367]; HBP [190]; TIP4P-QDP [125]; POL4D [159]; iAMOEBA [167]; CC-dpol-8s' [158]; Dang-Chang [152]; TL5P [166]; SWM4-NDP [159]; fm-TIP4P/F-TPSS-D3 [175]; TL4P [166]; TL3P [166]; MFP/TIP3P [149]. **(b):** MCDHO$_r$ [104]; MCDHO$_{ff}$ [104]; MCDHO$_{fc}$ [104]; IPOL-0.13-0.1 [118]; APOL-0.13 [118]; COS/D2 [170]; COS/G2 [368]; IPOL-0.16-0.1 [118]; SWM4-NDP [165]; COS/D [128]; IPOL-0.13 [118]; POL3 [118]; COS/B2 [95]; COS/G3 [368]; APOL-0.16 [118]; COS/B1 [95]; IPOL-0.16 [118]; STR/RF [95]; STR/1 [95].

2.2.3 The effect of internal degrees of freedom

The most widely-used water models assume that the intra-molecular degrees of freedom are frozen and thus treat the water molecule as a rigid object. To that end, the geometric characteristics of water models are usually based on experimental findings for an isolated molecule in the gas phase. The arguments for employing such a simplified model are both technical and physical (Berendsen et al. [349], Anderson et al. [38]). From the technical point of view, the computational time needed for simulating a system containing fully flexible molecules is higher, due to the introduction of bonded interactions and the lower simulation time-step needed (up to 5 times lower [141]) for the proper integration of Newton's equation. Although, this was a great issue in the early days of molecular simulations, nowadays with the huge increase in computational power and the availability of highly parallelizable open-source codes (LAMMPS [9], GROMACS [10], and NAMD [373]), such effects can be mitigated up to a point, especially for simulations of bulk fluids. A physical argument against the use of flexible models is that the internal vibrations in a water molecule are of quantum nature and thus cannot be properly modelled with classical mechanical approximations (Tironi et al. [374]). In addition, one can argue that at standard conditions $\hbar\omega_i \gg k_B T$ (where $\hbar$ is the Planck constant, and ω_i is the angular frequency of the i^{th} normal mode of vibration) and therefore the intra-molecular degrees of freedom are negligible [375].

On the other hand, arguments for employing a flexible water model are also common in literature. Lemberg and Stillinger [375] in 1975 presented the central force (CF) model for water, which includes intra-molecular degrees of freedom. This choice was based on the idea that even at low to moderate temperatures, the influence of zero-point motions and the possibility of static distortions due to the nature of hydrogen bonds still exist and should be reckoned with. Based on the CF model, the BJH [376] and RWK [377] water force fields modified the intra-molecular potential in a try to better capture the dynamics of the condensed phase. Lie and Clementi [35] extended the MCY model [357] to include intra-molecular vibrations, based on the idea that those motions in liquid water differ from the respective of an isolated water molecule, which are implicitly averaged and used in the rigid geometry. An interesting analysis on the effect of flexibility in the structural and dynamic properties of water for CF-type potentials is provided by Smith and Haymet [56]. Moreover, molecular simulations of flexible water make possible the investigation of properties related to its infrared and Raman spectra, and their relation with the hydrogen bonding network ([378], [379]).

Based on the context discussed above a reasonable question is: "…*how flexibility affects the prediction of self-diffusion coefficient*?". Teleman and co-workers ([41], [55]) worked towards answering this question by performing MD simulations of the original rigid (Berendsen et al. [349]) and a flexible version of SPC model (Anderson et al. [38]). In their first article [41] they concluded that the introduction of flexibility in the SPC model vastly affects the kinetic behaviour of the system resulting in approximately 40% higher self-diffusivity. However, in their second article [55], in which both a harmonic and an anharmonic potential was used to describe the intra-molecular vibrations, self-diffusivity was shown to be slower by 15 – 26 %. The reason for this behaviour was that the flexible model exhibited an increased dipole moment, which causes the strengthening of the cohesive forces in the fluid. The increased dipole moment is in fact a polarization response to the local electric field for the water molecule. The discrepancy between these two studies of Teleman and co-workers was attributed to the insufficient equilibration and the thermostat used in the simulations of the first paper [41].

Similar conclusions for various flexible realizations of the SPC model ([380], [38], [359], and [108]), were also drawn by the studies of Barrat and McDonnald [49], Lobaugh and Voth [77], English and MacElroy [91], Amira et al. [100], and Wu et al. [108]. The findings of these studies suggest that the self-diffusion coefficient decreases significantly when vibrational degrees of freedom are introduced to the SPC model, due to the increased dipole moment and radius of gyration of the flexible molecule. Wu et al. [108] specifically pointed out that the equilibrium bond length is a key factor affecting self-diffusivity, mainly due to its effect on the strength of the hydrogen bonds. Thus, the predictions from the flexible SPC models were shown to be closer to the experimental self-diffusivity value.

Other types of flexible models include the F3C by Levitt and co-workers [76], a force field specifically designed for simulations with macromolecules, and the TIP4P/2005f by Gonzalez and Abascal [141], which is the flexible version of the popular TIP4P/2005. According to the original papers, the self-diffusion coefficient of F3C is very close to the experimental value (deviation of approx. 4%), while TIP4P/2005f is less accurate compared to its rigid predecessor, underestimating the experimental value by approx. 16%.

At this point it is important to note that for none of the already discussed flexible water models the finite size dependency of the self-diffusion coefficient were taken into account, and thus the exact comparisons with the experimental values cannot be quantitatively accurate. In most of the above cases, a significant correction is needed due to the fact that the number of molecules used in the simulations was in the range of 100 – 300 molecules. In fact, the only corrected self-diffusion coefficient available in literature for flexible water models are given by Yu et al. [159], Wang et al. [167] and Spura et al. [175], for the polarizable force fields AMOEBA ([98], [103]), iAMOEBA [167] and fm-TIP4P/F-TPSS-D3 [175]. The values are shown in Figure 3 (a) and Table SI–1 of the Supporting Information.

The idea of further improving the structural, thermodynamic and kinetic property predictions of water by incorporating both flexibility and polarizability led to the design of many flexible polarizable force fields ([53], [60], [78], [86], [85], [98], [96], [381], [382], [111], [110], [383], [119], [98], [103], [124], [142], [151], [167], [384], [175]). The values for the reported self-diffusion coefficient from this type of force fields are gathered in Table SI–1 of the Supporting Information. In summary, some flexible polarizable models that provide quite accurate self-diffusivity values are the AMOEBA ([98], [103]), MB-pol ([384] and [385]), PFG [96], HBB2-pol [151], and POLIR [119]. As mentioned above, a purely quantitative analysis of the self-diffusivity predictions of these models is impossible due to divergence in the system size used in each study. However, the effect of grafting flexibility onto a rigid polarizable force field is the same as with the non-polarizable models. For instance, Jeon et al. [96] presented the Polarflex, a three-site flexible polarizable model for water, and compared it with its rigid version. Consistently to the studies of non-polarizable models, the self-diffusion coefficient was found to be lower for the flexible force field. Similarly, Fanourgakis and Xantheas [110] showed that the flexible version of their polarizable Thole-type model, known as TTM2.1F, was diffusing much slower (approx. 30%) compared to the rigid TTM-R [89].

2.2.4 Self-diffusion coefficient from Coarse-Grained models

Coarse-grained models have been widely employed in MD simulations to increase the accessible system size and time scales by using single particles (commonly called beads) to represent groups of nearby atoms. Nevertheless, this rough resolution of the smoothed potential energy surface can be a problem when dealing with small molecules such as water (Fuhrmans et al., [137]). Many models have been developed aiming at finding a balance between accurate representation of water properties and reasonable computational effort.

Fuhrmans et al. [137] modified SPC water model by introducing bundling through a restraining potential with tetrahedral shape geometry (four water molecules per bead). The higher hydrodynamic radius should give lower diffusion coefficient due to larger friction. However, the authors considered the SPC values for self-diffusion as four independent bundled water molecules, which gave similar but higher values (Table 1). This is believed to be likely due to coordinated movement enforced by the bundling.

Karamertzanis et al. [135] developed an anisotropic rigid-body potential to model the properties of water and the hydration free energies of neutral organic solutes. Their multipolal model includes average polarization effects of clusters of 225 – 250 water molecules and fits repulsion-dispersion parameters to liquid water experimental data. Although some properties like density are very close to the experimental value, self-diffusion was significantly underestimated (i.e., 1.4×10^{-9} m^2/s while the experimental value is 2.3×10^{-9} m^2/s at 298 K [289]).

Darre et al. [136] presented the WT4 potential, in which four interconnected beads in a tetrahedral conformation carry an explicit partial charge. Each cluster represents the movement of approximately eleven water molecules. The values of the self-diffusion coefficient obtained at different temperatures are in good agreement with experimental values.

A coarse-grained model based on Morse potential form (named CSJ) was described by Chiu et al. [134] with four water molecules per bead. The self-diffusion coefficient at 298 K is overestimated (4.3×10^{-9} m^2/s) when compared to the experimental value.

The ELBA force field, a new parameterisation of the Stockmayer potential introduced by Orsi and Essex [145], is an electrostatic based potential in which each water molecule is represented by a soft LJ sphere embedded with a point dipole. LJ and inertial parameters were tuned to capture the experimental data for the bulk density and the self-diffusion coefficient. As a result, the dynamic behaviour of water is in good agreement with experimental and molecular-scale models at 298 K and 1 bar, as clearly shown in Table 2. Table 2 shows a comparative assessment between coarse-grained models, as obtained from Orsi [176]. The ELBA force field was also used to evaluate properties of water confined within mesoporous material and representative results for diffusion coefficient behaviour along the pore radius have been reported (Yamashita and Daiguji, [268]).

Table 1: Diffusion coefficient values for SPC modified 4-water bead by Fuhrmans et al. [137].

Model	***D*** **(10^{-9} m^2/s) at 298 K**	***D*** **(10^{-9} m^2/s) at 323 K**
Model 1*	1.26 ± 0.05	1.80 ± 0.11
Model 2*	1.24 ± 0.07	1.81 ± 0.10
SPC	1.05	1.55

*The models differ by the force constant of the restraining potential and the C_{12} LJ parameter. Model 1 has a lower force constant and allows greater deformation of the water clusters. Model 2 has a fourfold higher force constant that keeps the tetrahedral conformation constant and avoids overlaps in the coarse-grained representation.

Table 2: Self-diffusion coefficient of water for different coarse-grained models at 298/300 K.

Model	***D*** **(10^{-9} m^2/s)**	**Water molecules → interaction sites**
ELBA (*)	2.16	1 → 1
SSD (*)	1.78 – 2.51	1 → 1
SSDQO (*)	2.21 – 2.26	1 → 1
M3B (*)	1.7	1 → 1
mW (*)	6.5	1 → 1
MARTINI (*)	2.0	4 → 1
P-MARTINI (*)	2.5	4 → 3
GROMOS (*)	6.9	5 → 2
WT4 (*)	2.23	11 → 4
Mie (8-6) CGW1-vle [184]	1.7	1 → 1
Mie (8-6) CGW1-ift [184]	7.4	1 → 1
Mie (8-6) CGW2-bio [184]	3.8	2 → 1
Experimental [289]	**2.3**	-

(*) References of studies reporting self-diffusivities can be found in Orsi [176].

2.3 The effect of temperature and pressure on self-diffusion coefficient

2.3.1 The effect of temperature on self-diffusion coefficient at ambient pressure

Extensive MD simulations in the range of 220 – 370 K at 1 bar have been reported in the literature (see also Table SI–2 in the Supporting Information). It should be noted, however, that only a limited number of studies have included system size corrections in the MD-calculated water self-diffusion coefficient. Such cases are the following: Wang et al. [167] reported values for iAMOEBA [167] and AMOEBA [103]; Kiss and Baranyai [179] used BK3 [160]; Tran et al. [189] used SSMP that was introduced in the same study; Qvist et al. [147] used SPC/E [39]; and Guillaud et al. [194] used TIP4P/2005f [141].

SPC/E is a rigid classical water force field; TIP4P/2005f is a flexible version of the classical rigid TIP4P/2005 water force field, while the remaining four are polarizable interaction potentials. An extensive discussion of such types of force field has been also presented earlier in Sections 2.2.1 – 2.2.3. Figure 4 shows a plot of the water self-diffusion coefficient as a function of temperature at 1 bar, considering only those studies that have reported corrections accounting for system size effects. We observe that an increase in temperature results in an increase of the self-diffusion coefficient of liquid water. The temperature dependence of the MD-calculated self-diffusion coefficient of water can be accurately described using either a Speedy–Angel power-law [386] or a Vogel–Fulcher–Tamann (VFT) equation [386]. Additional discussion on this issue will be provided in Section 2.3.3.

In Figure 4 the MD-calculated values for the self-diffusion coefficient of water are also compared with experimental data obtained from a Speedy–Angel-type correlation reported by Qvist et al. [147]. The authors reported that in the temperature range 253 – 293 K the experimental self-diffusion coefficient, obtained from NMR pulsed gradient spin echo [388] or tracer measurements [287], can be represented by the following power-law expression:

$$D_{NMR}/10^{-10}m^2s^{-1} = 159\left(\frac{T/K}{212.6} - 1\right)^{2.125} \tag{2}$$

Similarly Holtz et al. [389] reported that the available experimental data, in the temperature range 273 – 373 K, can be optimally fitted (i.e., with an error limit of $\leq 1\%$) with a Speedy–Angel power-law that has the following form:

$$D = D_o \left(\frac{T}{T_S} - 1\right)^{\gamma} \tag{3}$$

where $D_o = (1.635 \times 10^{-8} \pm 2.242 \times 10^{-11})$ m^2s^{-1}, $T_S = (215.05 \pm 1.20)$ K and, $\gamma = (2.063 \pm 0.051)$. As can be observed in Figure 4, at 1 bar all the water force fields considered, give accurate self-diffusion coefficient, with the least accurate being AMOEBA (underestimation) and SPC/E (overestimation).

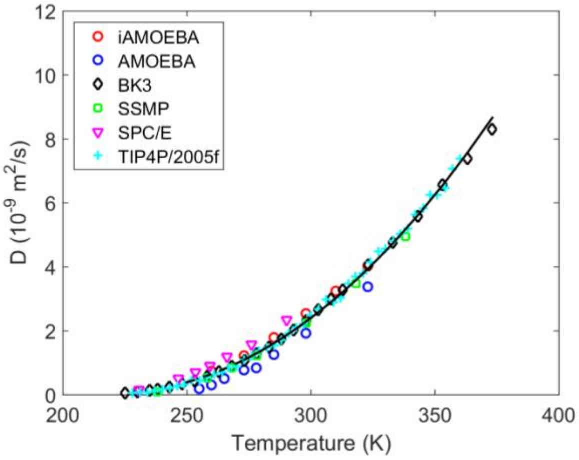
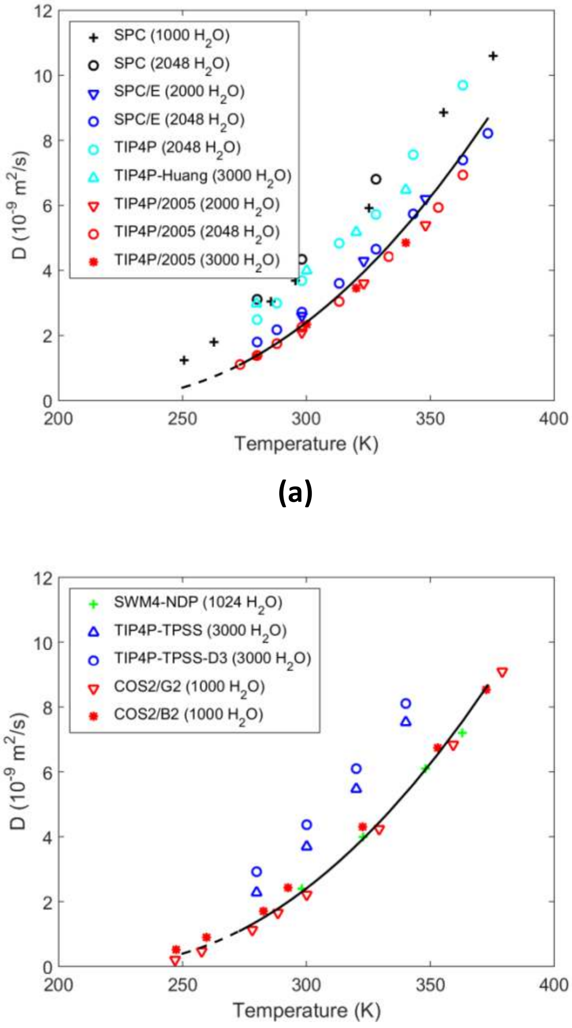


Figure 4. Water self-diffusion coefficient as a function of temperature at 1 bar. Symbols denote MD studies that have included system size corrections in the calculations: iAMOEBA [167]; AMOEBA [167]; BK3 [179]; SSMP [189]; SPC/E [147]; and TIP4P/2005f [194]. The black lines denote Speedy–Angel-type correlations of experimental data (solid line: experimental data of Holtz et al. [389] in the temperature range 273 – 373 K; dashed line: experimental data of Qvist et al. [147] in the temperature range 253 – 293 K).

Based on the discussion presented in Sections 2.1 and 2.2, we also examine the self-diffusion coefficient of water for those studies that lack corrections for system size effects, however, used 1,000 or more water molecules in the study. Figure 5 (a) shows a plot of the water self-diffusion coefficient as a function of temperature at 1 bar, considering studies ([368], [173], [139]) that used rigid non-polarizable water force fields, while in Figure 5 (b) all remaining available studies ([368], [165], and [192]), using polarizable and *ab initio* models, are collected. Among the rigid non-polarizable water force fields that are included in Figure 5 (a) are SPC [349], SPC/E [39], TIP4P [32], TIP4P-Huang [390], and TIP4P/2005 [105]. It can be seen in Figure 5 (a) that the earlier versions of the SPC- and TIP4P-type water force fields significantly over-predict the self-diffusion coefficient of water at 1 bar. The TIP4P-Huang (Huang et al. [390]) is a TIP4P-type empirical model, optimized to reproduce accurately the vapour-liquid equilibrium that also over-predicts the self-diffusion coefficient of water at 1 bar. On the other hand, for the subsequent modifications (i.e., SPC/E [39] and TIP4P/2005 [105]) the predictions of the self-diffusion coefficient of water at 1 bar are significantly improved.

Figure 5 (b) shows that the MD simulations reported by Koster et al. [192], using the water force fields TIP4P-TPSS and TIP4P-TPSS-D3, with 3,000 molecules, significantly over-estimate the self-diffusion coefficient of water at 1 bar. No further discussion was presented by the authors for the poor performance regarding the self-diffusion coefficient of these models. It should be noted that both TIP4P-TPSS and TIP4P-TPSS-D3 are force fields that were derived (Spura et al. [175]) from *ab initio* MD simulations by means of an improved force-marching scheme. On the other hand, the MD simulations that were reported by Yu and Gunsteren [368], with the polarizable models COS2/G2 and COS2/B2, using 1,000 H_2O molecules, show good agreement with the experimental values [Figure 5 (b)]. Similar behaviour is observed for the MD simulations that were reported by Stukan et al. [165] with the four-site, polarizable, SWM4-NDP (Lamourex et al. [107]) water model, using 1,024 H_2O molecules.



(a)

(b)

Figure 5. Water self-diffusion coefficient as a function of temperature at 1 bar: **(a)** Rigid classical force fields, and **(b)** Polarizable and *ab initio* force fields. Symbols denote MD studies that have considered more than 1,000 water molecules, without including any system size corrections in the calculation of the water self-diffusion coefficient. The black lines denote Speedy–Angel-type correlations of experimental data (solid line: experimental data of Holtz et al. [389] in the temperature range 273 – 373 K; dashed line: experimental data of Qvist et al. [147] in the temperature range 253 – 293 K). Sources for MD data: SPC, COS2/G2, and COS2/B2 using 1,000 H_2O (Yu and Gunsteren [368]); SWM4-NDP using 1,024 H_2O (Stukan et al. [165]); SPC/E and TIP4P/2005 using 2,000 H_2O (Moultos et al. [173]); SPC, SPC/E, TIP4P and TIP4P/2005 using 2,048 H_2O (Guevara-Carrion et al. [139]); TIP4P/2005, TIP4P-TPSS, TIP4P-TPSS-D3, and TIP4P-Huang using 3,000 H_2O (Koster et al. [192]).

The agreement between the experimental self-diffusion coefficient of water and those calculated with the ELBA coarse-grained model (as reported by Ding et al. [191]) deteriorates significantly for temperatures other than 298 K as clearly shown in Figure 6. Molinero and Moore [130] reported MD simulations of the self-diffusion coefficient of the mW coarse-grained model [130] and observed significant deviations from the experimental values. This observation was in good agreement with the work of Espinosa et al. [180]. The calculations using mW are also shown in Figure 6. The discrepancy between the two aforementioned coarse-grained models and the experimental values can be further visualized by comparing the calculated values for the activation energy, E_a. The activation energy can be obtained from the slope of the line when we plot the self-diffusion coefficient in an Arrhenius-type plot. The self-diffusion coefficient data for ELBA, from Ding et al. [191], result in a value for the activation energy, $E_a = 9.998$ kJ/mol, while the data for mW, from Espinosa et al. [180], result in a value $E_a = 12.890$ kJ/mol. When the aforementioned MD-calculated values are compared against the experimental value, $E_a = 16.566$ kJ/mol, result in 39.7% and 12.6% errors for ELBA and mW, respectively. Correspondingly, the intercept, $\ln D_o$, has a value equal to -15.913 for ELBA and -13.460 for mW, resulting in 20.5% and 1.9% errors respectively, when compared with the experimental value of -13.207.

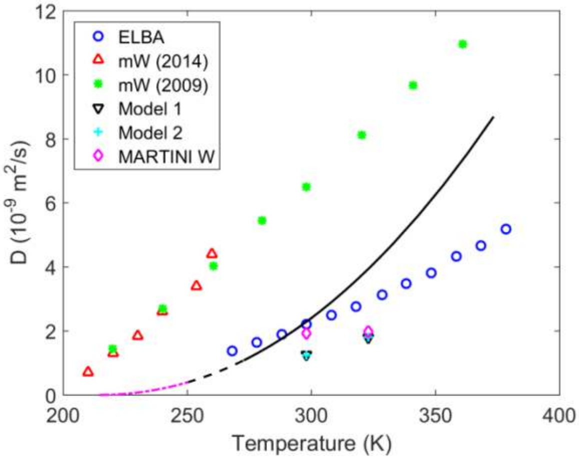


Figure 6. Water self-diffusion coefficient as a function of temperature at 1 bar for the coarse-grained water force fields ELBA (blue circles) reported by Ding et al. [191], mW (red triangles) reported by Espinosa et al. [180], mW (green stars) reported by Molinero and Moore [130]; and Model 1 (black triangles), Model 2 (cyan crosses) and MARTINI W (magenta diamonds) reported by Fuhrmans et al. [137]. The black lines denote Speedy–Angel-type correlations of experimental data (solid black line: experimental data of Holtz et al. [389] in the temperature range 273 – 373 K; dashed black line: experimental data of Qvist et al. [147] in the temperature range 253 – 293 K; dashed-dotted magenta line: extrapolation to lower temperatures of the correlation by Qvist et al. [147]).

2.3.2 *The effect of supercooled conditions on self-diffusion coefficient*

Figure 4 provides a plot of the water self-diffusion coefficient as a function of temperature at 1 bar, considering only the studies that have reported corrections accounting for system size effects. The same data are also used in Figure 7, in which the water self-diffusion coefficient is plotted as a function of the inverse temperature. Speedy–Angel-type correlations of the experimental data ([389], [147]) are also shown in Figure 4. Furthermore, the MD data of the specific six studies have been correlated using three different types of equations. Namely, an Arrhenius (ARH) law given by:

$$D_{ARH} = D_0 exp\left(-\frac{\alpha}{T}\right) \tag{4}$$

a Vogel – Fulcher – Tamann (VFT) equation:

$$D_{VFT} = exp\left[\frac{-\alpha}{(T-\beta)} - \gamma\right] \tag{5}$$

and a Speedy – Angel (SA) power law described by the following equation:

$$D_{SA} = D_o\left(\frac{T}{215.05} - 1\right)^{\gamma} \tag{6}$$

where $D_o, \alpha, \beta, \gamma$ are fit parameters given in Table 3. For the case of the Arrhenius law, $\alpha = \frac{E_a}{R}$, where *R* is the gas constant and E_a is the Arrhenius activation energy (in kJ/mol). In Table 3 the values for the percentage average absolute deviation (*% AAD*), defined as $\% AAD = 100 \times \left|\frac{D^{calc} - D^{exp}}{D^{exp}}\right|$ are also shown. The superscripts *calc* and *exp* denote the calculated and experimental values of the self-diffusion coefficient of water respectively.

Table 3. Parameters for the MD self-diffusion coefficient of water calculated using different correlations and % average absolute deviation *(% AAD*) between experimental data and correlations.

Correlation	D_o **(m^2/s)**	α **(K)**	β **(K)**	γ	***% AAD***
***ARH*-type**	2.1529×10^{-6}	2.0446×10^{3}	na	na	42.90
***VFT*-type**	na	5.6714×10^{3}	149.4743	16.0620	5.91
***SA*-type**	1.6035×10^{-8}	na	na	2.0255	7.61

na: not applicable

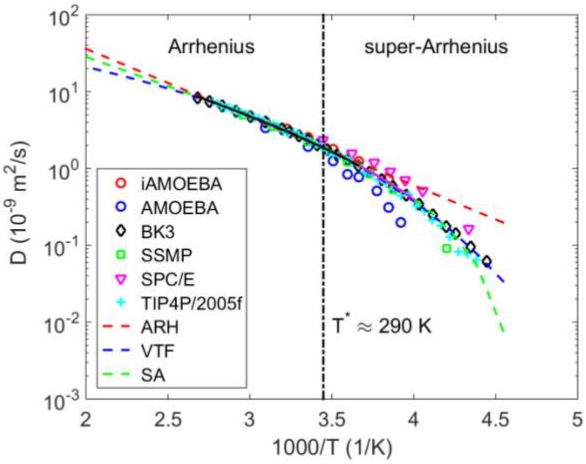


Figure 7. Water self-diffusion coefficient as a function of the inverse temperature at 1 bar. Symbol notation is the same as in Figure 4. The solid lines denote Speedy–Angel-type correlations of experimental data (black line: experimental data of Holtz et al. [389] in the temperature range 273 – 373 K; magenta line: experimental data of Qvist et al. [147] in the temperature range 253 – 293 K). The dashed lines correspond to correlations of all the MD data that included corrections based on system size effects. Colour code. Arrhenius (ARH) law: red line; Vogel–Fulcher–Tamann (VFT) equation: blue line; Speedy – Angel (SA) power law: green line.

As can be seen in Figure 7 for temperatures higher than approximately 290 K the MD data for the water self-diffusion coefficient are in excellent agreement with the Arrhenius law, a behaviour known as “Arrhenius”. On the other hand, for temperatures lower than approximately 290 K significant deviations from the Arrhenius law begin to appear, a behaviour known as “super-Arrhenius”. The deviations become stronger as we enter deeper in the supercooled region (i.e., lower temperatures). For temperatures lower than 235 K (i.e., a region also known as “no man’s land” [391]) the VFT-type equation seems to follow closer the MD self-diffusion coefficient data for the BK3 water force-field.

The value of the crossover temperature, T_x=290 K, is obtained from the study of Xu et al. [392]. The authors presented experimental measurements for the self-diffusion coefficient of water and reported that the Stokes-Einstein (SE) relation, $D \sim (\tau / T)^{-1}$ (where τ is the translational relaxation time), breaks down for temperatures below T_x. The SE relation, which is regarded as one of the *“hallmarks of transport in liquids*” according to ref [392], is replaced by the “fractional-SE” relation, $D \sim (\tau / T)^{-t}$, for temperatures below T_x, with $t \approx 0.62$. Xu et al. [392] also reported MD simulations using the TIP5P [360] water force field and identified that the “fractional-SE” relation, with $t \approx 0.77$, is applicable for temperatures lower than $T_x \approx 320$ K. The authors pointed out that the crossover temperature, T_x, seems to roughly coincide with the onset of the increase of the population of water molecules with LDA-like structure (i.e., low density amorphous solid water). At the same time a decrease occurs for the population of water molecules with HDA-like structure (i.e., high density amorphous solid water).

In the related literature ([11], [392], [393], [394]) different values for the crossover temperature, T_x, have been used and consequently the discussion on where the “Arrhenius” and “super-Arrhenius” regions are located, can change accordingly. Let, for example, consider $T_x \cong T_S \approx 225$ K, which is the temperature where thermodynamic and dynamic properties exhibit power law divergences. In that case, for $T > T_x$ the self-diffusion coefficient of water obeys “Arrhenius” behaviour, termed also as “strong” behaviour. On the other hand, for $T < T_x$ the self-diffusion coefficient of water obeys “super-Arrhenius” behaviour, termed also as “fragile” behaviour. Thus during cooling of water a “fragile”-to-“strong” (FTS) liquid transition will occur upon crossing T_x [393]. Alternatively, the extent to which the shear viscosity, η, deviates from the Arrhenius law, $\eta = \eta_0 \exp\left(-\frac{E}{k_B T}\right)$, constitutes the basis for classifying the liquids as either "strong" or "fragile" [11]. An FTS liquid transition has been reported by Starr et al. [79] who performed MD simulations for the self-diffusion coefficient of water using the SPC/E [39] force-field in a wide range of temperatures, T, and densities, ρ. Their study covered the following region of the $T-\rho$ plane: ($210 < T < 300$ K and $0.9 < \rho < 1.4$ g cm^{-3}).

The behaviour of the self-diffusion of water at the supercooled conditions and the connection to other water anomalies has attracted significant scientific attention. This issue has been addressed by both experimental and computational studies. Mallamace et al. [394] analysed experimental measurements in the pressure range 0.1 – 800 MPa and temperature range 252 – 400 K for the isothermal compressibility, K_T, defined as $K_T = -\left(\frac{\partial \ln \rho}{\partial \ln P}\right)_T$, and the coefficient of isobaric thermal expansion, α_P, defined as $\alpha_P = -\left(\frac{\partial \ln \rho}{\partial T}\right)_P$. The authors found that a temperature T^* exists ($T^* \sim 315 \pm 5$ K), such that K_T shows a minimum for all pressures considered. Furthermore, all the $\alpha_P(T)$ curves that are measured at different pressures cross at the cross-over temperature, T^*, resulting thus at a "singular and universal expansivity point" with a value equal to $\alpha_P(T^*) \approx 0.44 \times 10^{-3}$ K^{-1}. The particular temperature T^* is the border between two distinct behaviours (indicating two distinct regions) that can be also clearly identified in the self-diffusion coefficient of water. Namely, for $T < T^*$ the self-diffusion coefficient of water has a maximum value that, as T increases, shifts to lower values of P and eventually disappears near T^*. This is the "super-Arrhenius" region. On the other hand, for $T > T^*$ the self-diffusion coefficient of water has a more regular behaviour and obeys an Arrhenius law, shown in Eq. (4).

Subsequently, we used the MD data from the six studies (at 1 bar) that have reported self-diffusion coefficient of water, accounting for corrections for system size effects, to calculate the corresponding parameters for an Arrhenius-type equation. Results for the fitting of each water force field separately are shown in Table 4, along with the combined fitting for all six water force fields. Furthermore, we examine two different temperature ranges for fitting the MD data and we compare with the results obtained from experimental measurements. Namely, we consider: (i) the entire temperature range, and (ii) temperatures that are higher than approximately 270 K. In agreement with the previous discussion, we observe clearly that when we limit the fitting to the higher temperature range, a significant improvement is obtained upon comparison with the experimental data. From the six models considered in Table 4, the correlations of BK3 and iAMOEBA show better agreement with the experimental measurements for the self-diffusion coefficient of water at 1 bar, while the correlations of SPC/E and AMOEBA exhibit the highest errors.

Table 4. Parameters of fitting the MD self-diffusion coefficient of water at 1 bar, using an Arrhenius-type equation, for various water force fields.

Study	**Model**	***T*-range (K)**	**E_a (kJ/mol) All *T*'s**	**ln(D_o (m^2/s)) All *T*'s**	**% *AAD* in E_a All *T*'s**	**E_a (kJ/mol) *T*>270 K**	**ln(D_o (m^2/s)) *T*>270 K**	**% *AAD* in E_a *T*>270 K**
Qvist et al. [147]	SPC/E	230–290	19.978	-11.58	20.59	17.891	-12.46	8.00
Wang et al. [98]	iAMOEBA	260–323	17.148	-12.92	3.51	16.511	-13.16	0.33
Wang et al. [98]	AMOEBA	255–323	22.319	-11.17	34.73	20.842	-11.73	25.81
Kiss & Baranyai [179]	BK3	225–373	16.658	-13.19	0.56	15.912	-13.45	3.95
Tran et al. [189]	SSMP	238–338	18.508	-12.52	11.72	17.730	-12.80	7.03
Guillard et al. [194]	TIP4P/2005f	228–360	17.474	-12.87	5.48	17.346	-12.91	4.70
	Combined	**225–373**	**17.247**	**-12.96**	**4.11**	**16.825**	**-13.11**	**1.56**
Experimental: [147], [389]		**273–373**	**16.566**	**-13.21**				

Scala et al. [395] used the SPC/E [39] water force field to calculate the liquid entropy *S*, the vibrational entropy, S_{vib}, of the liquid constrained in one typical basin of the potential energy landscape, and the configurational entropy, S_{conf}, (defined as: $S_{conf} \equiv S - S_{vib}$) for the same state points considered in the earlier study of Starr et al. [79]. Scala et al. observed that both S_{conf} and *D* exhibit maxima which become more pronounced with decreasing temperature. Furthermore, they observed that the maxima occur at $\rho \approx 1.15$ g cm^{-3}. Figure 8 clearly demonstrates the remarkable correlation between the qualitative behaviours exhibited by both S_{conf} and *D*. For the case of SPC/E water force field and the range of parameters examined, it was also found that the Adams-Gibbs equation, given as $D \sim \exp\left(-\frac{B}{TS_{conf}}\right)$, holds.

An alternative approach to connect thermodynamic and dynamic (i.e., transport) properties of dense fluids is also provided by excess entropy scaling relationships for transport properties. The excess entropy, S_{ex}, is defined as the difference, $S_{ex} \equiv S - S_{ig}$, between the entropy of the fluid, *S*, and the entropy of the ideal gas, S_{ig}. Transport properties including diffusivity, viscosity and thermal conductivity can be conveniently reduced to dimensionless form using reduction factors based on kinetic theory. It has been shown, initially by Rosenfeld [397], and subsequently by others ([396], [398]) that for a wide range of simple liquids the following semi-empirical scaling relationship is valid: $X^*(T) \sim \exp(b(\rho)S_{ex})$, where X^* denotes dimensionless transport properties, $b(\rho)$ is a *T*-independent parameter that depends on both the nature of the interactions and the transport property, and ρ is constant. Chopra et al. [399] used the following dimensionless, translational self-diffusion coefficient, $D^* = D\frac{(\rho/M)^{1/3}}{(k_BT/M)^{1/2}}$, where *M* is the molecular weight. S_{ex} accounts for all intermolecular correlations (i.e., two-, three-, and higher body). Chopra et al. considered also the simpler case of only the translational contributions to the excess entropy and accounting only for the two-body contributions, $S_{(2)}$. The authors employed the SPC/E water force field and (i) confirmed the validity of the Rosenfeld-type scaling for the self-diffusion coefficient of water and (ii) confirmed the behaviour described by Starr et al. [79] in Figure 8.

Yan et al. [400] used the TIP5P [360] water model to investigate the relationship between the excess entropy and the anomalies of water. They found that the two-body excess entropy adequately predicts the regions of structural, dynamic, and thermodynamic anomalies of water as well as the location of the Widom line (see also Section 2.3.3. for additional details). In two recent studies, using the TIP4P water force field, Gallo et al. ([182]) and Corradini et al. ([188]) have shown that if S_{ex} is approximated with $S_{(2)}$, (i.e., the two-body term of the excess entropy), the same FTS transition of the diffusion coefficient is found. Namely, the aforementioned simulation studies indicate that the two-body term shows the FTS crossover and, therefore, captures the features of water behaviour also in the high-density side.

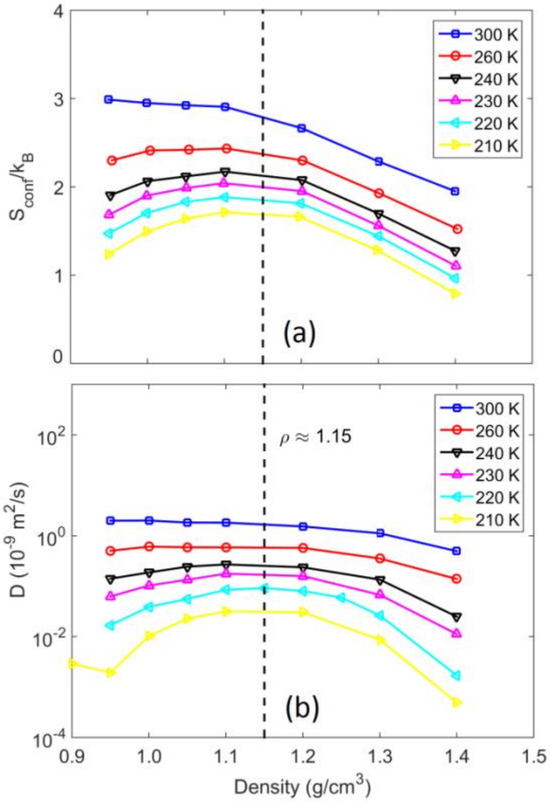


Figure 8. Density dependence for: **(a)** SPC/E water configurational entropy (Scala et al. [395]), and **(b)** water self-diffusion coefficient using SPC/E model (Starr et al. [79]). Symbols denote MD simulations for six isothermal paths (from top to bottom: 300 K, 260 K, 240 K, 230 K, 220 K, and 210 K).

2.3.3 The effect of temperature on self-diffusion coefficient at high pressures

As discussed in the previous section, Mallamace et al. [394] analysed experimental measurements in the pressure range 0.1 – 800 MPa and temperature range 252 – 400 K, and pointed out the existence of a temperature T^* ($T^* \sim 315 \pm 5$ K) that clearly identifies the border between two distinct behaviours for the self-diffusion coefficient of water.

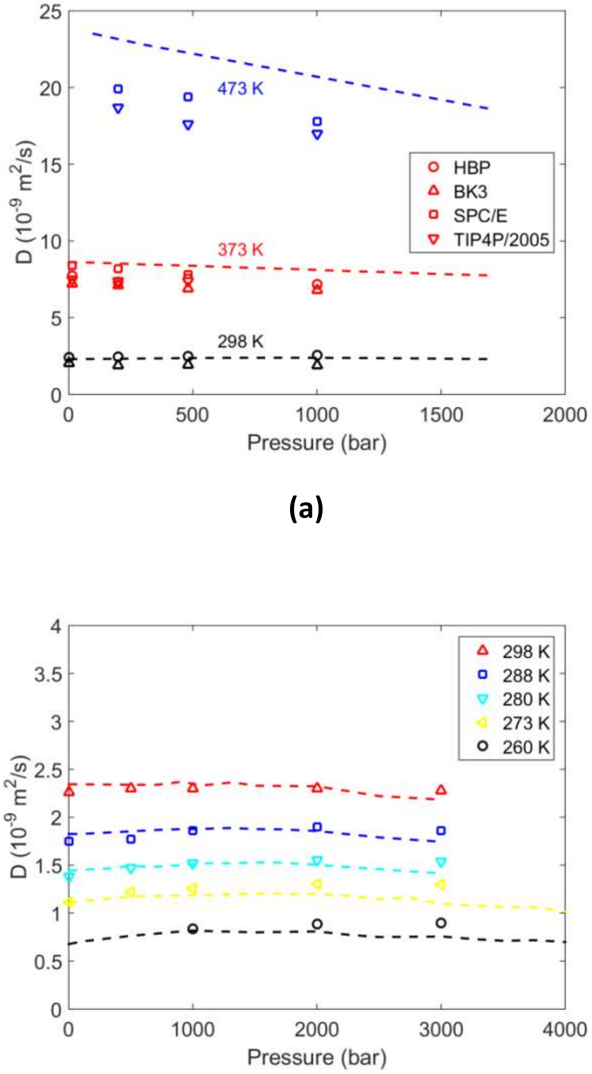
Starr et al. [79] reported extensive MD simulations for the self-diffusion coefficient of water using the SPC/E [39] force-field in a wide range of temperatures, T, and densities, ρ. However, due to computational limitations they performed simulations with 216 water molecules. They also reported that no significant effect in their limited study of larger systems (i.e., 1,728 water molecules at 190 and 200 K and 1 g cm^{-3}) was observed. The discussion presented previously in Section 2.1 clearly indicates that at least 1,000 water molecules are required to significantly reduce the errors introduced by the finite system size effects. Subsequently, Mittal et al. [112], and Chopra et al. [399] performed similar simulations with a larger number (500) of SPC/E water molecules. The use of a larger system is expected to shift the calculated self-diffusion coefficient to higher values. Both studies were in reasonable agreement with the experimental behaviour described by Mallamace et al. [394].

Only a limited number of MD studies have considered the effect of pressure on the self-diffusion coefficient of water and simultaneously addressed adequately the issue of system size effects. Studies that provided corrected MD values for the water self-diffusion coefficient include Jiang et al. [190] who reported results using the HBP, BK3, and TIP4P/2005 water force fields, and Tran et al. [189] who reported results using the SSMP and TIP4P-Ew force fields. These studies explored the effect of pressure on the water self-diffusion coefficient for various isotherms. Kiss and Baranyai [179] used BK3 [160] and examined the effect of temperature on the water self-diffusion coefficient at 1,500 bar.

A number of studies, that used more than 1,000 water molecules, have also examined the effect of pressure on the self-diffusion coefficient of water, without providing any further corrections to the MD values, to account for system size effects. Xu et al. [106] used 1,728 ST2 water molecules, Guevara-Carrion et al. [139] used 2,048 TIP4P/2005 water molecules, Moultos et al. [173] used 2,000 SPC, SPC/E, and TIP4P/2005 water molecules. Furthermore, a detailed list of studies in which less than 1,000 water molecules were used can be found in the Supporting Information (Table SI–1)

To examine the applicability of the observation by Mallamace et al. [394] to the MD-calculated self-diffusion coefficient of water, we plot them as a function of pressure for various isotherms. As shown in Figure 9, the overall picture is consistent with the conclusions reported by Mallamace et al. [394]. We observe a weak dependence on pressure for the lower temperatures, which increases at higher temperatures. The agreement between the MD and the experimental values is better at lower temperatures, while deviations increase at higher temperatures. Figure 9 (a) shows the pressure dependence of *D* for the HBP, BK3, SPC/E and TIP4P/2005 water force fields, at 298, 373, and 473 K. The MD data are compared with the experimental values reported by Krynicki et al. [289]. Figure 9 (b) shows the pressure dependence of *D* for the TIP4P/2005 water force fields, at 260, 273, 280, 288, and 298 K (i.e., case with $T < T^*$). MD data are compared with the experimental data of Prielmeier et al. [292]. The MD data follow closely the experimental values and indicate the existence of a maximum value. The existence of the maximum in Figure 9 (b) would be clearer if data at higher pressures were available.

To this purpose, in Figure 10 we show a plot of the MD simulation for various force fields at 298 K. For this temperature, MD simulations are available for pressures up to 10 kbar for the cases of TIP4P-Ew and SSMP, reported by Tran et al. [189]. Both water force fields exhibit a maximum for the self-diffusion coefficient at 298 K. Furthermore, excellent agreement between experimental values and MD simulations are found for the case of SSMP.



(a)

(b)

Figure 9. Self-diffusion coefficient of water as a function of pressure for various isotherms. Symbols denote the MD simulations and dashed lines denote experimental measurements. Lines and symbols of the same colour correspond to the same temperature. **(a)** MD data for HBP and BK3 water models are from Jiang et al. [190] (with corrections for system size effects included), while for SPC/E and TIP4P/2005 are from Moultos et al. [173] (using 2,000 water molecules). **(b)** MD data for TIP4P/2005 are from Guevara-Carrion et al. [139] (using 2,048 water molecules). Experimental values for (a) are from Krynicki et al. [289], while for (b) from Prielmeier et al. [292].

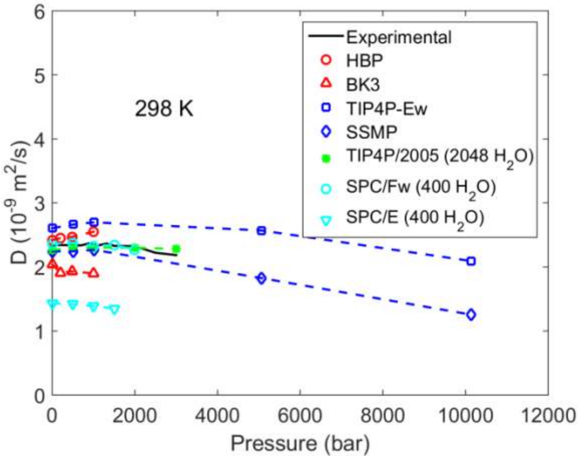


Figure 10. Self-diffusion coefficient of water plotted as a function of pressure at 298 K. Symbols denote the MD simulations and black solid line denotes experimental measurements (Prielmeier et al. [292]). The dashed lines connecting the MD data points are guides to the eye only. The MD data for HBP and BK3 water models (from Jiang et al. [190]) and for TIP4P-Ew and SSMP (from Tran et al. [189]) have included corrections for system size effects. Data for TIP4P/2005 are from Guevara-Carrion et al. [139] (using 2,048 water molecules), while for SPC/Fw and SPC/E are from Raabe and Sadus [148] (using 400 H_2O molecules).

In addition to studying the effect of pressure and temperature on the self-diffusion coefficient under constant temperature or pressure conditions respectively, the behaviour of the self-diffusivity along the two-phase (i.e., Vapour – Liquid equilibrium, VLE) coexistence curve is also of interest. Figure 11 shows the available MD calculations of the self-diffusion coefficient plotted as a function of temperature, along the liquid branch of the VLE curve. The experimental data used for the comparison are from the work of Yoshida et al. [295].

Bauer and Patel [126] introduced the polarizable water force field TIP4P-QDP-LJ and used it to calculate water self-diffusion coefficient, among other properties. The reported values for self-diffusivity are corrected in order to account for system size effects. Figure 11 shows excellent agreement with the experimental values, for the entire range considered (i.e., up to 600 K). The model predicts the following critical properties: $T_c = 623$ K, $P_c = 250.9$ atm, and $\rho_c = 0.351$ g cm^{-3}. These values should be compared against the experimental: $T_c = 647.1$ K, $P_c = 218$ atm, and $\rho_c = 0.322$ g cm^{-3}.

In Figure 11 simulation data from two versions of the coarse-grained model introduced by Lobanova et al. [184] are also shown. The model employs a single interaction site (bead) to represent a water molecule. Based on the use of different target properties during the parameter optimization two versions were introduced. Namely, the Mie (8-6) CGW1-vle model was parameterised to match the saturated-liquid density and vapour pressure; while the Mie (8-6) CGW1-ift model was parameterised to match the saturated liquid density and vapour–liquid interfacial tension. The authors attributed the overestimation of the water self-diffusion coefficient by the Mie (8-6) CGW1-ift model to the fact that the coarse-grained models have a higher mobility since the water molecules are not slowed down by the re-orientation of the hydrogen atoms and the formation/break-up of hydrogen bonds. Significant over-estimation of the diffusion coefficient occurred at low temperatures, and became comparable with the experimental values at the higher-temperature limit considered (approx. 350 – 400 K). On the other hand, the authors attributed the under-estimation of the water self-diffusion coefficient by the Mie (8-6) CGW1-vle model to the fact that the large values of the energetic well of the potential, resulting from the use of the vapour pressure as the target property. A third version was also developed, Mie (8-6) CGW2-bio, where two water molecules were considered per coarse-grained bead. For the particular version only a single value at 298 K and 1 bar has been reported (see also Table 2).

Finally, the simulations reported by Guissani and Guillot [59] using 256 SPC/E [39] water molecules, and by Yoshida et al. [295] using 256 TIP4P water molecules are shown also in Figure 11. Very good agreement is observed between the MD simulations and the experimental values for both the SPC/E and TIP4P water force fields. However, no corrections for system size effects were included in the reported self-diffusion coefficient. Therefore, upon inclusion of the corrections a shift to higher values is expected for both SPC/E and TIP4P, resulting eventually in the over-estimation of the self-diffusivity. This behaviour is consistent with the discussion presented in Sections 2.1 and 2.3.1 (see also Figures 4 and 5 (a)).

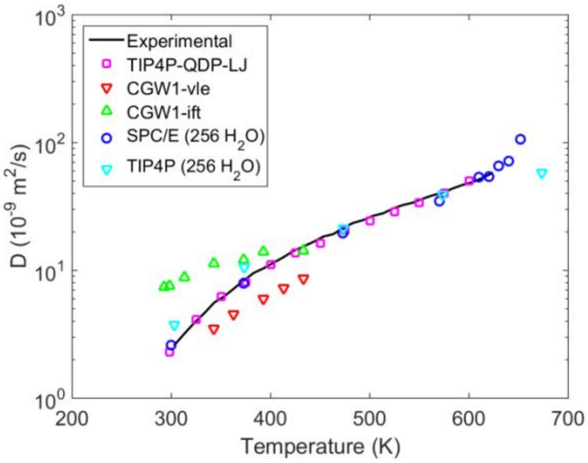


Figure 11. Self-diffusion coefficient of liquid water as a function of temperature along the VLE line. Symbols denote the MD simulations and black solid line denotes experimental measurements by Yoshida et al. [295]. Sources for MD data: TIP4P-QDP-LJ [126]; Mie (8-6) CGW1-vle and Mie (8-6) CGW1-ift [184]; SPC/E [59]; TIP4P [295].

The study of diffusion phenomena at near-critical or supercritical conditions for water is significant for geological processes. Despite their importance, only a limited number of simulation studies have explored this region for the case of water. Nieto-Draghi et al. [92] calculated water self-diffusion coefficient for the following four force fields: TIP4P [32], TIP5P [360], SPC/E [39], and DEC [87]. In all simulations they used 256 water molecules. They reported good agreement at high densities (e.g., between 2% and 5% at $\rho = 0.65$ g cm^{-3}), while the highest disagreement ($\approx 15\%$) was found for the low densities and was attributed to the lack of polarizability of the models. For all force fields considered, over-predictions of the self-diffusivities were observed. Please note that the deviations are expected to increase further, if corrections for system size effects are incorporated. Shvab and Sadus [187] reported calculations for water self-diffusion coefficient using the TIP4P/2005 [105] and TIP4P/2005f [141] force fields, at 670 K, using 1,728 H_2O molecules, without corrections for system size effects. They found better agreement for the flexible force field. The rigid force field was found to underestimate the water self-diffusion coefficient by approximately 2 – 10% in the first half of the density range. They attributed the higher values of TIP4P/2005f to the elongated O-H bond, which results in a higher dipole moment. Yoshida et al. [116] reported self-diffusivities using 1,000 TIP4P H_2O molecules, at 673 K, without corrections for system size effects. On the other hand, Tainter et al. [183] calculated water self-diffusion coefficient using the E3B3 (which accounts for three-body interactions) and TIP4P/2005 [105] force fields at 673 K, with their study also accounting for system size corrections. The authors used experimental values for the shear viscosity to correct for finite-size effects, instead of using MD-calculated values, as already discussed earlier.

Figure 12 shows a comparison of the MD-calculated values for the water self-diffusion coefficient, using the aforementioned models, with the experimental measurements reported by Lamb et al. [290]. The authors measured experimentally the self-diffusion coefficient of compressed supercritical water as a function of pressure, in the temperature range 673 to 973 K, using the NMR spin-echo technique. The specific experimental data are probably the only available water self-diffusion data at supercritical conditions. For all four models considered, we observe a good agreement between experimental and MD values for the self-diffusivity, especially for densities that are higher than the critical density.

Gallo et al. [182] in a seminal study used available experimental data and performed extended MD simulations with the TIP4P/2005 water model (4,096 water molecules), to study the thermodynamic properties of water in the temperature range 600 to 800 K and the pressure range 175 to 400 bar. They demonstrated that the lines connecting the maxima of the response functions (i.e., the constant pressure-specific heat, C_P; the isobaric thermal expansion coefficient, α_P; and the isothermal compressibility factor, K_T) converge in a single line (i.e., Widom Line – WL) as they approach the critical point. Note that a similar WL has also been found in the deeply supercooled region.

The WL, found in the supercritical region, delineates a crossover from liquid-like to gas-like behaviour. This behaviour is clearly visible in other transport properties as well. For example, if we plot the shear viscosity as a function of temperature, for various isobars, we can observe that in the liquid-like portion, all curves show a strong decrease of viscosity with temperature. In the gas-like portion, the change of slopes is not as strong. The same picture was obtained by Galo et al. [182] for the case of the inverse self-diffusivity of TIP4P/2005 [105] water. In a subsequent study, Corradini et al. [188] extended the previous analysis to TIP3P [32], TIP4P [32], TIP5P [360], and SPC/E [39] water force fields and obtained similar behaviours.

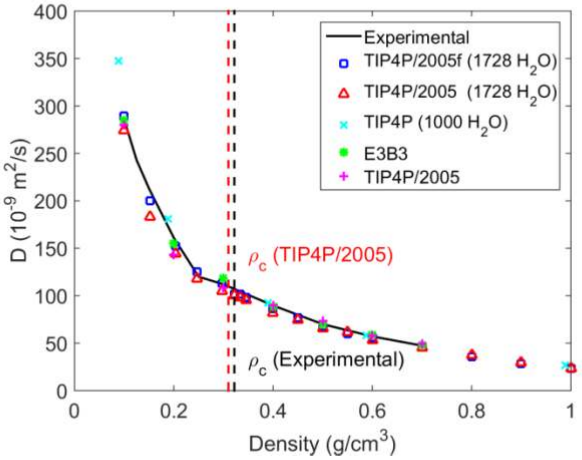


Figure 12. Self-diffusion coefficient as a function of density for supercritical water along the isotherm of 673 K. Symbols denote the MD simulations and black solid line denotes experimental measurements by Lamb et al. [290]. The vertical dashed lines denote the critical density values. Experimental (black): $\rho_c = 0.322$ g cm^{-3}; TIP4P/2005 (red): $\rho_c = 0.31$ g cm^{-3}. Sources for MD data: E3B3 and TIP4P/2005 (magenta cross) are at 673 K from Tainter et al. [183] with system size corrections incorporated. TIP4P/2005 (red triangles) and TIP4P/2005f are at 670 K from Shvab and Sadus [187] using 1,728 H_2O molecules, while TIP4P are at 673 K from Yoshida et al. [116] using 1,000 H_2O molecules, without any further corrections for system size effects.

3. Self-diffusion coefficient of water in confinement

The self-diffusion of confined water has been evaluated in the recent literature for a variety of confining systems. These systems constitute of materials differing in their chemical nature, shape, size, and surface charge distribution, features that significantly impact structural and transport properties of the confined fluid near the interface. Carbon compounds, minerals, zeolites, gold plates, surfactants, and biomolecules have been employed as the confining material in calculating water self-diffusion coefficient via MD simulations. Figure 13 presents the distribution of published articles in the open literature (in %, out of 109 papers) with calculated self-diffusion coefficient of water in different confining materials, showing the predominance of minerals and carbon compounds (see also Table SI–3 of the Supporting information).

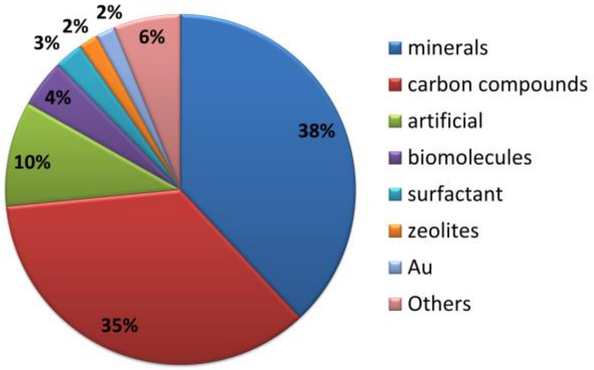


Figure 13. Distribution of published articles in the open literature (in %) with calculated self-diffusion coefficient of water in different confining materials.

3.1 Carbon compounds

Most of the data found in the literature are related to carbon compounds as the confining material. Usually analysed at room temperature, water self-diffusivity is commonly calculated through Einstein's and Green-Kubo's method using mostly the SPC/E [39] force field, but also SPC [358], TIP3P [32], and variations of TIP4P [32]. The values for water self-diffusion coefficient differ considerably even between the same confining material depending on density, temperature, and size of confinement.

Striolo [198] has proposed that the diffusion of water in carbon nanotubes can be described by three different mechanisms depending on the time evolution of the mean squared displacement. When water molecules move in a chaotic manner and overcome one another in the direction of motion, the mean squared displacement varies linearly with time, which entails a Fickian regime. Nevertheless, when water molecules are confined in such a way that resembles an one-dimensional path, the mean squared displacement scales with the square root of time, and such a mechanism is called single-file diffusion. The intermediary mechanism is characterized by a ballistic regime where the mean square displacement is proportional to the square of time. In a subsequent work, Striolo [199] has shown that water diffusion in a carbon nanotube doped with carboxyl group (which makes the surface hydrophilic) obeys different mechanisms compared to water diffusion in a pure hydrophobic carbon nanotube. Moreover, the self-diffusion coefficient of water is significantly lower in the doped carbon nanotube.

Geometry is a key factor on transport properties of confined fluids. Nie et al. [200] calculated SPC/E [39] water self-diffusion coefficient in carbon nanotubes built with three different geometries for the cross-sectional area: circular, square, and triangular. By varying the chirality of the nanotube, the same trend is observed for all three different geometries, finding the lowest self-diffusion coefficient values for water molecules confined by a CNT (8,8), although the values are different for different cross-sectional areas.

A question that might emerge in these calculations is how one can separate the effect of the interface and the effect of confinement. Zheng et al. [201] investigated such a limit using TIP4P-Ew water molecules within carbon nanotubes. They claimed that the effect of the confinement is relevant for nanotubes up to 16 Å of diameter. The volume fraction, ϑ, of water molecules that feel the interactions with the wall constitutes a scaling parameter for the water self-diffusion coefficient in confinement. Chiavazzo et al. [202] showed that the relation between the self-diffusion coefficient of water within carbon nanotubes and the bulk water self-diffusion coefficient scales linearly with ϑ.

Martí and Godillo [203] analysed the SPC/E [39] water self-diffusion coefficient in carbon nanotubes with different chiralities at high temperatures (between 573 and 773 K). The logarithm of such self-diffusion coefficient depends almost linearly with the inverse of temperature, especially for CNT (10,10) and CNT (12,12), which shows that an Arrhenius behaviour may also be present in confinement.

Investigating spatial variation of the diffusion coefficient and its directional components, Farimani and Aluru [204] calculated the diffusion coefficient for SPC/E [39] water confined by (10,10), (20,20) and (30,30) carbon nanotubes and noticed that diffusion enhancement is evident near the surface for all studied cases. The spatial variation of axial diffusion coefficient depends on the size of the nanotube, being sharper in the (20,20). As the diameter increases, a bulk-like region is observed at the centre of the nanotube and the effect of surface diminishes as expected. For carbon nanotubes with diameter d < 2.2 nm, the average axial diffusion coefficient is lower than the bulk because confinement plays a dominant role. For 2.3 nm < d < 6.0 nm, diffusion coefficient is higher than the bulk one, reaching a maximum at d = 2.7 nm due to surface contribution to depletion of hydrogen bonds and the existence of a bulk region for normal diffusion of molecules. For d > 6.0 nm, the average self-diffusion coefficient is close to the bulk value. The average axial self-diffusion coefficient for carbon nanotubes with different diameters is shown in Figure 14. Data from Liu and Wang [205] are also included for comparison, showing some differences between the two works. As the carbon nanotube diameter increases, the water self-diffusion coefficient approaches the bulk value.

Farimani and Aluru [204] also presented an evaluation of the diffusion mechanisms described previously (Striolo [198]) and claimed that for diameters d < 1.5 nm the diffusion mechanism is non-Fickian; i.e., it might be either a transition state (for the (7,7) carbon nanotube) or single-file diffusion, in the case of (8,8) nanotube. For 1.6 nm< d < 2.3 nm and d > 4.0 nm, Fickian diffusion is observed. When 2.4 nm < d < 4.0 nm, a transition between a Fickian and a ballistic mechanism is observed.

Carbon compounds were also widely studied as slit pores in the form of parallel sheets of graphite (Hirunsit and Balbuena [206]; Sanghi and Aluru [207]) and graphene (Mozaffari [208]; Muscatello et al*.* [209]). Sendner et al*.* [210] confined water between plates of a diamond-like structure and analysed the perpendicular diffusion coefficient as the surface hydrophobicity was changing. Using the SPC/E [39] force field, they found that when the material becomes more hydrophilic, surface binding and trapping of water alter the pure diffusive regime observed previously.

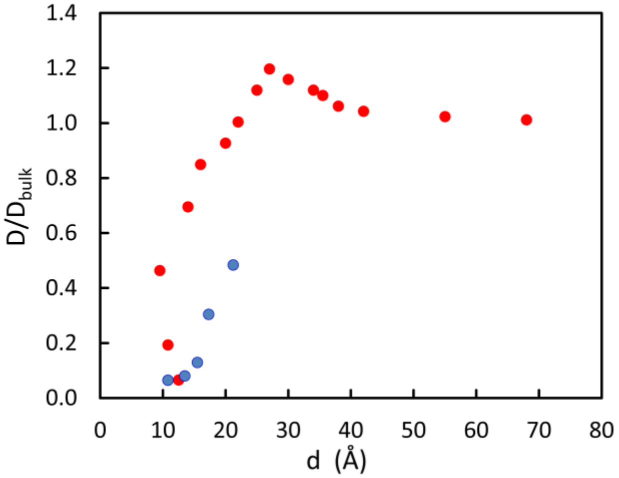


Figure 14. Ratio between axial self-diffusion coefficient of water confined in carbon nanotubes and bulk water self-diffusion coefficient as a function of the carbon nanotube diameter. Blue circles, 298 K, 1000 kg·m^{-3}, SPC water model (Liu and Wang, [205]). Red circles, 300 K, 1000 kg·m^{-3}, SPC/E water model (Farimani and Aluru, [204]).

Nguygen and Bhatia [211] studied water dynamics in activated carbon fibers, due to their importance on adsorption-based processes. The authors tried to capture the influence of structural disorder and to create a more realistic model to evaluate water diffusion on nanoporous carbons. A transition between Fickian and single-file diffusion mechanisms that depend on the temperature was found. They observed that the self-diffusion coefficient increases with the temperature and is higher for lower adsorption loadings. Diallo et al. [212] also simulated water confined by activated carbon fibers. They evaluated the diffusion coefficient of supercooled water (220 ≤ T ≤ 280 K) and compared the results with experimental data from quasi-elastic neutron scattering. They concluded that the self-diffusion of confined water is lower than the self-diffusion coefficient of bulk water, but comparable to water in carbon nanotubes and other porous media of similar pore size.

Martí et al. studied the dynamic properties of water confined between graphite (Gordillo and Martí, [213]) and graphene (Martí et al., [214]) plates using a flexible SPC water force field and evaluated the changes with temperature. In other studies, they calculated the diffusion coefficient for SPC water at different densities (Martí et al. [215], Tahat and Martí, [216], Martí et al., [217]), showing its evolution with a growing distance from the surface. Mosaddeghi et al. [218] also investigated the confining effect of graphite on the water self-diffusion coefficient by changing the density and the slit pore size. The methods used to calculate the diffusion of SPC/E [39] water were Green-Kubo and Einstein's and the results were comparable, with restrictions for smaller sizes due to high oscillations of the velocity auto-correlation function.

Graphite was also used as a hydrophobic model for biomaterials. Surface properties influence material performance and their understanding is extremely important for biomedical applications (Spera et al., [219]). Water-surface interaction has considerable influence on the biocompatibility of implant materials (Wei et al., [220]), macromolecular association and protein assembly (Choudhurry and Pettit, [221]). Wei et al. [220] used MD simulations to understand the difference between biocompatibility of carbon (in graphite form) and TiO_2. They found that diffusion of SPC/E [39] water on graphite is higher than on titanium oxide due to the stronger interaction between water and TiO_2 surface, which could explain the greater affinity of the human organism with this material once the cells would interact with water instead of the material directly. This work showed that the surface chemistry has more impact on the diffusion of water compared to the slit pore size.

Kim et al. [222] reported the self-diffusion coefficient of SPC/E [39] water confined between two graphene plates and between plates of graphene and mica at the opposite ends of confinement. The presence of different surface features give rise to competition between ordering induced by water interaction with mica and pure diffusive flow induced by graphene.

3.2 Minerals

This important class of materials covers silica, clays, mica, hydroxyapatite, rutile and other known minerals. They are extremely relevant to a wide variety of processes, such as catalysis and separation (Spohr, [223]), nanofluidics (Leng and Cummings, [224]) and in the food and cosmetic industry (Porion et al., [225]). Particularly the presence of water gives rise to interesting phenomena, e.g., interfacial water tends to form hydrogen bonds with hydrophilic mineral surfaces, ordering the water layers and reducing diffusion (Ou et al., [226]).

Magnesium oxide [$Mg(OH)_2$] shows a potential for use in water environment remediation and industrial water treatment. Although magnesium oxide has a hydrophilic nature, unlike most minerals, Ou et al. [226] observed a modest effect on the dynamic behaviour of water near the $Mg(OH)_2$ confining surface and no adsorption sites. Their study with flexible SPC water found self-diffusion coefficient in the same order of magnitude as bulk water. They have also shown that the parallel diffusion is twice the value of the perpendicular diffusion, corroborating that water moves more freely in the unconfined directions, as expected.

The confinement of water between mica surfaces, which are highly hydrophilic, has an important relation to biolubrication, ion channels and clay swelling (Leng and Cummings [224], Li et al. [227]). Leng and Cummings [224] studied TIP4P water confined between two parallel mica surfaces at different pressures, 1 and 150 bar, and noted the same behaviour for both cases: significant drop of the diffusion coefficient near the wall to roughly four orders of magnitude lower than bulk value, indicating strong interactions of water with mica.

Feldspar, a mineral that hosts contaminants such as uranium within its intra-grain fractures, was used in the MD study by Kerisit and Liu [228] as confining material to study the self-diffusion coefficient of SPC/E [39] water. The value of the parallel diffusion coefficient increased with the distance from the surface, while the perpendicular one has a behaviour related to the density profile. Computing the average self-diffusion coefficient, they discovered the presence of an interfacial region 2.0 – 2.5 nm wide, where the self-diffusion coefficient in confinement is significantly smaller than in the bulk phase and that surface effects only become negligible for confinement width of several tens of nanometers.

The major component of carbonate rocks is calcite, an important mineral for CO_2 sequestration, oil exploration, and other geological processes. Mutisya et al. [229] found that the water dynamics are affected by the interaction between water and calcite surface reducing the self-diffusion coefficient and inducing water layering. The calculation of the parallel coefficient was performed according to the method of Liu et al. [230], using a flexible SPC/Fw water model. Mutisya et al. [229] found values smaller than the bulk self-diffusion for pores ranging from 1.0 to 6.0 nm wide, with confinement effects enhanced for the narrowest pore due to overlap of surface effects.

The interaction with the material surface can affect the local environment and modify water dynamics under confinement. This has been investigated by Prakash et al. ([231],[232]) for hydroxyapatite (i.e., a component of bone mineral phase which is used as scaffold for bone repair). Prakash et al. [232] characterized water transport properties by MD simulations applying different water potentials and found that the SPC/E [39] water together with the core-shell potential for hydroxyapatite is the most accurate combination for predicting diffusion properties. With these models, Prakash et al. [231] calculated the anisotropic self-diffusion coefficient of the second-order diffusion tensor and found that the perpendicular component is significantly lower than the parallel ones for all the studied widths. The calculation of transport properties showed a dependency on the size of the nanopore, confirming the work of Pham et al. [233], which showed this behaviour for water confined in hydroxyapatite pores from 2.0 to 6.0 nm wide at different temperatures.

Titanium dioxide (TiO_2) is present in many applications such as photo-catalysis, solar cells, optical sensors, bone implants, and biomedical coatings. Předota et al. [234] confined water in a TiO_2 slit pore and analysed the axial profile of parallel and perpendicular self-diffusion coefficient of SPC/E [39] water at 298, 448, and 523 K. The diffusion coefficient was shown to increase with temperature and, for all cases, the perpendicular component was found to be smaller than the parallel one. In the same study three regions between the confining walls were identified: the first layer near the surface where the self-diffusion coefficient is nearly zero, an inhomogeneous area were the diffusion changes with the surface distance, and a bulk-like region beyond a distance of 1.5 nm from the walls. Solveyra et al. [235] and Cao et al. [236] studied SPC/E [39] water self-diffusion inside rutile nanopores with different diameters and found that the self-diffusion coefficient are significantly reduced near the surface due to strong bonding with water. Solveyra et al. [235] suggested that, due to the first compact monolayer of water formed near surface, it is possible to compare the results with a less hydrophobic material of smaller radius.

Several works use silica as confining material to study water dynamics due to this mineral's importance in catalysis and separation technology. Either as parallel planes or cylindrical pores, self-diffusion of water was analysed to assess water behaviour with changes in pore size (Zhang et al. [237], Renou et al. [238], Dickey and Stevens [239]), temperature (Ishikawa et al. [240], Patsahan and Holovko [241]), surface composition (Siboulet et al. [242], Jeddi and Castrillón [243], and Lerbret et al. [244]), and water content (Spohr et al. [223]). The results show that, due to its hydrophilic nature, silica has a strong interaction with water which significantly decreases the diffusion coefficient near the surface due to partial adsorption of water layer near the walls. This effect was also noticed for higher temperatures. The diffusion coefficient increases with temperature, hydration, and with pore size, but decreases with density (Patsahan and Holovko [241]).

Silica can be also found as calcium silicate hydrate, which is present at the construction industry, as it is important for the strength, cohesion, and durability of the cement paste. Qomi et al. [245] analysed how different compositions of calcium and silicon affect physicochemical properties of water confined in these hydrophilic media. The self-diffusion coefficient was found to increase with increasing density. This anomalous behaviour is explained by a decrease on the diffusion energy barrier, which is the activation energy required for a water molecule to escape its dynamical cage. The mobility of water near the walls was strongly composition dependent and much slower than in the bulk phase due to strong interactions with the surface. This behaviour was confirmed by Hou and co-workers ([246]– [248]).

Another class of minerals is formed by clays. Mass transfer through clay nanopores is important for groundwater hydrology, petroleum and gas engineering, and environmental applications (Boek [250], Boţan et al. [251]). Boţan et al. [251] employed the method by Liu et al. [230] to calculate the diffusion of SPC/E [39] water inside Na-montmorillonite pores from 2.0

to 9.0 nm wide and found that the self-diffusion at 300 K is reduced to 70% of the bulk value near the walls due to the higher density and surface effects. Boek [250] studied the parallel self-diffusion of water in montmorillonite for the cases of sodium, potassium, and lithium as the monovalent cation using the TIP4P water force field. He found smaller values of the diffusion coefficient for K-montmorillonite in comparison to the other metals. Rao et al. [252] also analysed water inside Na-montmorillonite and showed results for higher pressures and temperatures.

Other types of clays were also used as confining media for studying water dynamics: Zhou et al. [253] built sepiolite cells and showed that water confined inside this magnesium-rich clay has a much lower self-diffusion coefficient compared to water confined in montmorillonite. Smirnov and Bougeard [254] investigated SPC water dynamics between kaolinite surfaces, where the diffusion coefficient was calculated to be less than 5% of the bulk value near the walls. Michot et al. [255] evaluated SPC/E water diffusion confined between saponite, for different temperatures (i.e., 250 to 350 K) and obtained Arrhenius plots for the parallel component of the diffusion tensor.

3.3 Biomolecules

Stanley et al. [256] performed MD simulations to study the relation between dynamic transitions of biomolecules and dynamic properties of water. The TIP5P [360], and ST2 [28] potentials were chosen to describe water confined by lysozyme and DNA. It was shown that the self-diffusion coefficient of water exhibits Arrhenius behaviour at lower temperatures and a crossover to non-Arrhenius behaviour at approx. 245 K. The possibility that protein glass transition results from a change in behaviour of hydration water was stated in the same study. Sega et al. [257] investigated the diffusion behaviour of water close to a protein (GME ganglioside), considering the anisotropic nature of the fluid diffusion. For SPC water, they found that the parallel component is higher than the perpendicular one and both of them are one order of magnitude lower than the bulk near the protein surface.

Interested in chitosan/chitin films for food packaging, McDonnell et al. [258] evaluated the effects of increasing humidity on properties such as solvation, oxygen permeability, and diffusivity. Concerning the self-diffusivity of TIP4P water, they found an increase of one order of magnitude when the relative humidity varied from 15% to 95%. A strong O_2 attraction to protonated amine groups is overcome by water self-diffusivity, which means that reducing the latter will reduce the overall oxygen permeability.

Hua et al. [259] studied water dynamics to understand the kinetics of hydrophobic collapse and molecular self-assembly on biological environment. SPC water confined between BphC enzyme, a two-domain protein, showed lower self-diffusivity near the surface. Its mobility was also affected by surface geometry, hydrophobicity, and size of confinement – for domain separation of 2.0 nm, the water behaviour was bulk-like at the centre of the inter-domain region.

3.4 Other confining media

Data are also available for theoretical confining media and some less frequently used materials, which are summarized in this section. Other confining materials with available self-diffusion coefficient data are ionomers (Berrod et al., [260]), aluminum phosphate nanotubes (Gavazzoni et al., [261]), polyamide RO membranes (Ding et al., [262]), boron nitride nanotubes (Won and Aluru [263]), and surfactants such as Newton Black films (Di Napoli and Gamba, [264]).

Several works are dedicated in the study of dynamical properties of water confined between general hydrophobic/hydrophilic media described by LJ potential. Beckstein and Samson [265], Brovchenko et al. [266], Cui [267], Yamashita and Daiguji [268], and Köhler et al. [269] confined water inside a cylindrical pore and analysed the influence of properties such as density, temperature, and pore radius on water self-diffusion. The authors agreed that hydrophilic walls slightly decrease diffusion in comparison to the bulk value, while hydrophobic walls can increase water self-diffusion up to three times the bulk value. The parallel and perpendicular components were also considered and for all cases the value was higher for the perpendicular component. Brovchenko et al. [266] found that the perpendicular components are closer in value to the parallel ones if the confining media is hydrophobic.

Kumar and co-workers ([270], [271]), Bai and Zheng [272], and Choudhurry [273] studied water under parallel plates. They evaluated the behaviour with temperature changes, density variations, high pressure and hydrophobic/hydrophilic nature. Bauer et al. [274] used different water force fields for the calculation of self-diffusivity inside hydrophobic plates and found that TIP4P showed an enhancement on the parallel component of the diffusion coefficient relative to bulk. This was explained based on a reduction on the molecular dipole moment of water in comparison to the average bulk value, weakening the intermolecular interaction of confined water and enhancing diffusion. Han et al. [275] observed a transition from a ballistic to a diffusive regime for TIP5P [360] water confined within hydrophobic parallel plates at different temperatures.

Different geometries were also considered as confining media for studying water dynamics. Marañón Di Leo and Marañón [276] confined SPC/E [39] water within rectangular prismatic nanotubes and calculated values for parallel and perpendicular components of the diffusion coefficient for water in both hydrophilic and hydrophobic walls, considering SPC/E bulk water diffusion value as 2.265 x 10^{-9} m^2/s. These microporous crystalline structures have high selectivity, chemical stability and mechanical strength, and therefore are widely used as membranes for adsorption. Han et al. [277] evaluated kinetic and structural properties of TIP4P-Ew water confined inside 1-D and 3-D pore zeolites and studied the self-diffusivity to get insights on the effect of confinement in water dynamics, finding that the self-diffusion coefficient inside 1-D hydrophobic pores zeolites was approximately one order of magnitude higher than the self-diffusivity computed in the 3-D pores. Shirono and Daiguji [278] calculated water's self-diffusion coefficient inside zeolites considering the polarization of water by using the SPC-FQ potential. The calculated value agreed with the SPC/E calculations and the experimental data and they concluded that the variation of the dipole moment does not affect the dynamic properties.

Ju et al. [279] analysed the effect of pore width on water confined between two parallel Au plates at 400 K. Using the F3C [76] water potential, it was shown that for all plate distances the parallel component of the diffusion coefficient was larger than the perpendicular one but both increased with the gap size. Due to the interaction between water and Au atoms, the molecules near the surface were adsorbed forming a water layer, while for the largest gap (2.5 nm) the central region showed bulk-like behaviour.

Lane et al. [280] used gold as a substrate to study the properties of confined water between self-assembly monolayers (SAMs) of alkanethiols. SAMs are often used on surface modification to control surface interactions at the atomic level and are very important for nanofluidics and biomedical systems. They simulated water dynamics with the SPC/E [39] potential at 300 K and showed that there is an increment in the diffusion coefficient increasing water thickness. They concluded that geometry and water ordering, due to surface interaction, reduce diffusion by a factor of 100 in comparison to bulk water.

3.5 Methods and system size effect

The usual way to calculate the self-diffusion coefficient through MD simulation data is by applying either Einstein, or its analogue, Green-Kubo method. Such an approach is a possibility to interpret the time evolution of the particles mean squared displacement, or the time integral of the velocity auto-correlation function. This possibility is restricted to some assumptions that are frequently overlooked. The most important of these restrictions is the fluid density homogeneity. Although this is the case for bulk systems, for confined media such a hypothesis is invalid. The solid walls impose an inherent inhomogeneity on the confined fluid. This spatial variation of the fluid density inside the pore must be considered, especially close to the wall surface where the magnitude of such a variation can be extremely large. Moreover, for a confined fluid, the self-diffusion coefficient is no longer a simple scalar, but a diagonal second-order tensor, with components differing in different directions (Franco et al., [281]).

Notwithstanding the exposed rationality, in most of the literature, we continue to observe the employment of the Einstein, or Green-Kubo, method to calculate self-diffusion coefficient of confined fluids. There have been some developments of new methods to calculate the self-diffusion coefficient of confined fluids, considering the tensorial nature of such a coefficient and the intrinsic inhomogeneity of the confined media (Liu et al., [230]; Franco et al., [282]; Mittal et al., [283]; von Hansen et al., [284]; Carmer et al., [285]).

As well as for the bulk fluid, the system size effect in the calculation of the self-diffusion coefficient within MD simulations with periodic boundary conditions must be taken into account. Recently, Simonnin et al. [286] derived analytical expressions that consider the hydrodynamic effects between periodic images for LJ particles confined within slit-pores. They found that the finite-size effects are minimized in elongated boxes (for a ratio of approximately than 2.8 between the height, *H*, and the length, *L*). Nevertheless, for other pore geometries, no correction for finite-size effects in confinement is currently available in the open literature to the best of our knowledge. Table 5 shows the ratio *H*/*L* for several calculations of the confined water parallel self-diffusion coefficient in different minerals at 300 K.

Table 5. Aspect ratio (*H*/*L*) for confined SPC/E water self-diffusion coefficient in different minerals at 300 K.

Ref.	Mineral	$D_{\text{parallel}}/D_{\text{bulk}}$	H/L
Kerisit and Liu [228]	Feldspar	0.817	1.95
Kerisit and Liu [228]	Feldspar	0.913	3.89
Ou et al. [226]	$Mg(OH)_2$	0.494	3.30
Mutisya et al. [229]	Calcite	0.574	0.56

4. Conclusions and Future Outlook

In the current review we presented a detailed overview of molecular scale simulation studies examining the self-diffusion coefficient of water. In Section 2 we discussed issues related to the self-diffusion coefficient of water in the bulk phase, while in Section 3 we discussed the effect of confinement on the self-diffusion coefficient of water.

Numerous researchers, utilizing a wide range of different force fields (e.g., rigid, flexible, polarizable, *ab initio*, etc.) have calculated the water self-diffusivity at a limited number of state points. However, only a handful of studies have performed a consistent and systematic exploration of the $P-T$, or $P-\rho$ plane. The particular problem is further exacerbated by the common practice of using a few hundred molecules, which can lead to a significant deviation between the simulated (i.e., finite system size) and real (i.e., thermodynamic limit) self-diffusivity. A notable exception is the recent works of Gallo et al. [182], and Corradini et al. [188] who considered the TIP4P/2005, TIP3P, TIP4P, TIP5P, and SPC/E water force fields, in a wide temperature and pressure range, limited however, within the supercritical region. The authors used 4,096 water molecules minimizing thus the finite size effects. On the other hand, within the supercooled region, the extensive studies of Starr et al. [79], Mittal et al. [112], and Chopra et al. [399] were limited by the use of less than 1,000 SPC/E water molecules. In addition, the studies of Guevara-Carrion et al. [139] that used 2,048 TIP4P/2005 water molecules; Moultos et al. [173] that used 2,000 SPC/E, and TIP4P/2005 water molecules; and the study of Jiang et al. [190] that reported results using the HBP, BK3, and TIP4P/2005 water force fields, explore only a limited range of the $P-T$ plane of interest.

Therefore, to the best of our knowledge to this day, there is no specific molecular simulation study, using any water force field, that can satisfy simultaneously the following two criteria: (i) performed MD simulations of the water self-diffusivity at a wide T and P range, including the supercritical and the supercooled regions, and (ii) correctly accounting for system size effects by either incorporating corrections to the reported self-diffusivity values or by using a large number of water molecules (e.g., larger than 1,000). Consequently, the conclusions regarding the performance of the examined water force fields, with respect to the self-diffusivity, need to be based on partial information. The discussion is further hampered by the lack of experimental measurements at various regions of interest that could be used for force field validations.

Nevertheless, based on the available information the following recommendations can be made regarding the computation of the water self-diffusivity. Six water force fields seem to be promising in providing reasonable predictions in a wide *T* and *P* range: Namely, the three polarizable force fields TIP4P-QDP-LJ, BK3, and HBP, the two-body, rigid TIP4P/2005, and flexible TIP4P/2005f, and the three-body E3B3. These force fields are good candidates for identifying the best model to consider in a future systematic study of the self-diffusivity of water. Among the issues that need to be discussed further, is the computational cost associated with using each one of the aforementioned force fields, considering the amount of computations that a systematic study would require.

Regarding the case of water in bulk, possible future contributions in the following research directions would be beneficial:

- Performing MD simulations with the most successful force fields, at high pressures, in order to verify if the self-diffusion coefficient exhibit maxima at isotherms (when T<315 K).
- A systematic study for *T*'s in the supercooled region, including corrections for system size effects.
- Delineating the crossover temperature where the Stokes-Einstein theory is replaced by the fractional Stokes-Einstein and calculation of the fractional exponent, *t*. This effort would require the systematic study, using MD simulations, of the shear viscosity in addition to the self-diffusivity.
- Improve the performance of coarse-grained models regarding their ability to calculate accurately the water self-diffusivity in a wide *T* and *P* range.

On the other hand, regarding the case of water under confinement, possible future contributions in the following areas would be beneficial:

- The establishment of a methodology to accurately calculate the self-diffusion coefficient in confined media via MD, including an adequate theoretical framework to account for system size effects.

- A broader comparison between different force fields is still lacking, including the most successful ones for the bulk phase, to calculate confined water self-diffusion coefficient.

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SUPPLEMENTARY MATERIAL

Self-Diffusion Coefficient of Bulk and Confined Water: A Critical Review of Classical Molecular Simulation Studies

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Contents

TABLE SI-1. Available MD simulation data of the self-diffusion coefficient of water at ambient conditions. "**Ref #**" corresponds to the reference (see Reference list at page 71) of the study reporting the self-diffusion coefficient value. "***T***", "**P**", and "***ρ***" correspond to the conditions at which the simulations are performed. "**SSE correction**" indicates if the data are corrected for system size effects (see ref [76]). "**H_2O Ref #**" lists the original H_2O model development papers.

Ref #	Authors	Year	*T* (K)	*P* (bar)	ρ (g/cm^3)	*D* (m^2/s) (x 10^9)	Statistical Error	SSE correction	Number of H_2O molecules	H_2O force field	H_2O Ref #
3	Rahman et al.	1975	295.15		1	0.73	N/A	No	216	CF	3
4	Stillinger & Rahman	1978	302.65	1.01325		1.1	N/A	No	216	CF modified	4
5	Impey et al.	1982	294		1	2.3	0.2	No	125	MCY	175
6	Jorgensen et al.	1983	294.15	1.01325		4.3	10%	No	125	BF	176
	"----//----"	1983	293.15	1.01325		3.2	10%	No	125	TIPS2	177
9	Lie & Clementi	1986	300		0.998	1.8	N/A	No	343	MCYL	9
	"----//----"	1986	299		0.998	1.9	N/A	No	343	MCYL	9
	"----//----"	1986	300.6		0.998	1.9	N/A	No	343	MCYL	9
	"----//----"	1986	300.6		0.998	2.1	N/A	No	343	MCYL	9
10	Neumann	1986	293		1.0	2.8	N/A	No	256	TIP4P	6
11	Wojcik & Clementi	1986	296		1	2.25	N/A	No	512	MCY	175
	"----//----"	1986	304		1	1.3	N/A	No	512	MCY + *ab initio* 3 body	11
12	Anderson et al.	1987	300		1	2.54	N/A	No	125	SPC modified (flex.)	12
13	Berendsen et al.	1987	306		0.998	2.50	N/A	No	216	SPC/E	13
	"----//----"	1987	308		0.97	4.30	N/A	No	217	SPC	178
14	Reddy & Berkowitz	1987	268		0.999	1.36	N/A	No	216	TIP4P	6
	"----//----"	1987	298		0.999	2.96	N/A	No	216	TIP4P	6
15	Teleman et al.	1987	301			4.4	0.1	No	216	SPC-type; R1 (rigid)	15

	"----//----"	1987	301			2.6	0.1	No	216	SPC-type; R2 (rigid)	15
	"----//----"	1987	301			6.10	0.2	No	216	SPC-type; F (flexible)	15
16	Ahlstrom et al.	1989	303			8.9	N/A	No	216	PSPC - GD	16
	"----//----"	1989	301			0.80	N/A	No	216	PSPC - P(P)	16
	"----//----"	1989	300			0.77	N/A	No	216	PSPC - P(I)	16
	"----//----"	1989	302			0.04	N/A	No	216	PSPC - LD	16
	"----//----"	1989	302			2.0	N/A	No	216	PSPC	16
17	Watanabe & Klein	1989	298		0.997	2.4	0.4	No	216	SPC/E	13
	"----//----"	1989	298		0.997	3.6	0.5	No	216	SPC	178
	"----//----"	1989	298		0.997	3.3	0.5	No	216	TIP4P	6
	"----//----"	1989	298		0.997	1.1	0.3	No	216	WK	17
18	Caldwell et al.	1990	303		0.991	3.1	0.5	No	216	POL1	179
	"----//----"	1990	300		0.998	2.5	N/A	No	216	SPC/E	13
19	Wallqvist et al.	1990			1.0	1.3	0.1	No	216	NEMO	19
20	Ruff & Diestler	1990	298	1		2.2	N/A	No	256	BJH	203
21	Sprik et al.	1990	295	0		1.5	0.4	No	216	Pol	21
22	Straatsma & McCammon	1990	303.6	1.7	0.994	3.1	N/A	No	216	STR/1	22
26	Sprik	1991	300	600	1	2.4	N/A	No	216	Pol.	26
27	Zhu et al.	1991	298		0.997	1.6	N/A	No	256	MST-FP	27
28	Zhu et al.	1991	298	1.01325	0.997	7.1	N/A	No	256	SPC-FP	28
29	Wallqvist & Teleman	1991	300			3.6	0.2	No	216	SPC-flex (harmonic)	29
	"----//----"	1991	300			3.1	0.2	No	216	SPC-flex (unharmonic)	182
	"----//----"	1991	300			4.2	0.2	No	216	SPC-rigid	178
30	Smith & Haymet	1992	298		1	1.44	0.06	No	216	CF	4
	"----//----"	1992	298		1	1.16	0.06	No	216	RCF (rigid)	30
	"----//----"	1992	298		1	3.7	0.1	No	216	SPC	178
31	van Belle et al.	1992	300		1	4.6	0.2	No	216	SPC	178
	"----//----"	1992	300		1	2.4	0.2	No	216	PSPC	16
	"----//----"	1992	300		1	2.7	0.3	No	216	PSPC-PPD	31
34	Rick et al.	1994	298		1	1.9	0.1	No	256	TIP4P-FQ	34
	"----//----"	1994	298		1	1.7	0.1	No	256	SPC-FQ	34
35	Smith & Dang	1994	298		0.997	2.4	0.3	No	216	RPOL	180

	"----//----"	1994	298		0.997	2.4	0.4	No	216	SPC/E	13
36	Svishchev & Kusalik	1994	298.15		0.998	2.15	N/A	No	108	SPC/E	13
	"----//----"	1994	298.15		0.998	2.24	N/A	No	256	SPC/E	13
37	Padro et al.	1994	298		1	2.5	N/A	No	216	SPC (flex)	178
39	Astrand et al.	1995	300			1.0	N/A	No	216	NEMO modified	39
40	Soetens & Millot	1995	298.15		1	1.7	N/A	No	216	SPEP/SPEP	40
	"----//----"	1995	298.15		1	1.4	N/A	No	216	SPEP/TPEP	40
	"----//----"	1995	298.15		1	6.1	N/A	No	216	TPEP/TPEP	40
	"----//----"	1995	298.15		1	4.4	N/A	No	216	SPEP/1SITE	40
41	Duan et al.	1995	307.15	1		3.06	N/A	No	256	RWK2	181
42	Mountain	1995	303		0.997	2.7	N/A	No	216	RPOL	180
43	Brodholt et al.	1995	298.15		1	2.3	N/A	No	256	TIP4P-Polarizable	43
44	Svishchev et al.	1996	298		0.997	2.6	2%	No	256	PPC	44
47	Taylor et al.	1996	298		1	3.02	N/A	No	526	SPC/E	13
49	Dang & Chang	1997	298		0.995	2.1	0.1	No	550	TIP4P-type (Polarizable)	49
50	Levitt et al.	1997	273		0.999	1.6	N/A	(see ref)	216	F3C	50
	"----//----"	1997	298		0.997	2.4	0.23	(see ref)	216	F3C	50
51	Lobaugh & Voth	1997	300		0.996	4.2	N/A	No	125	Quantum SPC/F	51
	"----//----"	1997	300		0.996	3.0	0.2	No	125	Classical SPC/F	182
	"----//----"	1997	300		0.996	3.8	N/A	No	125	Quantum SPC/F_2	51
	"----//----"	1997	300		0.996	2.2	0.2	No	125	Classical SPC/F_2	51
52	de Leeuw & Parker	1998	300		1.15	1.15	N/A	No	256	SW	52
55	Nymand & Linse	2000	303.15		Exp. Dens.	0.786	0.002	No	216	NEMO (SC)	39
	"----//----"	2000	303.15		Exp. Dens.	0.813	0.002	No	216	NEMO (ES)	39
	"----//----"	2000	303.15		Exp. Dens.	0.837	0.002	No	512	NEMO (ES)	39
	"----//----"	2000	303.15		Exp. Dens.	1.20	0.002	No	216	NEMO (RF)	39
	"----//----"	2000	303.15		Exp. Dens.	1.00	0.002	No	512	NEMO (RF)	39
	"----//----"	2000	303.15		Exp. Dens.	1.17	0.002	No	216	NEMO (RF)	39
	"----//----"	2000	303.15		Exp. Dens.	2.75	0.002	No	216	SPC/E (RF)	13
	"----//----"	2000	303.15		Exp. Dens.	3.13	0.002	No	216	SPC/E (RF)	13
	"----//----"	2000	303.15		Exp. Dens.	0.799	0.002	No	216	NEMO (SC)	39
	"----//----"	2000	303.15		Exp. Dens.	0.820	0.002	No	216	NEMO (ES)	39

	"----//----"	2000	303.15		Exp. Dens.	0.855	0.002	No	512	NEMO (ES)	39
	"----//----"	2000	303.15		Exp. Dens.	1.20	0.002	No	216	NEMO (RF)	39
	"----//----"	2000	303.15		Exp. Dens.	1.00	0.002	No	512	NEMO (RF)	39
	"----//----"	2000	303.15		Exp. Dens.	1.16	0.002	No	216	NEMO (RF)	39
	"----//----"	2000	304.15		Exp. Dens.	2.77	0.002	No	216	SPC/E (RF)	13
	"----//----"	2000	305.15		Exp. Dens.	3.13	0.002	No	216	SPC/E (RF)	13
56	Guo & Zhang	2001	303		0.999	2.63	0.06	No	256	SPC/E	13
57	Mahoney & Jorgensen	2001	298.15	1.01325		3.85	0.09	No	267	SPC	178
	"----//----"	2001	298.15	1.01325		2.49	0.05	No	267	SPC/E	13
	"----//----"	2001	298.15	1.01325		5.19	0.08	No	267	TIP3P	6
	"----//----"	2001	298.15	1.01325		3.31	0.08	No	267	TIP4P	6
	"----//----"	2001	298.15		0.993	5.06	0.09	No	267	TIP3P	6
	"----//----"	2001	298.15		0.990	3.29	0.05	No	267	TIP4P	6
	"----//----"	2001	298.15		0.999	2.62	0.04	No	267	TIP5P	183
58	Stern et al.	2001	298.15	1.01325		1.81	0.06	No	256	POL5/TZ	58
	"----//----"	2001	298.15	1.01325		1.25	0.05	No	256	POL5/QZ	58
59	van Maaren & van der Spoel	2001	300		0.997	3.66	0.19	No	820	SWFLEX-AI	59
	"----//----"	2001	300		0.997	3.58	0.02	No	820	SWFLEX-ISO	59
	"----//----"	2001	300		0.996	3.22	0.15	No	820	SWRIGID-AI	59
	"----//----"	2001	300		0.993	3.30	0.34	No	820	SWRIGID-ISO	59
60	Lefohn et al.	2001	300		1.0	1.5	N/A	No	256	2S-PF (Two-State PolarFlex)	60
	"----//----"	2001	300		1.0	1.9	N/A	No	256	3S-PF (Three-State PolarFlex)	60
63	Burnham & Xantheas	2002	300		1.046	2.23	N/A	No	64	TTM2-R	63
64	Guo et al.	2002	303.8		0.999	2.63	0.06	No	256	SPC/E	13
	"----//----"	2002	273.5		1.011	1.27	0.03	No	256	SPC/E	13
65	English & MacElroy	2002	298.15		0.997	2.3	0.1	No	256	SPC/F (flexible)	182
	"----//----"	2002	298.15		0.997	3.4	0.1	No	256	TIP4P	6
	"----//----"	2002	298.15		0.997	2.0	0.1	No	256	TIP4P-FQ	34
68	Tan et al.	2003	298	668.745	0.997	2.24	N/A	No	256	SSD0 (original)	184
	"----//----"	2003	298	1.01325	0.958	2.37	N/A	No	256	SSD0 (original)	184
	"----//----"	2003	298	1.01325	0.99	2.13	N/A	No	256	SSD1 (optimized)	68
69	Yu et al.	2003	300	1.01325		4.3	N/A	No	1331	SPC	69

	"----//----"	2003	300	1.01325		4.0	N/A	No	1331	STR/1	22
	"----//----"	2003	300	1.01325		3.5	N/A	No	1331	STR/RF	69
	"----//----"	2003	300	1.01325		2.7	N/A	No	1331	COS/B1	69
	"----//----"	2003	300	1.01325		2.6	N/A	No	1331	COS/B2	69
70	Jeon et al.	2003	300		0.997	2.44	0.04	No	256	PRG (PolarFlex Rigid Gausian)	70
	"----//----"	2003	300		0.997	2.40	0.03	No	256	PRG (PolarFlex Rigid Gausian)	70
	"----//----"	2003	300		0.997	2.29	0.07	No	256	PFG (PolarFlex Flexible Gausian)	70
	"----//----"	2003	300		0.997	2.28	0.04	No	256	PFG (PolarFlex Flexible Gausian)	70
	"----//----"	2003	300		0.997	3.0	N/A	No	256	SPC/F (flexible)	182
71	English & MacElroy	2003	260		1.002	0.83	N/A	No	500	F-SPC	182
	"----//----"	2003	298		0.997	2.3	N/A	No	500	F-SPC	182
	"----//----"	2003	298		0.996	2.1	N/A	No	502	TIP4P-FQ	182
72	Ren & Ponder	2003	298		1.0004	2.02	0.05	No	216	AMOEBA	72
73	Spangberg & Hermansson	2003	298		0.998	2.32	0.10		128	SPC/E	13
	"----//----"	2003	298		0.998	2.43	0.03		256	SPC/E	13
	"----//----"	2003	298		0.997	2.57	0.03		512	SPC/E	13
	"----//----"	2003	298		0.998	2.58	0.03		1024	SPC/E	13
	"----//----"	2003	298		0.978	4.08	0.05		512	SPC	178
74	Amira et al.	2004	300		1.000	2.55	N/A	No	512	SPC+CCL	74
	"----//----"	2004	300		1.000	2.57	N/A	No	512	F-SPC	182
75	Horn et al.	2004	272.2	1.01325	0.9996	1.2	0.02	No	512	TIP4P-Ew	75
	"----//----"	2004	297.4	1.01325	0.9954	2.4	0.06	No	512	TIP4P-Ew	75
76	Yeh & Hummer	2004	298	1		6.05	N/A	YES		TIP3P	6
77	Yu & Gunsteren	2004	302.8		0.9972	2.3	N/A	No	1000	COS/G2	77
	"----//----"	2004	302.0		1.0000	2.6	N/A	No	1000	COS/G3	77
79	Saint-Martin et al.	2005	298.15	1.01325		1.16	N/A	No	1000	MCDHO$_{fc}$	185
	"----//----"	2005	298.15	1.01325		1.09	N/A	No	1000	MCDHO$_{ff}$	186
	"----//----"	2005	298.15	1.01325		0.92	N/A	No	1000	MCDHO$_{r}$	79
	"----//----"	2005	298.15	1.01325		0.9	N/A	No	1000	MCD	79
80	Abascal & Vega	2005	298.15	1	0.9979	2.08	N/A	No	530	TIP4P/2005	80

82	Lamoureux et al.	2006	298.15	1.01325		2.33	0.02	No	250	SWM4-NDP	82
83	Wu et al.	2006	298.16	1.01325	0.977	4.02	0.01	No	216	SPC	178
	"----//----"	2006	298.16	1.01325	0.999	2.41	0.08	No	216	SPC/E	13
	"----//----"	2006	298.16	1.01325	0.986	5.3	0.07	No	216	TIP3P	6
	"----//----"	2006	298.16	1.01325	1.01	2.76	0.07	No	216	SPC/Fd	187
	"----//----"	2006	298.16	1.01325	1.004	2.62	0.01	No	216	F3C	50
	"----//----"	2006	298.16	1.01325	1.034	3.53	0.11	No	216	TIP3P/Fs	188
	"----//----"	2006	298.16	1.01325	1.012	2.32	0.05	No	216	SPC/Fw	83
84	Paesani et al.	2006	298.15	1.01325	0.999	2.4	0.1	No	216	q-SPC/Fw	84
	"----//----"	2006	298.15	1.01325	0.991	3.2	0.1	No	216	SPC/Fw	83
85	Fanourgakis et al.	2006	300	1.01325		1.4	N/A	No	256	TTM2.1-F	85
86	Donchev et al.	2006	298.15	1.01325		1.2	N/A	No	256	QMPFF2	86
	"----//----"	2006	298.15	1.01325		1.9	N/A	No	256	QMPFF2	86
	"----//----"	2006	298.15	1.01325		2.6	N/A	No	256	NCC	189
	"----//----"	2006	298.15	1.01325		1.3	N/A	No	256	NEMO	19
	"----//----"	2006	298.15	1.01325		2.2	N/A	No	256	TTM2-R	63
89	Hofmann et al.	2007	298	1	1.06	1.42	N/A	No		Hofmann et al.	89
90	De Fusco et al.	2007	300	1.01325	1.105	2.63	N/A	No	216	DPP	90
93	Kolafa	2008	298.15	-0.97	0.997048	2.52	0.05	No	1000	POL3	190
	"----//----"	2008	298.15	1	0.997048	2.51	0.05	No	1000	IPOL-0.13	93
	"----//----"	2008	298.15	1	0.997048	3.01	0.06	No	1000	IPOL-0.16	93
	"----//----"	2008	298.15	1	0.997048	2.04	0.04	No	1000	IPOL-0.13-0.1	93
	"----//----"	2008	298.15	1	0.997048	2.37	0.04	No	1000	IPOL-0.16-0.1	93
	"----//----"	2008	298.15	1	0.997048	2.14	0.02	No	1000	APOL-0.13	93
	"----//----"	2008	298.15	1	0.997048	2.61	0.05	No	1000	APOL-0.16	93
94	Mankoo & Keyes	2008	300		0.997	2.38	N/A	No	256	POLIR	94
95	Liem & Popelier	2008	300	1.01325	0.996	1.44	N/A	No	216	QCT	95
96	Kumar & Skinner	2008	298			2.49	0.04	No	256	SPC/E	13
	"----//----"	2008	298			3.44	0.07	No	256	TIP4P	191
	"----//----"	2008	298			2.36	0.05	No	256	Kumar et al.	96
97	Akin-Ojo et al.	2008	298		0.997	2.8	0.2	No	216	MP2f	97
	"----//----"	2008	298		0.997	2.6	0.3	No	216	BLYPf	97

	"----//----"	2008	298		0.997	1.9	0.1	No	216	B3LYPf	97
99	Vega et al.	2009	298	1		5.51	N/A	No	360	TIP3P	6
	"----//----"	2009	298	1		3.22	N/A	No	360	TIP4P	191
	"----//----"	2009	298	1		2.77	N/A	No	360	TIP5P	183
	"----//----"	2009	298	1		2.07	N/A	No	360	TIP4P/2005	80
100	Walsh & Liang	2009	298		1.0004	2.02	N/A	No	512	AMOEBA	78
	"----//----"	2009	298		0.98	2.52	N/A	No	512	DMIP	100
101	Bauer et al.	2009	298	1.01325		2.15	N/A	Yes	216	TIP4P-FQ	34
	"----//----"	2009	298	1.01325		2.46	N/A	Yes	216	TIP4P-QDP	101
	"----//----"	2009	298	1.01325		2.04	N/A	Yes	216	QDP-P1	101
102	Bauer & Patel	2009	298	1.01325	0.998	2.3	0.04	Yes	216	TIP4P-QDP-LJ	102
103	Liu et al.	2009	298.15	1.01325		1.8	0.1	No	216	q-SPC/Fw	84
	"----//----"	2009	298.15	1.01325		5	0.1	No	216	q-SPC/Fw	84
	"----//----"	2009	298.15	1.01325		2.5	0.1	No	216	q-SPC/Fw	84
104	Kunz & van Gunsteren	2009	298.15	1.01325		2.5	N/A	No	1000	COS/D	104
105	Akin-Ojo & Wang	2009	298.15			3.7	N/A	Yes	216	MP2$_f$_hb	104
106	Molinero & Moore	2009	298			6.50	N/A	No		mW	106
108	Te & Ichiye	2010	298	1		2.22	N/A	No	256	SSDQO1	108
109	Shaik et al.	2010	298	1.01325		2.27	N/A	No	216	Optimized QCT	109
	"----//----"	2010	298	1.01325		2.62	N/A	No	216	TIP5P	183
110	Chiu et al.	2010	298		0.998	4.3	N/A	No	400/3200	CSJ W4	110
	"----//----"	2010	298		1.005	1.6	N/A	No	400/3200	MARTINI W	192
	"----//----"	2010	298		0.993	6.6	N/A	No	400/3200	SSRBK W	193
111	Karamertzanis et al.	2010	298.15	1.01325		1.4	N/A	No	542	Karamertzanis et al.	111
112	Daree et al.	2010	300	1	1.0001	2.23	N/A	No	497	WT4	112
113	Fuhrmans et al.	2010	298	1		1.26	0.05	No	1068	Model 1 Fuhrmans et al.	113
	"----//----"	2010	298	1		1.24	0.07	No	1068	Model 2 Fuhrmans et al.	113
	"----//----"	2010	298	1		1.92	0.03	No	1068	MARTINI W	192
	"----//----"	2010	298	1		4.21	0.19	No	1068	SPC	178
115	Guevara-Carrion et al.	2011	298.15	1		4.34	N/A	No	2048	SPC	178
	"----//----"	2011	298.15	1		2.72	N/A	No	2048	SPC/E	13
	"----//----"	2011	298.15	1		3.69	N/A	No	2048	TIP4P	191

	"----//----"	2011	298.15	1		2.25	N/A	No	2048	TIP4P/2005	80
116	Tainter et al.	2011	298	1.01325	993.5	2.3	0.02	Yes	500	E3B	116
117	Gonzalez & Abascal	2011	298	1	0.9977	1.93	N/A	No	500	TIP4P/2005f	117
	"----//----"	2011	298	1	0.9979	2.08	N/A	No	500	TIP4P/2005	80
118	Hasegawa & Tanimura	2011	298	1	0.9932	1.83	0.02	No	216	Hasegawa & Tanimura	118
119	Alejandre et al.	2011	300	1	0.9947	2.2	N/A	No	500	TIP4Q	119
120	Viererblova & Kolafa	2011	298.15	1.01325		2.461	0.015	Yes	360	POL4D	120
121	Orsi & Essex	2011	298.15	1.01325		2.5	1%	No	4000	ELBA	121
122	Wang & Hou	2011	298			2.984	0.005	No	624	TIP3P	6
	"----//----"	2011	298			3.097	N/A	No	928	TIP3P	6
124	Raabe & Sadus	2012	298.15	1		2.432	0.023	No	400	SPC/E	13
	"----//----"	2012	298.15	1		2.359	0.035	No	400	SPC/Fw	83
	"----//----"	2012	298.15	1		3.861	0.03	No	400	SPC	178
125	Leontyev & Stuchebrukhov	2012	298.15	1.01325	0.9986	6.1	0.1	Yes	2048	MFP/TIP3P	125
	"----//----"	2012	298.15	1.01325	0.9986	6.1	0.1	Yes	2048	TIP3P	6
126	Daree et al.	2012	300	1		4.3	N/A	No	2002	SPC	178
	"----//----"	2012	300	1		2.9	N/A	No	2002/182	Hybrid SPC/WT4	126
	"----//----"	2012	300	1		2.23	N/A	No	182	WT4	112
127	Babin et al.	2012	298.15		0.997	2.3	5	No	256	HBB2-pol	127
128	Tazi et al.	2012	300		0.998	2.97	0.05	Yes	64-4096	SPC/E	13
	"----//----"	2012	300		0.998	2.49	0.06	Yes	2048	TIP4P/2005	80
	"----//----"	2012	300		0.998	2.72	0.09	Yes	512	Dang-Chang	49
132	Lee	2013	300		0.9965	2.78	0.06	No	1024	SPC/E	13
133	Chen et al.	2013	298.15	1.01325		5.06	N/A	No	256	TIP3P	6
	"----//----"	2013	298.15	1.01325		3.29	N/A	No	256	TIP4P	191
	"----//----"	2013	298.15	1.01325		2.62	N/A	No	256	TIP5P	183
	"----//----"	2013	298.15	1.01325		2.4	N/A	No	256	TIP4P-Ew	75
	"----//----"	2013	298.15	1.01325		2.49	N/A	No	256	SPC/E	13
	"----//----"	2013	298.15	1.01325		2.52	N/A	No	256	TIP4P(M)	133
134	Akin-Ojo & Szalewicz	2013	298.15			2.4	N/A	Yes	256	CC-pol-8s'	134
	"----//----"	2013	298.15			2.6	N/A	Yes	256	CC-dpol-8s'	134
135	Yu et al.	2013	298.15	1.01325		3.92	N/A	Yes	267	TIP4P	191

	"----//----"	2013	298.15	1.01325		2.74	N/A	Yes	512	TIP4P-Ew	75
	"----//----"	2013	298.15	1.01325		2.49	0.09	Yes	average of 360 and 530	TIP4P/2005	80
	"----//----"	2013	298.15	1.01325		3.06	N/A	Yes	267	TIP5P	183
	"----//----"	2013	298.15	1.01325		2.8	0.1	No	256/512	TIP5P-Ew	194
	"----//----"	2013	298.15	1.01325		2.97	0.05	Yes	216	SPC/E	13
	"----//----"	2013	298.15	1.01325		2.14	0.19	Yes	1000	SWM6	135
	"----//----"	2013	298.15	1.01325		2.14	N/A	Yes	512	AMOEBA	78
	"----//----"	2013	298.15	1.01325		2.3	N/A	No	1000	COS/G2	77
	"----//----"	2013	298.15	1.01325		2.23	N/A	No	64	TTM2-R	195
	"----//----"	2013	298.15	1.01325		2.37	N/A	No	256	TTM3-F	196
	"----//----"	2013	298.15	1.01325		2.26	N/A	No	256	GCPM	197
	"----//----"	2013	298.15	1.01325		2.461	0.012	Yes	360	POL4D	120
	"----//----"	2013	298.15	1.01325		2.43	N/A	No	300/432	BKd3	198
	"----//----"	2013	298.15	1.01325		6.14	0.06	Yes	256	TIP3P	6
	"----//----"	2013	298.15	1.01325		2.85	0.28	Yes	1000	SWM4-NDP	82
136	Kiss & Baranay	2013	298.15	1.01325		2.28	0.04	Yes		BK3	136
137	Corsetti et al.	2013	300		1	1.92	Yes (Fig. 12)	No	200	TIP4P	191
138	Han et al.	2013	298.15	1.01325		2.7	N/A	No	267	XP3P	138
139	Baker & Best	2013	298.15	1.01325		2.81	0.03	No		SWM4A-OPT	139
140	Nagarajan et al.	2013	300			1.24	0.0376	No		Bundled water model	140
141	Stukan et al.	2013	298.15	1.01325		2.4	N/A	No	1024	SWM4-NDP	82
142	Troster et al.	2013	300		0.9965	3.4	N/A	Yes	728/1500/3374	TL3P	142
	"----//----"	2013	300		0.9965	3	N/A	Yes	728/1500/3375	TL4P	142
	"----//----"	2013	300		0.9965	2.8	N/A	Yes	728/1500/3376	TL5P	142
143	Wang et al.	2013	298	1.01325		2.53	N/A	Yes	216/512/1000	iAMOEBA	143
	"----//----"	2013	298	1.01325		1.93	N/A	Yes	216/512/1001	AMOEBA	78
144	Arismendi-Arrieta et al.	2014	298.15		1	2.35	N/A	No	256	NCC(Q)	144
145	Braun et al.	2014	300		1.008	5.81	0.02	No	2100	TIP3P	6
	"----//----"	2014	300		0.995	2.64	0.02	No	2100	SPC/E	13
	"----//----"	2014	300		1.040	0.72	0.02	No	525	BMW	199
146	Bachmann & van Gunsteren	2014	298.15	1.01325	0.972	4.2	N/A	No	1000	SPC	178

	"----//----"	2014	298.15	1.01325	0.999	2	N/A	No	1000	COS/G2	77
	"----//----"	2014	298.15	1.01325	0.996	0.8	N/A	No	1000	COS/D	104
	"----//----"	2014	298.15	1.01325	0.999	2.2	N/A	No	1000	COS/D2	146
147	Fuentes-Azcatl & Alejandre	2014	300	1	0.9967	2.1048	N/A	No	500	TIP4P/2005	80
	"----//----"	2014	300	1	0.9958	2.0963	N/A	No	500	TIP4P/ε	147
148	Troster et al.	2014	300	1		2.3	N/A	Yes		TL6P	148
	"----//----"	2014	300	1		2.2	N/A	Yes		TL6PSk	148
149	Moultos et al.	2014	298.15	1		3.6	0.5	No	2000	SPC	178
	"----//----"	2014	298.15	1		2.6	0.1	No	2000	SPC/E	13
	"----//----"	2014	298.15	1		2.1	0.1	No	2000	TIP4P/2005	80
150	Izadi et al.	2014	298.15	1	0.995	2.44	N/A	No		TIP4P-Ew	75
	"----//----"	2014	298.15	1	0.994	2.54	N/A	No		SPC/E	13
	"----//----"	2014	298.15	1	0.98	5.5	N/A	No		TIP3P	6
	"----//----"	2014	298.15	1	0.979	2.78	N/A	No		TIP5P	183
	"----//----"	2014	298.15	1	0.997	2.3	0.02	No		OPC	150
151	Spura et al.	2014	298.15	1.01325		2.88	N/A	Yes	125/216/343	fm-TIP4P/F-TPSS-D3	151
152	Orsi	2014	298.15	1.01325	0.99945	2.16	0.01	No		ELBA	121
	"----//----"	2014	298.15	1.01325	0.9769	4.42	0.03	No		SPC	178
	"----//----"	2014	298.15	1.01325	0.9984	2.78	0.02	No		SPC/E	13
	"----//----"	2014	298.15	1.01325	0.99586	4.3	0.02	No		TIP3P-Ew	200
	"----//----"	2014	298.15	1.01325	0.99714	2.53	0.01	No		TIP4P-Ew	75
	"----//----"	2014	298.15	1.01325	0.99846	2.28	0.02	No		TIP4P/2005	80
153	Bachmann & van Gunsteren	2014	298.15	1.01325	0.972	4.1	N/A	No	1000	SPC	178
	"----//----"	2014	298.15	1.01325	0.999	2	N/A	No	1000	COS/G2	195
	"----//----"	2014	298.15	1.01325	0.996	0.8	N/A	No	1000	COS/D	104
154	Medders et al.	2014	298.15	1.01325		1.2	0.1	No	256	MB-pol	201
	"----//----"	2014	298.15	1.01325		2.2	0.3	No	256	MB-pol	201
159	Tainter et al.	2015	298.15	1.01325		2.27	N/A	Yes	500	E3B2	202
	"----//----"	2015	298.15	1.01325		2.32	N/A	Yes	500	TIP4P/2005	80
	"----//----"	2015	298.15	1.01325		1.98	N/A	Yes	500	E3B3	159
160	Lobanova et al.	2015	298	1.01325	0.997	1.7	N/A	No		Mie (8-6) CGW1-vle	160

	"----//----"	2015	298	1.01325	0.998	7.4	N/A	No		Mie (8-6) CGW1-ift	160
	"----//----"	2015	298	1.01325	0.999	3.8	N/A	No		CGW2	160
	"----//----"	2015	298	1.01325	1	5.8	N/A	No		Mie (9-6)	160
165	Tran et al.	2016	300	1.01325	0.995	2.24	Yes (Fig. 5)	Yes	512	SSMP	165
166	Jiang et al.	2016	298.15	1		2.42	0.01	Yes	512	HBP	166
	"----//----"	2016	298.15	1		2.04	0.05	Yes	512	BK3	136
	"----//----"	2016	298.15	1		2.1	0.01	Yes	512	TIP4P/2005	80
172	Abbaspour et al.	2018	300	1.01325	0.9966	2.61	N/A	No	500	HFD-Like potential	172

<u>TABLE SI-2.</u> Available MD simulation data of the self-diffusion coefficient of water at other conditions. "**Ref #**" corresponds to the reference (see Reference list at page 71) of the study reporting the self-diffusion coefficient value. "***T***", "**P**", and "***ρ***" correspond to the conditions at which the simulations are performed. "**SSE correction**" indicates if the data are corrected for system size effects (see ref [76]). "**H_2O Ref #**" lists the original H_2O model development papers.

Ref #	**Authors**	**Year**	***T* (K)**	***P* (bar)**	***ρ* (g/cm^3)**	***D* (m^2/s) (x 10^9)**	**Statistical Error**	**SSE correction**	**Number of H_2O molecules**	**H_2O force field**	**H_2O Ref #**
1	Rahman & Stillinger	1971	307.5		1	4.2	N/A	No	216	BNS (modified)	1
	"----//----"	1971	265			1.50	N/A	No	216	BNS (modified)	1
2	Stillinger & Rahman	1974	270.15		1	1.3	N/A	No	216	ST2	2
	"----//----"	1974	283.15		1	1.9	N/A	No	216	ST2	2
	"----//----"	1974	314.15		1	4.3	N/A	No	216	ST2	2
	"----//----"	1974	391.15		1	8.4	N/A	No	216	ST2	2
5	Impey et al.	1982	242		1	0.50	0.08	No	125	MCY	175
	"----//----"	1982	282		1	1.81	0.07	No	125	MCY	175
	"----//----"	1982	286		1	2.12	0.15	No	125	MCY	175
	"----//----"	1982	294		1	2.3	0.2	No	125	MCY	175
	"----//----"	1982	360		1	5.1	0.2	No	125	MCY	175
7	Jansco et al.	1984	336.15		0.9718	2.4	0.15	No	200	BJH	203
	"----//----"	1984	350.15		1.346	2.7	0.2	No	200	BJH	203
8	Ferrario & Tani	1985	243.15	60	0.985	0.8	N/A	No	343	TIP4P	6
	"----//----"	1985	298.15	370	0.983	45	N/A	No	343	TIP4P	6
	"----//----"	1985	348.15	1030	0.978	7.6	N/A	No	343	TIP4P	6

12	Anderson et al.	1987	259		1	0.76	N/A	No	125	SPC modif. (flex.)	12
	"----//----"	1987	300		1	2.54	N/A	No	125	SPC modif. (flex.)	12
	"----//----"	1987	350		1	5.60	N/A	No	125	SPC modif. (flex.)	12
14	Reddy & Berkowitz	1987	268		0.999	1.36	N/A	No	216	TIP4P	6
	"----//----"	1987	268		1.083	1.47	N/A	No	216	TIP4P	6
	"----//----"	1987	268		1.149	1.27	N/A	No	216	TIP4P	6
	"----//----"	1987	298		0.999	2.96	N/A	No	216	TIP4P	6
	"----//----"	1987	298		1.083	2.88	N/A	No	216	TIP4P	6
	"----//----"	1987	298		1.149	2.38	N/A	No	216	TIP4P	6
23	Barrat & McDonald	1990	270	1500		2.3	0.2	No	N/A	SPC-type; R1 (rigid)	23
	"----//----"	1990	270	1000		1.1	0.1	No	N/A	SPC-type; R2 (rigid)	23
	"----//----"	1990	270	-200		1.7	0.2	No	N/A	SPC-type; F (flex)	23
	"----//----"	1990	300	2000		4.5	0.5	No	N/A	SPC-type; R1 (rigid)	23
	"----//----"	1990	300	1500		2.4	0.2	No	N/A	SPC-type; R2 (rigid)	23
	"----//----"	1990	300	200		3.0	0.3	No	N/A	SPC-type; F (flex)	23
24	Brodholt & Wood	1990	300.91	470	1	3.2	N/A	No	108	TIP4P	6
	"----//----"	1990	338.70	1240	1	4.63	N/A	No	108	TIP4P	6
	"----//----"	1990	373.60	1610	1	7.86	N/A	No	108	TIP4P	6
	"----//----"	1990	436.74	3000	1	11.9	N/A	No	108	TIP4P	6
	"----//----"	1990	498.99	4070	1	15.8	N/A	No	108	TIP4P	6
	"----//----"	1990	670.94	7780	1	20.8	N/A	No	108	TIP4P	6
	"----//----"	1990	717.70	9020	1	22.3	N/A	No	108	TIP4P	6
	"----//----"	1990	862.12	11800	1	28.8	N/A	No	108	TIP4P	6
	"----//----"	1990	1250.00	20000	1	38.9	N/A	No	108	TIP4P	6
	"----//----"	1990	1849.40	30900	1	44.2	N/A	No	108	TIP4P	6
	"----//----"	1990	2344.10	38200	1	69.5	N/A	No	108	TIP4P	6
	"----//----"	1990	1996.00	302600	1.9	3.79	N/A	No	108	TIP4P	6

25	Frattini et al.	1990	256			1.09	N/A	No	108	TIP4P	6
	"----//----"	1990	275			1.85	N/A	No	108	TIP4P	6
	"----//----"	1990	310			3.92	N/A	No	256	TIP4P	6
	"----//----"	1990	347			6.83	N/A	No	108	TIP4P	6
	"----//----"	1990	383			8.71	N/A	No	108	TIP4P	6
32	Sciortino et al.	1992	273		0.75	0.281	N/A	No	216	ST2	2
	"----//----"	1992	273		0.80	0.212	N/A	No	216	ST2	2
	"----//----"	1992	273		0.85	0.331	N/A	No	216	ST2	2
	"----//----"	1992	273		0.90	0.843	N/A	No	216	ST2	2
	"----//----"	1992	273		0.95	1.146	N/A	No	216	ST2	2
	"----//----"	1992	273		1.00	1.647	N/A	No	216	ST2	2
	"----//----"	1992	235		0.835	0.007	N/A	No	216	ST2	2
	"----//----"	1992	235		0.886	0.008	N/A	No	216	ST2	2
	"----//----"	1992	235		0.950	0.054	N/A	No	216	ST2	2
	"----//----"	1992	235		1.00	0.145	N/A	No	216	ST2	2
33	Guissani & Guillot	1993	300		VLE	2.6	0.1	No	256	SPC/E	13
	"----//----"	1993	373		VLE	7.9	N/A	No	256	SPC/E	13
	"----//----"	1993	473		VLE	19.6	N/A	No	256	SPC/E	13
	"----//----"	1993	570		VLE	34.7	N/A	No	256	SPC/E	13
	"----//----"	1993	610		VLE	53.6	N/A	No	256	SPC/E	13
	"----//----"	1993	620		VLE	54.1	N/A	No	256	SPC/E	13
	"----//----"	1993	630		VLE	65.6	N/A	No	256	SPC/E	13
	"----//----"	1993	640		VLE	71.7	N/A	No	256	SPC/E	13
	"----//----"	1993	652		VLE	106.0	N/A	No	256	SPC/E	13
37	Padro et al.	1994	298		1	2.5	N/A	No	216	SPC (flex)	178
	"----//----"	1994	523		0.75	2.6	N/A	No	216	SPC (flex)	178
38	Baez & Clancy	1994	328.3	1	0.9872	3.57	2.9E-01	No	360	SPC/E	13
	"----//----"	1994	307.4	1	1.0013	2.51	2.2E-01	No	360	SPC/E	13

	"----//----"	1994	282.2	1	1.0160	1.51	1.1E-01	No	360	SPC/E	13
	"----//----"	1994	261.2	1	1.0217	1.08	1.9E-01	No	360	SPC/E	13
	"----//----"	1994	250.2	1	1.0251	0.586	7.6E-02	No	360	SPC/E	13
	"----//----"	1994	240.4	1	1.0262	0.501	6.9E-02	No	360	SPC/E	13
	"----//----"	1994	229.9	1	1.0267	0.311	4.8E-02	No	360	SPC/E	13
	"----//----"	1994	220.6	1	1.0251	0.164	3.2E-02	No	360	SPC/E	13
	"----//----"	1994	209.5	1	1.0237	5.50E-02	2.1E-03	No	360	SPC/E	13
	"----//----"	1994	200.2	1	1.0185	1.65E-02	7.2E-04	No	360	SPC/E	13
	"----//----"	1994	190.3	1	1.0097	1.14E-03	2.1E-05	No	360	SPC/E	13
41	Duan et al.	1995	307.15	1		3.06	N/A	No	256	RWK2	181
	"----//----"	1995	373.15	21		7.66	N/A	No	256	RWK2	181
	"----//----"	1995	473.15	2083		12.7	N/A	No	256	RWK2	181
	"----//----"	1995	513.15	3109		14.5	N/A	No	256	RWK2	181
42	Mountain	1995	303		0.997	2.7	N/A	No	216	RPOL	180
	"----//----"	1995	579		0.720	34	N/A	No	216	RPOL	180
	"----//----"	1995	678		0.660	46	N/A	No	216	RPOL	180
	"----//----"	1995	297	490		2.5	N/A	No	216	ST2	2
	"----//----"	1995	575	890		34	N/A	No	216	ST2	2
	"----//----"	1995	667	1400		45	N/A	No	216	ST2	2
43	Brodholt et al.	1995	298.15		1	2.3	N/A	No	256	TIP4P-Polarizable	43
	"----//----"	1995	573.15		0.712	23.3	N/A	No	256	TIP4P-Polarizable	43
	"----//----"	1995	573.15		0.921	12.5	N/A	No	256	TIP4P-Polarizable	43
	"----//----"	1995	298.15		1	2.3	N/A	No	256	SPC/E	13
	"----//----"	1995	573.15		0.712	19.5	N/A	No	256	SPC/E	13
	"----//----"	1995	573.15		0.921	11.8	N/A	No	256	SPC/E	13
44	Svishchev et al.	1996	263		0.9981	0.95	2%	No	256	PPC	44

	"----//----"	1996	298		0.9970	2.6	2%	No	256	PPC	44
	"----//----"	1996	373		0.9583	9.6	2%	No	256	PPC	44
	"----//----"	1996	473		0.8647	18.8	2%	No	256	PPC	44
	"----//----"	1996	573		0.7123	33.2	2%	No	256	PPC	44
45	Gallo et al.	1996	284.5		0.984	1.3000	0.1	No	216	SPC/E	13
46	"----//----"	1996	258.5		0.986	0.5200	5.0E-02	No	216	SPC/E	13
	"----//----"	1996	238.2		0.987	0.1400	1.0E-02	No	216	SPC/E	13
	"----//----"	1996	224.0		0.984	0.0440	4.0E-03	No	216	SPC/E	13
	"----//----"	1996	213.6		0.977	0.0110	4.0E-03	No	216	SPC/E	13
	"----//----"	1996	209.3		0.970	0.0051	9.0E-04	No	216	SPC/E	13
	"----//----"	1996	206.3		0.966	0.0018	1.1E-03	No	216	SPC/E	13
47	Taylor et al.	1996	268		1	1.69	N/A	No	526	SPC/E	13
	"----//----"	1996	283		1	2.17	N/A	No	526	SPC/E	13
	"----//----"	1996	298		1	3.02	N/A	No	526	SPC/E	13
	"----//----"	1996	323		1	4.56	N/A	No	526	SPC/E	13
	"----//----"	1996	348		1	5.64	N/A	No	526	SPC/E	13
	"----//----"	1996	373		1	7.74	N/A	No	526	SPC/E	13
48	Bagchi et al.	1997	277.2	-5		1.60	0.08	No	512	SPC/E	13
	"----//----"	1997	277.2	1209		1.63	0.07	No	512	SPC/E	13
	"----//----"	1997	277.2	2428		1.64	0.08	No	512	SPC/E	13
	"----//----"	1997	277.2	3236		1.55	0.03	No	512	SPC/E	13
	"----//----"	1997	277.2	3993		1.57	0.08	No	512	SPC/E	13
	"----//----"	1997	277.2	6574		1.42	0.05	No	512	SPC/E	13
	"----//----"	1997	277.2	8637		1.23	0.05	No	512	SPC/E	13
	"----//----"	1997	277.2	12156		1.01	0.04	No	512	SPC/E	13
50	Levitt et al.	1997	273		0.999	1.6	N/A	(see ref)	216	F3C	50
	"----//----"	1997	298		0.997	2.4	0.23	(see ref)	216	F3C	50
	"----//----"	1997	323		0.988	3.2	N/A	(see ref)	216	F3C	50

	"----//----"	1997	348	0.975	4.2	N/A	(see ref)	216	F3C	50
	"----//----"	1997	373	0.958	6.6	N/A	(see ref)	216	F3C	50
	"----//----"	1997	398	0.939	7.1	N/A	(see ref)	216	F3C	50
	"----//----"	1997	423	0.916	9.8	N/A	(see ref)	216	F3C	50
	"----//----"	1997	448	0.890	12.4	N/A	(see ref)	216	F3C	50
	"----//----"	1997	473	0.861	16.1	N/A	(see ref)	216	F3C	50
	"----//----"	1997	498	0.829	19.1	N/A	(see ref)	216	F3C	50
	"----//----"	1997	573	0.717	33.8	N/A	(see ref)	216	F3C	50
53	Starr et al.	1999	190	1.00	2.40E-04	4E-06	No	216	SPC/E	13
	"----//----"	1999	200	1.00	1.50E-03	4E-05	No	216	SPC/E	13
	"----//----"	1999	210	0.90	2.92E-03	4E-05	No	216	SPC/E	13
	"----//----"	1999	210	0.95	1.93E-03	4E-05	No	216	SPC/E	13
	"----//----"	1999	210	1.00	1.03E-02	4E-04	No	216	SPC/E	13
	"----//----"	1999	210	1.05	2.27E-02	4E-04	No	216	SPC/E	13
	"----//----"	1999	210	1.10	3.17E-02	4E-04	No	216	SPC/E	13
	"----//----"	1999	210	1.20	3.04E-02	4E-04	No	216	SPC/E	13
	"----//----"	1999	210	1.30	8.71E-03	4E-05	No	216	SPC/E	13
	"----//----"	1999	210	1.40	4.90E-04	4E-06	No	216	SPC/E	13
	"----//----"	1999	220	0.95	1.68E-02	4E-04	No	216	SPC/E	13
	"----//----"	1999	220	1.00	3.89E-02	4E-04	No	216	SPC/E	13
	"----//----"	1999	220	1.05	5.58E-02	4E-04	No	216	SPC/E	13
	"----//----"	1999	220	1.10	8.47E-02	4E-04	No	216	SPC/E	13
	"----//----"	1999	220	1.15	9.18E-02	4E-04	No	216	SPC/E	13
	"----//----"	1999	220	1.20	8.01E-02	4E-04	No	216	SPC/E	13
	"----//----"	1999	220	1.25	5.94E-02	4E-04	No	216	SPC/E	13
	"----//----"	1999	220	1.30	2.63E-02	4E-04	No	216	SPC/E	13
	"----//----"	1999	220	1.40	1.69E-03	4E-05	No	216	SPC/E	13
	"----//----"	1999	230	0.95	6.25E-02	4E-04	No	216	SPC/E	13
	"----//----"	1999	230	1.00	0.103	4E-03	No	216	SPC/E	13
	"----//----"	1999	230	1.05	0.134	4E-03	No	216	SPC/E	13
	"----//----"	1999	230	1.10	0.177	4E-03	No	216	SPC/E	13

"----//----"	1999	230	1.20	0.159	4E-03	No	216	SPC/E	13
"----//----"	1999	230	1.30	6.72E-02	4E-04	No	216	SPC/E	13
"----//----"	1999	230	1.40	1.12E-02	4E-04	No	216	SPC/E	13
"----//----"	1999	240	0.95	0.141	4E-03	No	216	SPC/E	13
"----//----"	1999	240	1.00	0.187	4E-03	No	216	SPC/E	13
"----//----"	1999	240	1.05	0.244	4E-03	No	216	SPC/E	13
"----//----"	1999	240	1.10	0.270	4E-03	No	216	SPC/E	13
"----//----"	1999	240	1.20	0.237	4E-03	No	216	SPC/E	13
"----//----"	1999	240	1.30	0.135	4E-03	No	216	SPC/E	13
"----//----"	1999	240	1.40	2.49E-02	4E-04	No	216	SPC/E	13
"----//----"	1999	260	0.95	0.504	4E-03	No	216	SPC/E	13
"----//----"	1999	260	1.00	0.608	4E-03	No	216	SPC/E	13
"----//----"	1999	260	1.05	0.591	4E-03	No	216	SPC/E	13
"----//----"	1999	260	1.10	0.588	4E-03	No	216	SPC/E	13
"----//----"	1999	260	1.20	0.574	4E-03	No	216	SPC/E	13
"----//----"	1999	260	1.30	0.354	4E-03	No	216	SPC/E	13
"----//----"	1999	260	1.40	0.139	4E-03	No	216	SPC/E	13
"----//----"	1999	300	0.95	1.99	4E-02	No	216	SPC/E	13
"----//----"	1999	300	1.00	2.00	4E-02	No	216	SPC/E	13
"----//----"	1999	300	1.05	1.83	4E-02	No	216	SPC/E	13
"----//----"	1999	300	1.10	1.82	4E-02	No	216	SPC/E	13
"----//----"	1999	300	1.20	1.53	4E-02	No	216	SPC/E	13
"----//----"	1999	300	1.30	1.12	4E-02	No	216	SPC/E	13
"----//----"	1999	300	1.40	0.495	4E-03	No	216	SPC/E	13
"----//----"	1999	350	0.90	6.11	4E-02	No	216	SPC/E	13
"----//----"	1999	350	1.00	4.97	4E-02	No	216	SPC/E	13
"----//----"	1999	350	1.10	3.81	4E-02	No	216	SPC/E	13
"----//----"	1999	350	1.20	2.70	4E-02	No	216	SPC/E	13
"----//----"	1999	350	1.30	1.80	4E-02	No	216	SPC/E	13
"----//----"	1999	350	1.40	1.39	4E-02	No	216	SPC/E	13
"----//----"	1999	190	1.00	2.40E-04	4E-06	No	216	SPC/E	13

	"----//----"	1999	200		1.00	1.50E-03	4E-05	No	216	SPC/E	13
	"----//----"	1999	210		1.00	1.03E-02	4E-04	No	216	SPC/E	13
	"----//----"	1999	220		1.00	3.89E-02	4E-04	No	216	SPC/E	13
	"----//----"	1999	230		1.00	0.103	4E-03	No	216	SPC/E	13
	"----//----"	1999	240		1.00	0.187	4E-03	No	216	SPC/E	13
	"----//----"	1999	260		1.00	0.608	4E-03	No	216	SPC/E	13
	"----//----"	1999	300		1.00	2.00	4E-02	No	216	SPC/E	13
	"----//----"	1999	350		1.00	4.97	4E-02	No	216	SPC/E	13
54	Svishchev & Zassetsky	2000	238			0.24	N/A	No	256	PPC	44
	"----//----"	2000	263			0.72	N/A	No	256	PPC	44
	"----//----"	2000	298			2.15	N/A	No	256	PPC	44
	"----//----"	2000	473			21.7	N/A	No	256	PPC	44
61	Guillot & Guissani	2001	254.61		0.997	0.59	N/A	No	256	DEC	61
	"----//----"	2001	297.09		0.997	2.52	N/A	No	256	DEC	61
	"----//----"	2001	304.37		0.997	2.90	N/A	No	256	DEC	61
	"----//----"	2001	377.18		0.997	6.93	N/A	No	256	DEC	61
	"----//----"	2001	481.55		0.997	13.62	N/A	No	256	DEC	61
	"----//----"	2001	678.16		0.997	22.39	N/A	No	256	DEC	61
	"----//----"	2001	673		0.10	291.18	N/A	No	256	DEC	61
	"----//----"	2001	673		0.30	109.41	N/A	No	256	DEC	61
	"----//----"	2001	673		0.66	45.88	N/A	No	256	DEC	61
	"----//----"	2001	673		0.99	21.18	N/A	No	256	DEC	61
57	Mahoney & Jorgensen	2001	298.15	1.01325	0.999	2.62	0.04	No	267	TIP5P	183
	"----//----"	2001	298.15	506.625	1.026	2.65	0.05	No	267	TIP5P	183
	"----//----"	2001	298.15	1013.25	1.053	2.66	0.05	No	267	TIP5P	183
	"----//----"	2001	298.15	1519.875	1.072	2.60	0.04	No	267	TIP5P	183
	"----//----"	2001	298.15	2026.5	1.092	2.63	0.05	No	267	TIP5P	183
	"----//----"	2001	298.15	3039.75	1.128	2.67	0.05	No	267	TIP5P	183

	"----//----"	2001	348.15	1.01325	0.951	6.78	0.10	No	267	TIP5P	183
	"----//----"	2001	348.15	506.625	0.985	6.97	0.14	No	267	TIP5P	183
	"----//----"	2001	348.15	1013.25	1.011	6.71	0.09	No	267	TIP5P	183
	"----//----"	2001	348.15	1519.875	1.034	6.38	0.09	No	267	TIP5P	183
	"----//----"	2001	348.15	2026.5	1.055	6.33	0.12	No	267	TIP5P	183
	"----//----"	2001	348.15	3039.75	1.091	5.89	0.11	No	267	TIP5P	183
	"----//----"	2001	248.15	1.01325	0.981	0.14	0.02	No	267	TIP5P	183
	"----//----"	2001	260.65	1.01325	0.988	0.43	0.03	No	267	TIP5P	183
	"----//----"	2001	273.15	1.01325	1.007	1.01	0.02	No	267	TIP5P	183
	"----//----"	2001	285.65	1.01325	1.005	1.87	0.08	No	267	TIP5P	183
	"----//----"	2001	298.15	1.01325	0.999	2.62	0.04	No	267	TIP5P	183
	"----//----"	2001	310.65	1.01325	0.989	3.70	0.09	No	267	TIP5P	183
	"----//----"	2001	323.15	1.01325	0.978	4.74	0.08	No	267	TIP5P	183
	"----//----"	2001	335.65	1.01325	0.967	6.33	0.07	No	267	TIP5P	183
	"----//----"	2001	348.15	1.01325	0.951	6.78	0.10	No	267	TIP5P	183
62	Errington & Debenedetti	2001	400		0.85	12.085	N/A	No	256	SPC/E	13
	"----//----"	2001	400		0.90	9.561	N/A	No	256	SPC/E	13
	"----//----"	2001	400		0.95	9.515	N/A	No	256	SPC/E	13
	"----//----"	2001	400		1.00	8.519	N/A	No	256	SPC/E	13
	"----//----"	2001	400		1.05	7.361	N/A	No	256	SPC/E	13
	"----//----"	2001	400		1.10	7.072	N/A	No	256	SPC/E	13
	"----//----"	2001	400		1.15	6.444	N/A	No	256	SPC/E	13
	"----//----"	2001	400		1.20	5.375	N/A	No	256	SPC/E	13
	"----//----"	2001	400		1.25	4.728	N/A	No	256	SPC/E	13
	"----//----"	2001	400		1.30	3.808	N/A	No	256	SPC/E	13
	"----//----"	2001	350		0.85	6.871	N/A	No	256	SPC/E	13
	"----//----"	2001	350		0.90	6.260	N/A	No	256	SPC/E	13
	"----//----"	2001	350		0.95	5.704	N/A	No	256	SPC/E	13
	"----//----"	2001	350		1.00	5.778	N/A	No	256	SPC/E	13
	"----//----"	2001	350		1.05	4.906	N/A	No	256	SPC/E	13

"----//----"	2001	350	1.10	4.165	N/A	No	256	SPC/E	13
"----//----"	2001	350	1.15	3.932	N/A	No	256	SPC/E	13
"----//----"	2001	350	1.20	3.583	N/A	No	256	SPC/E	13
"----//----"	2001	350	1.25	3.042	N/A	No	256	SPC/E	13
"----//----"	2001	350	1.30	2.493	N/A	No	256	SPC/E	13
"----//----"	2001	320	0.85	4.341	N/A	No	256	SPC/E	13
"----//----"	2001	320	0.90	4.397	N/A	No	256	SPC/E	13
"----//----"	2001	320	0.95	3.604	N/A	No	256	SPC/E	13
"----//----"	2001	320	1.00	3.525	N/A	No	256	SPC/E	13
"----//----"	2001	320	1.05	3.327	N/A	No	256	SPC/E	13
"----//----"	2001	320	1.10	3.140	N/A	No	256	SPC/E	13
"----//----"	2001	320	1.15	2.861	N/A	No	256	SPC/E	13
"----//----"	2001	320	1.20	2.749	N/A	No	256	SPC/E	13
"----//----"	2001	320	1.25	2.175	N/A	No	256	SPC/E	13
"----//----"	2001	320	1.30	1.751	N/A	No	256	SPC/E	13
"----//----"	2001	300	0.85	3.217	N/A	No	256	SPC/E	13
"----//----"	2001	300	0.90	2.830	N/A	No	256	SPC/E	13
"----//----"	2001	300	0.95	2.489	N/A	No	256	SPC/E	13
"----//----"	2001	300	1.00	2.350	N/A	No	256	SPC/E	13
"----//----"	2001	300	1.05	2.465	N/A	No	256	SPC/E	13
"----//----"	2001	300	1.10	2.453	N/A	No	256	SPC/E	13
"----//----"	2001	300	1.15	2.047	N/A	No	256	SPC/E	13
"----//----"	2001	300	1.20	1.832	N/A	No	256	SPC/E	13
"----//----"	2001	300	1.25	1.583	N/A	No	256	SPC/E	13
"----//----"	2001	300	1.30	1.418	N/A	No	256	SPC/E	13
"----//----"	2001	280	0.85	1.766	N/A	No	256	SPC/E	13
"----//----"	2001	280	0.90	1.473	N/A	No	256	SPC/E	13
"----//----"	2001	280	0.95	1.466	N/A	No	256	SPC/E	13
"----//----"	2001	280	1.00	1.539	N/A	No	256	SPC/E	13

"----//----"	2001	280	1.05	1.614	N/A	No	256	SPC/E	13
"----//----"	2001	280	1.10	1.471	N/A	No	256	SPC/E	13
"----//----"	2001	280	1.15	1.438	N/A	No	256	SPC/E	13
"----//----"	2001	280	1.20	1.200	N/A	No	256	SPC/E	13
"----//----"	2001	280	1.25	1.113	N/A	No	256	SPC/E	13
"----//----"	2001	280	1.30	0.880	N/A	No	256	SPC/E	13
"----//----"	2001	260	0.85	0.872	N/A	No	256	SPC/E	13
"----//----"	2001	260	0.90	0.754	N/A	No	256	SPC/E	13
"----//----"	2001	260	0.95	0.750	N/A	No	256	SPC/E	13
"----//----"	2001	260	1.00	0.844	N/A	No	256	SPC/E	13
"----//----"	2001	260	1.05	0.902	N/A	No	256	SPC/E	13
"----//----"	2001	260	1.10	0.980	N/A	No	256	SPC/E	13
"----//----"	2001	260	1.15	1.047	N/A	No	256	SPC/E	13
"----//----"	2001	260	1.20	0.874	N/A	No	256	SPC/E	13
"----//----"	2001	260	1.25	0.691	N/A	No	256	SPC/E	13
"----//----"	2001	260	1.30	0.537	N/A	No	256	SPC/E	13
"----//----"	2001	240	0.85	0.287	N/A	No	256	SPC/E	13
"----//----"	2001	240	0.90	0.231	N/A	No	256	SPC/E	13
"----//----"	2001	240	0.95	0.247	N/A	No	256	SPC/E	13
"----//----"	2001	240	1.00	0.369	N/A	No	256	SPC/E	13
"----//----"	2001	240	1.05	0.478	N/A	No	256	SPC/E	13
"----//----"	2001	240	1.10	0.493	N/A	No	256	SPC/E	13
"----//----"	2001	240	1.15	0.465	N/A	No	256	SPC/E	13
"----//----"	2001	240	1.20	0.447	N/A	No	256	SPC/E	13
"----//----"	2001	240	1.25	0.366	N/A	No	256	SPC/E	13
"----//----"	2001	240	1.30	0.285	N/A	No	256	SPC/E	13
"----//----"	2001	220	0.85	0.043	N/A	No	256	SPC/E	13
"----//----"	2001	220	0.90	0.032	N/A	No	256	SPC/E	13
"----//----"	2001	220	0.95	0.045	N/A	No	256	SPC/E	13

	"----//----"	2001	220	1.00	0.096	N/A	No	256	SPC/E	13
	"----//----"	2001	220	1.05	0.163	N/A	No	256	SPC/E	13
	"----//----"	2001	220	1.10	0.180	N/A	No	256	SPC/E	13
	"----//----"	2001	220	1.15	0.222	N/A	No	256	SPC/E	13
	"----//----"	2001	220	1.20	0.206	N/A	No	256	SPC/E	13
	"----//----"	2001	220	1.25	0.154	N/A	No	256	SPC/E	13
	"----//----"	2001	220	1.30	0.102	N/A	No	256	SPC/E	13
64	Guo et al.	2002	303.8	0.999	2.63	6E-02	No	256	SPC/E	13
	"----//----"	2002	273.5	1.011	1.27	3E-02	No	256	SPC/E	13
	"----//----"	2002	253.5	1.015	0.668	2E-02	No	256	SPC/E	13
	"----//----"	2002	232.5	1.014	0.235	8E-03	No	256	SPC/E	13
	"----//----"	2002	212.5	1.004	0.049	4E-03	No	256	SPC/E	13
71	English & MacElroy	2003	260	1.002	0.83	N/A	No	500	F-SPC	182
	"----//----"	2003	298	0.997	2.3	N/A	No	500	F-SPC	182
	"----//----"	2003	350	0.965	6.1	N/A	No	500	F-SPC	182
	"----//----"	2003	400	0.920	10.5	N/A	No	500	F-SPC	182
	"----//----"	2003	260	0.999	0.34	N/A	No	500	TIP4P-FQ	34
	"----//----"	2003	298	0.996	2.1	N/A	No	500	TIP4P-FQ	34
	"----//----"	2003	350	0.961	6.3	N/A	No	500	TIP4P-FQ	34
	"----//----"	2003	400	0.912	13.3	N/A	No	500	TIP4P-FQ	34
66	Nieto-Draghi et al.	2003	275.05	0.995	1.8903	N/A	No	256	TIP5P	183
	"----//----"	2003	447.75	0.995	16.0616	N/A	No	256	TIP5P	183
	"----//----"	2003	673.97	0.995	24.6765	N/A	No	256	TIP5P	183
	"----//----"	2003	951.79	0.995	32.2135	N/A	No	256	TIP5P	183
	"----//----"	2003	1251.41	0.995	38.7636	N/A	No	256	TIP5P	183
	"----//----"	2003	275.12	0.995	2.5231	N/A	No	256	TIP4P	191
	"----//----"	2003	298.12	0.995	3.0361	N/A	No	256	TIP4P	191

"----//----"	2003	448.87		0.995	14.4801	N/A	No	256	TIP4P	191
"----//----"	2003	673.95		0.995	23.0858	N/A	No	256	TIP4P	191
"----//----"	2003	954.07		0.995	30.1370	N/A	No	256	TIP4P	191
"----//----"	2003	1251.40		0.995	36.8058	N/A	No	256	TIP4P	191
"----//----"	2003	274.99		0.995	1.5138	N/A	No	256	DEC	61
"----//----"	2003	299.22		0.995	2.5231	N/A	No	256	DEC	61
"----//----"	2003	447.66		0.995	11.1746	N/A	No	256	DEC	61
"----//----"	2003	673.93		0.995	21.2801	N/A	No	256	DEC	61
"----//----"	2003	951.77		0.995	29.6940	N/A	No	256	DEC	61
"----//----"	2003	448.83		0.995	12.4871	N/A	No	256	DEC	61
"----//----"	2003	673		0.1005	32.7354	N/A	No	256	TIP5P	183
"----//----"	2003	673		0.2007	17.6682	N/A	No	256	TIP5P	183
"----//----"	2003	673		0.2990	12.2422	N/A	No	256	TIP5P	183
"----//----"	2003	673		0.5002	7.3543	N/A	No	256	TIP5P	183
"----//----"	2003	673		0.6612	5.3363	N/A	No	256	TIP5P	183
"----//----"	2003	673		0.9956	2.4664	N/A	No	256	TIP5P	183
"----//----"	2003	673		0.1005	34.7982	N/A	No	256	TIP4P	191
"----//----"	2003	673		0.2007	18.1166	N/A	No	256	TIP4P	191
"----//----"	2003	673		0.2990	12.6457	N/A	No	256	TIP4P	191
"----//----"	2003	673		0.5002	7.5785	N/A	No	256	TIP4P	191
"----//----"	2003	673		0.6612	5.6951	N/A	No	256	TIP4P	191
"----//----"	2003	673		0.9956	2.2870	N/A	No	256	TIP4P	191
"----//----"	2003	673		0.1005	30.9417	N/A	No	256	SPC/E	13
"----//----"	2003	673		0.2007	16.5022	N/A	No	256	SPC/E	13
"----//----"	2003	673		0.2990	11.7040	N/A	No	256	SPC/E	13
"----//----"	2003	673		0.5002	7.3543	N/A	No	256	SPC/E	13
"----//----"	2003	673		0.6612	5.3812	N/A	No	256	SPC/E	13
"----//----"	2003	673		0.9956	2.3767	N/A	No	256	SPC/E	13

67	Yamaguchi et al.	2003	273	0.90	0.024	N/A	No	512	SPC/E	13
	"----//----"	2003	273	0.96	0.030	N/A	No	512	SPC/E	13
	"----//----"	2003	273	1.00	0.030	N/A	No	512	SPC/E	13
	"----//----"	2003	273	1.04	0.027	N/A	No	512	SPC/E	13
	"----//----"	2003	273	1.10	0.020	N/A	No	512	SPC/E	13
	"----//----"	2003	273	1.14	0.014	N/A	No	512	SPC/E	13
	"----//----"	2003	273	1.20	0.007	N/A	No	512	SPC/E	13
	"----//----"	2003	298	0.90	0.132	N/A	No	512	SPC/E	13
	"----//----"	2003	298	0.96	0.130	N/A	No	512	SPC/E	13
	"----//----"	2003	298	1.00	0.121	N/A	No	512	SPC/E	13
	"----//----"	2003	298	1.04	0.107	N/A	No	512	SPC/E	13
	"----//----"	2003	298	1.10	0.080	N/A	No	512	SPC/E	13
	"----//----"	2003	298	1.14	0.061	N/A	No	512	SPC/E	13
	"----//----"	2003	298	1.20	0.036	N/A	No	512	SPC/E	13
	"----//----"	2003	323	0.90	0.302	N/A	No	512	SPC/E	13
	"----//----"	2003	323	0.96	0.285	N/A	No	512	SPC/E	13
	"----//----"	2003	323	1.00	0.262	N/A	No	512	SPC/E	13
	"----//----"	2003	323	1.04	0.225	N/A	No	512	SPC/E	13
	"----//----"	2003	323	1.10	0.174	N/A	No	512	SPC/E	13
	"----//----"	2003	323	1.14	0.137	N/A	No	512	SPC/E	13
	"----//----"	2003	323	1.20	0.089	N/A	No	512	SPC/E	13
	"----//----"	2003	373	0.90	0.887	N/A	No	512	SPC/E	13
	"----//----"	2003	373	0.96	0.793	N/A	No	512	SPC/E	13
	"----//----"	2003	373	1.00	0.692	N/A	No	512	SPC/E	13
	"----//----"	2003	373	1.04	0.596	N/A	No	512	SPC/E	13
	"----//----"	2003	373	1.10	0.466	N/A	No	512	SPC/E	13
	"----//----"	2003	373	1.14	0.386	N/A	No	512	SPC/E	13
	"----//----"	2003	373	1.20	0.275	N/A	No	512	SPC/E	13

78	Ren & Ponder	2004	255.912			0.218	N/A	No	512	AMOEBA	78
	"----//----"	2004	260.685			0.322	N/A	No	512	AMOEBA	78
	"----//----"	2004	260.685			0.322	N/A	No	512	AMOEBA	78
	"----//----"	2004	265.061			0.541	N/A	No	512	AMOEBA	78
	"----//----"	2004	273.547			0.792	N/A	No	512	AMOEBA	78
	"----//----"	2004	277.26			0.854	N/A	No	512	AMOEBA	78
	"----//----"	2004	285.481			1.292	N/A	No	512	AMOEBA	78
	"----//----"	2004	298.343			1.939	N/A	No	512	AMOEBA	78
	"----//----"	2004	323.138			3.380	N/A	No	512	AMOEBA	78
	"----//----"	2004	348.199			5.228	N/A	No	512	AMOEBA	78
	"----//----"	2004	248.221			0.198	N/A	No	512	AMOEBA-v	78
	"----//----"	2004	260.685			0.510	N/A	No	512	AMOEBA-v	78
	"----//----"	2004	273.68			0.959	N/A	No	512	AMOEBA-v	78
	"----//----"	2004	277.26			1.105	N/A	No	512	AMOEBA-v	78
	"----//----"	2004	298.343			2.106	N/A	No	512	AMOEBA-v	78
	"----//----"	2004	323.271			3.599	N/A	No	512	AMOEBA-v	78
	"----//----"	2004	348.066			5.688	N/A	No	512	AMOEBA-v	78
	"----//----"	2004	298	1		1.9194	N/A	No	512	AMOEBA	78
	"----//----"	2004	298	1000		1.628	N/A	No	512	AMOEBA	78
	"----//----"	2004	298	2000		1.6493	N/A	No	512	AMOEBA	78
	"----//----"	2004	348	1		5.1753	N/A	No	512	AMOEBA	78
	"----//----"	2004	348	1000		5.0403	N/A	No	512	AMOEBA	78
	"----//----"	2004	348	2000		4.6493	N/A	No	512	AMOEBA	78
75	Horn et al.	2004	235.1	1.01325	0.9845	0.17	0.01	No	512	TIP4P-Ew	75
	"----//----"	2004	272.2	1.01325	0.9996	1.2	0.02	No	512	TIP4P-Ew	75
	"----//----"	2004	297.4	1.01325	0.9954	2.4	0.06	No	512	TIP4P-Ew	75
	"----//----"	2004	321.6	1.01325	0.9843	3.9	0.06	No	512	TIP4P-Ew	75

	"----//----"	2004	346.9	1.01325	0.9688	5.7	0.04	No	512	TIP4P-Ew	75
	"----//----"	2004	371.6	1.01325	0.9492	7.8	0.1	No	512	TIP4P-Ew	75
	"----//----"	2004	398.4	1.01325	0.9254	10.3	0.1	No	512	TIP4P-Ew	75
77	Yu & Gunsteren	2004	247.07	1.01325		0.201	N/A	No	1000	COS/G2	77
	"----//----"	2004	257.69	1.01325		0.463	N/A	No	1000	COS/G2	77
	"----//----"	2004	278.21	1.01325		1.125	N/A	No	1000	COS/G2	77
	"----//----"	2004	288.46	1.01325		1.661	N/A	No	1000	COS/G2	77
	"----//----"	2004	300.18	1.01325		2.222	N/A	No	1000	COS/G2	77
	"----//----"	2004	329.30	1.01325		4.241	N/A	No	1000	COS/G2	77
	"----//----"	2004	359.16	1.01325		6.845	N/A	No	1000	COS/G2	77
	"----//----"	2004	379.12	1.01325		9.100	N/A	No	1000	COS/G2	77
	"----//----"	2004	247.44	1.01325		0.525	N/A	No	1000	COS/B2	69
	"----//----"	2004	259.71	1.01325		0.899	N/A	No	1000	COS/B2	69
	"----//----"	2004	282.78	1.01325		1.698	N/A	No	1000	COS/B2	69
	"----//----"	2004	292.67	1.01325		2.433	N/A	No	1000	COS/B2	69
	"----//----"	2004	322.71	1.01325		4.303	N/A	No	1000	COS/B2	69
	"----//----"	2004	353.11	1.01325		6.733	N/A	No	1000	COS/B2	69
	"----//----"	2004	372.53	1.01325		8.527	N/A	No	1000	COS/B2	69
	"----//----"	2004	250.7326	1.01325		1.247	N/A	No	1000	SPC	178
	"----//----"	2004	262.6374	1.01325		1.796	N/A	No	1000	SPC	178
	"----//----"	2004	285.7143	1.01325		3.042	N/A	No	1000	SPC	178
	"----//----"	2004	295.6044	1.01325		3.678	N/A	No	1000	SPC	178
	"----//----"	2004	325.2747	1.01325		5.921	N/A	No	1000	SPC	178
	"----//----"	2004	355.3114	1.01325		8.849	N/A	No	1000	SPC	178
	"----//----"	2004	375.2747	1.01325		10.593	N/A	No	1000	SPC	178
81	Xu et al.	2005	239.72	4000		1.63E-01	N/A	No	512	TIP5P	183
	"----//----"	2005	249.44	4000		3.17E-01	N/A	No	512	TIP5P	183
	"----//----"	2005	259.97	4000		5.12E-01	N/A	No	512	TIP5P	183

"----//----"	2005	279.66	4000	1.05E+00	N/A	No	512	TIP5P	183
"----//----"	2005	299.62	4000	1.80E+00	N/A	No	512	TIP5P	183
"----//----"	2005	319.31	4000	2.91E+00	N/A	No	512	TIP5P	183
"----//----"	2005	219.75	2000	5.82E-03	N/A	No	512	TIP5P	183
"----//----"	2005	229.88	2000	3.12E-02	N/A	No	512	TIP5P	183
"----//----"	2005	234.25	2000	5.46E-02	N/A	No	512	TIP5P	183
"----//----"	2005	239.72	2000	1.25E-01	N/A	No	512	TIP5P	183
"----//----"	2005	249.44	2000	2.63E-01	N/A	No	512	TIP5P	183
"----//----"	2005	259.61	2000	5.55E-01	N/A	No	512	TIP5P	183
"----//----"	2005	280.08	2000	1.17E+00	N/A	No	512	TIP5P	183
"----//----"	2005	299.62	2000	2.00E+00	N/A	No	512	TIP5P	183
"----//----"	2005	319.86	2000	3.32E+00	N/A	No	512	TIP5P	183
"----//----"	2005	349.53	2000	5.67E+00	N/A	No	512	TIP5P	183
"----//----"	2005	219.75	1000	1.28E-03	N/A	No	512	TIP5P	183
"----//----"	2005	229.88	1000	8.24E-03	N/A	No	512	TIP5P	183
"----//----"	2005	239.41	1000	3.21E-02	N/A	No	512	TIP5P	183
"----//----"	2005	245.79	1000	9.06E-02	N/A	No	512	TIP5P	183
"----//----"	2005	249.77	1000	1.96E-01	N/A	No	512	TIP5P	183
"----//----"	2005	259.61	1000	4.37E-01	N/A	No	512	TIP5P	183
"----//----"	2005	278.81	1000	1.30E+00	N/A	No	512	TIP5P	183
"----//----"	2005	298.17	1000	2.11E+00	N/A	No	512	TIP5P	183
"----//----"	2005	319.86	1000	3.60E+00	N/A	No	512	TIP5P	183
"----//----"	2005	350.19	1000	5.67E+00	N/A	No	512	TIP5P	183
"----//----"	2005		4000	see Fig. 4b	N/A	No	1728	ST2	2
"----//----"	2005		3000	see Fig. 4b	N/A	No	1728	ST2	2
"----//----"	2005		2000	see Fig. 4b	N/A	No	1728	ST2	2
"----//----"	2005		1000	see Fig. 4b	N/A	No	1728	ST2	2
"----//----"	2005		0	see Fig. 4b	N/A	No	1728	ST2	2

88	Yoshida et al.	2006	473.15	0.001	2.31E-02	2E-03	No	256	TIP4P-FQ	34
	"----//----"	2006	473.15	0.002	1.09E-02	6E-04	No	256	TIP4P-FQ	34
	"----//----"	2006	473.15	0.005	4.43E-03	2E-04	No	256	TIP4P-FQ	34
	"----//----"	2006	473.15	0.01	2.19E-03	6E-05	No	256	TIP4P-FQ	34
	"----//----"	2006	573.15	0.001	2.91E-02	2E-03	No	256	TIP4P-FQ	34
	"----//----"	2006	573.15	0.002	1.36E-02	4E-04	No	256	TIP4P-FQ	34
	"----//----"	2006	573.15	0.005	5.40E-03	1E-04	No	256	TIP4P-FQ	34
	"----//----"	2006	573.15	0.01	2.82E-03	9E-05	No	256	TIP4P-FQ	34
	"----//----"	2006	573.15	0.05	5.52E-04	2E-05	No	256	TIP4P-FQ	34
	"----//----"	2006	573.15	0.1	2.73E-04	4E-06	No	256	TIP4P-FQ	34
	"----//----"	2006	673.15	0.001	3.48E-02	1E-03	No	256	TIP4P-FQ	34
	"----//----"	2006	673.15	0.002	1.74E-02	3E-04	No	256	TIP4P-FQ	34
	"----//----"	2006	673.15	0.005	6.72E-03	2E-04	No	256	TIP4P-FQ	34
	"----//----"	2006	673.15	0.01	3.40E-03	2E-04	No	256	TIP4P-FQ	34
	"----//----"	2006	673.15	0.05	6.64E-04	1E-05	No	256	TIP4P-FQ	34
	"----//----"	2006	673.15	0.1	3.38E-04	7E-06	No	256	TIP4P-FQ	34
86	Donchev et al.	2006	250		0.1387	N/A	No	256	QMPFF2	86
	"----//----"	2006	260		0.2709	N/A	No	256	QMPFF2	86
	"----//----"	2006	273		0.4656	N/A	No	256	QMPFF2	86
	"----//----"	2006	280		0.7085	N/A	No	256	QMPFF2	86
	"----//----"	2006	290		0.9238	N/A	No	256	QMPFF2	86
	"----//----"	2006	298		1.1875	N/A	No	256	QMPFF2	86
	"----//----"	2006	310		1.6940	N/A	No	256	QMPFF2	86
	"----//----"	2006	320		2.0617	N/A	No	256	QMPFF2	86
	"----//----"	2006	363		4.1980	N/A	No	256	QMPFF2	86
	"----//----"	2006	250		0.4366	N/A	No	256	QMPFF2	86
	"----//----"	2006	260		0.7212	N/A	No	256	QMPFF2	86
	"----//----"	2006	273		1.0406	N/A	No	256	QMPFF2	86
	"----//----"	2006	280		1.2766	N/A	No	256	QMPFF2	86
	"----//----"	2006	290		1.5959	N/A	No	256	QMPFF2	86

	"----//----"	2006	298		1.8457	N/A	No	256	QMPFF2	86
	"----//----"	2006	310		2.4838	N/A	No	256	QMPFF2	86
	"----//----"	2006	320		2.8931	N/A	No	256	QMPFF2	86
	"----//----"	2006	363		5.2165	N/A	No	256	QMPFF2	86
87	Mittal et al.	2006	300	0.85	2.941	N/A	No	500	SPC/E	13
	"----//----"	2006	300	0.90	2.786	N/A	No	500	SPC/E	13
	"----//----"	2006	300	0.95	2.770	N/A	No	500	SPC/E	13
	"----//----"	2006	300	1.00	2.561	N/A	No	500	SPC/E	13
	"----//----"	2006	300	1.05	2.485	N/A	No	500	SPC/E	13
	"----//----"	2006	300	1.10	2.470	N/A	No	500	SPC/E	13
	"----//----"	2006	300	1.15	2.176	N/A	No	500	SPC/E	13
	"----//----"	2006	300	1.20	1.872	N/A	No	500	SPC/E	13
	"----//----"	2006	300	1.25	1.690	N/A	No	500	SPC/E	13
	"----//----"	2006	300	1.30	1.385	N/A	No	500	SPC/E	13
	"----//----"	2006	280	0.85	1.730	N/A	No	500	SPC/E	13
	"----//----"	2006	280	0.90	1.453	N/A	No	500	SPC/E	13
	"----//----"	2006	280	0.95	1.629	N/A	No	500	SPC/E	13
	"----//----"	2006	280	1.00	1.659	N/A	No	500	SPC/E	13
	"----//----"	2006	280	1.05	1.731	N/A	No	500	SPC/E	13
	"----//----"	2006	280	1.10	1.721	N/A	No	500	SPC/E	13
	"----//----"	2006	280	1.15	1.445	N/A	No	500	SPC/E	13
	"----//----"	2006	280	1.20	1.273	N/A	No	500	SPC/E	13
	"----//----"	2006	280	1.25	1.095	N/A	No	500	SPC/E	13
	"----//----"	2006	280	1.30	0.898	N/A	No	500	SPC/E	13
	"----//----"	2006	260	0.85	0.839	N/A	No	500	SPC/E	13
	"----//----"	2006	260	0.90	0.705	N/A	No	500	SPC/E	13
	"----//----"	2006	260	0.95	0.772	N/A	No	500	SPC/E	13
	"----//----"	2006	260	1.00	0.805	N/A	No	500	SPC/E	13
	"----//----"	2006	260	1.05	0.925	N/A	No	500	SPC/E	13

	"----//----"	2006	260		1.10	1.012	N/A	No	500	SPC/E	13
	"----//----"	2006	260		1.15	0.936	N/A	No	500	SPC/E	13
	"----//----"	2006	260		1.20	0.931	N/A	No	500	SPC/E	13
	"----//----"	2006	260		1.25	0.709	N/A	No	500	SPC/E	13
	"----//----"	2006	260		1.30	0.554	N/A	No	500	SPC/E	13
	"----//----"	2006	240		0.85	0.284	N/A	No	500	SPC/E	13
	"----//----"	2006	240		0.90	0.222	N/A	No	500	SPC/E	13
	"----//----"	2006	240		0.95	0.267	N/A	No	500	SPC/E	13
	"----//----"	2006	240		1.00	0.322	N/A	No	500	SPC/E	13
	"----//----"	2006	240		1.05	0.438	N/A	No	500	SPC/E	13
	"----//----"	2006	240		1.10	0.479	N/A	No	500	SPC/E	13
	"----//----"	2006	240		1.15	0.538	N/A	No	500	SPC/E	13
	"----//----"	2006	240		1.20	0.400	N/A	No	500	SPC/E	13
	"----//----"	2006	240		1.25	0.370	N/A	No	500	SPC/E	13
	"----//----"	2006	240		1.30	0.303	N/A	No	500	SPC/E	13
	"----//----"	2006	220		0.85	0.047	N/A	No	500	SPC/E	13
	"----//----"	2006	220		0.90	0.024	N/A	No	500	SPC/E	13
	"----//----"	2006	220		0.95	0.041	N/A	No	500	SPC/E	13
	"----//----"	2006	220		1.00	0.076	N/A	No	500	SPC/E	13
	"----//----"	2006	220		1.05	0.163	N/A	No	500	SPC/E	13
	"----//----"	2006	220		1.10	0.162	N/A	No	500	SPC/E	13
	"----//----"	2006	220		1.15	0.186	N/A	No	500	SPC/E	13
	"----//----"	2006	220		1.20	0.168	N/A	No	500	SPC/E	13
	"----//----"	2006	220		1.25	0.125	N/A	No	500	SPC/E	13
	"----//----"	2006	220		1.30	0.089	N/A	No	500	SPC/E	13
89	Hofmann et al.	2007	268	270	1.09	0.61	N/A	No		Hofmann et al.	89
	"----//----"	2007	298	1	1.06	1.42	N/A	No		Hofmann et al.	89
	"----//----"	2007	298	2100	1.12	1.31	N/A	No		Hofmann et al.	89
	"----//----"	2007	423	100	0.92	9.97	N/A	No		Hofmann et al.	89

91	Yoshida et al	2007	673.15	SC	0.01	2523.56	N/A	No	1000	TIP4P	191
	"----//----"	2007	673.15	SC	0.00	6608.27	N/A	No	1000	TIP4P	191
	"----//----"	2007	673.15	SC	0.04	731.62	N/A	No	1000	TIP4P	191
	"----//----"	2007	673.15	SC	0.09	347.48	N/A	No	1000	TIP4P	191
	"----//----"	2007	673.15	SC	0.19	181.13	N/A	No	1000	TIP4P	191
	"----//----"	2007	673.15	SC	0.39	92.44	N/A	No	1000	TIP4P	191
	"----//----"	2007	673.15	SC	0.59	58.12	N/A	No	1000	TIP4P	191
	"----//----"	2007	673.15	SC	0.99	26.96	N/A	No	1000	TIP4P	191
	"----//----"	2007	673.15	SC	1.19	14.52	N/A	No	1000	TIP4P	191
	"----//----"	2007	673.15	SC	1.49	4.60	N/A	No	1000	TIP4P	191
92	Kumar et al.	2007	220	2000		5.95E-03	N/A	No	512	TIP5P	183
	"----//----"	2007	230	2000		3.28E-02	N/A	No	512	TIP5P	183
	"----//----"	2007	240	2000		1.45E-01	N/A	No	512	TIP5P	183
	"----//----"	2007	250	2000		2.83E-01	N/A	No	512	TIP5P	183
	"----//----"	2007	260	2000		5.52E-01	N/A	No	512	TIP5P	183
	"----//----"	2007	270	2000		6.90E-01	N/A	No	512	TIP5P	183
	"----//----"	2007	280	2000		1.35E+00	N/A	No	512	TIP5P	183
	"----//----"	2007	290	2000		1.68E+00	N/A	No	512	TIP5P	183
	"----//----"	2007	300	2000		2.10E+00	N/A	No	512	TIP5P	183
	"----//----"	2007	320	2000		4.10E+00	N/A	No	512	TIP5P	183
	"----//----"	2007	230	1000		5.12E-03	N/A	No	512	TIP5P	183
	"----//----"	2007	240	1000		4.10E-02	N/A	No	512	TIP5P	183
	"----//----"	2007	250	1000		1.81E-01	N/A	No	512	TIP5P	183
	"----//----"	2007	260	1000		4.42E-01	N/A	No	512	TIP5P	183
	"----//----"	2007	270	1000		6.90E-01	N/A	No	512	TIP5P	183
	"----//----"	2007	280	1000		1.16E+00	N/A	No	512	TIP5P	183
	"----//----"	2007	290	1000		1.68E+00	N/A	No	512	TIP5P	183
	"----//----"	2007	300	1000		2.10E+00	N/A	No	512	TIP5P	183
	"----//----"	2007	320	1000		3.81E+00	N/A	No	512	TIP5P	183

	"----//----"	2007	230	0		3.54E-04	N/A	No	512	TIP5P	183
	"----//----"	2007	240	0		5.12E-03	N/A	No	512	TIP5P	183
	"----//----"	2007	250	0		7.43E-02	N/A	No	512	TIP5P	183
	"----//----"	2007	260	0		2.83E-01	N/A	No	512	TIP5P	183
	"----//----"	2007	270	0		5.12E-01	N/A	No	512	TIP5P	183
	"----//----"	2007	280	0		1.25E+00	N/A	No	512	TIP5P	183
	"----//----"	2007	290	0		1.45E+00	N/A	No	512	TIP5P	183
	"----//----"	2007	300	0		2.10E+00	N/A	No	512	TIP5P	183
	"----//----"	2007	320	0		3.28E+00	N/A	No	512	TIP5P	183
98	Yoshida et al	2008	303.15	VLE	0.99	3.75	N/A	No	256	TIP4P	191
	"----//----"	2008	373.15	VLE	0.96	10.56	N/A	No	256	TIP4P	191
	"----//----"	2008	473.15	VLE	0.86	21.26	N/A	No	256	TIP4P	191
	"----//----"	2008	573.15	VLE	0.70	39.00	N/A	No	256	TIP4P	191
	"----//----"	2008	673.15	VLE	0.59	58.04	N/A	No	256	TIP4P	191
98	Yoshida et al.	2008	303.15	VLE	1	2.61	0.12	No	256	TIP4P	191
	"----//----"	2008	313.15		0.997	3.2	0.04	No	256	TIP4P	191
	"----//----"	2008	323.15		0.992	3.89	0.06	No	256	TIP4P	191
	"----//----"	2008	333.15		0.988	4.62	0.03	No	256	TIP4P	191
	"----//----"	2008	343.15		0.982	5.6	0.08	No	256	TIP4P	191
	"----//----"	2008	353.15		0.976	6.25	0.07	No	256	TIP4P	191
	"----//----"	2008	363.15		0.97	7.22	0.06	No	256	TIP4P	191
	"----//----"	2008	373.15		0.963	8.36	0.3	No	256	TIP4P	191
	"----//----"	2008	383.15		0.955	9.57	0.08	No	256	TIP4P	191
	"----//----"	2008	393.15		0.947	10.4	0.1	No	256	TIP4P	191
	"----//----"	2008	403.15		0.939	11.5	0.3	No	256	TIP4P	191
	"----//----"	2008	413.15		0.93	12.7	0.2	No	256	TIP4P	191
	"----//----"	2008	423.15		0.921	14.2	0.2	No	256	TIP4P	191
	"----//----"	2008	433.15		0.911	15.4	0.1	No	256	TIP4P	191
	"----//----"	2008	443.15		0.901	16.7	0.2	No	256	TIP4P	191

	"----//----"	2008	453.15		0.891	18.4	0.2	No	256	TIP4P	191
	"----//----"	2008	463.15		0.88	19.2	0.1	No	256	TIP4P	191
	"----//----"	2008	473.15		0.869	21.5	0.4	No	256	TIP4P	191
	"----//----"	2008	483.15		0.856	23.5	0.2	No	256	TIP4P	191
	"----//----"	2008	493.15		0.844	24.7	0.1	No	256	TIP4P	191
	"----//----"	2008	503.15		0.831	26.7	0.1	No	256	TIP4P	191
	"----//----"	2008	513.15		0.817	27.9	0.2	No	256	TIP4P	191
	"----//----"	2008	523.15		0.802	30.4	0.2	No	256	TIP4P	191
	"----//----"	2008	533.15		0.787	32.4	0.3	No	256	TIP4P	191
	"----//----"	2008	543.15		0.771	33.8	0.1	No	256	TIP4P	191
	"----//----"	2008	553.15		0.754	36.3	1.5	No	256	TIP4P	191
	"----//----"	2008	563.15		0.735	38.6	0.9	No	256	TIP4P	191
	"----//----"	2008	573.15		0.715	40.4	0.8	No	256	TIP4P	191
	"----//----"	2008	583.15		0.694	43.6	1.1	No	256	TIP4P	191
	"----//----"	2008	593.15		0.67	46.5	1.2	No	256	TIP4P	191
	"----//----"	2008	603.15		0.644	48.9	0.6	No	256	TIP4P	191
	"----//----"	2008	613.15		0.613	52.7	1.4	No	256	TIP4P	191
	"----//----"	2008	623.15		0.577	57.5	0.6	No	256	TIP4P	191
95	Liem & Popelier	2008	300	1.01325	0.996	1.44	N/A	No	216	QCT	95
	"----//----"	2008	300	1.01325	0.996	1.44	N/A	No	216	QCT	95
	"----//----"	2008	300	1013.25	1.045	1.53	N/A	No	216	QCT	95
	"----//----"	2008	300	2026.5	1.086	1.42	N/A	No	216	QCT	95
	"----//----"	2008	300	4053	1.149	1.11	N/A	No	216	QCT	95
	"----//----"	2008	300	6079.5	1.2	0.88	N/A	No	216	QCT	95
	"----//----"	2008	300	8106	1.242	0.7	N/A	No	216	QCT	95
	"----//----"	2008	300	10132.5	1.274	0.58	N/A	No	216	QCT	95
99	Vega et al.	2009	278	1		3.71	N/A	No	360	TIP3P	6
	"----//----"	2009	288	1		4.34	N/A	No	360	TIP3P	6
	"----//----"	2009	298	1		5.51	N/A	No	360	TIP3P	6
	"----//----"	2009	308	1		6.21	N/A	No	360	TIP3P	6

	"----//----"	2009	318	1		6.32	N/A	No	360	TIP3P	6
	"----//----"	2009	278	1		2.08	N/A	No	360	TIP4P	191
	"----//----"	2009	288	1		2.71	N/A	No	360	TIP4P	191
	"----//----"	2009	298	1		3.22	N/A	No	360	TIP4P	191
	"----//----"	2009	308	1		4.12	N/A	No	360	TIP4P	191
	"----//----"	2009	318	1		4.9	N/A	No	360	TIP4P	191
	"----//----"	2009	278	1		1.11	N/A	No	360	TIP5P	183
	"----//----"	2009	288	1		1.74	N/A	No	360	TIP5P	183
	"----//----"	2009	298	1		2.77	N/A	No	360	TIP5P	183
	"----//----"	2009	308	1		3.68	N/A	No	360	TIP5P	183
	"----//----"	2009	318	1		4.81	N/A	No	360	TIP5P	183
	"----//----"	2009	278	1		1.27	N/A	No	360	TIP4P/2005	80
	"----//----"	2009	288	1		1.57	N/A	No	360	TIP4P/2005	80
	"----//----"	2009	298	1		2.07	N/A	No	360	TIP4P/2005	80
	"----//----"	2009	308	1		2.6	N/A	No	360	TIP4P/2005	80
	"----//----"	2009	318	1		3.07	N/A	No	360	TIP4P/2005	80
101	Bauer & Patel	2009	298		VLE	2.3	N/A	Yes	217	TIP4P-QDP-LJ	101
	"----//----"	2009	325		VLE	4.12	N/A	Yes	217	TIP4P-QDP-LJ	101
	"----//----"	2009	350		VLE	6.26	N/A	Yes	217	TIP4P-QDP-LJ	101
	"----//----"	2009	375		VLE	8.08	N/A	Yes	217	TIP4P-QDP-LJ	101
	"----//----"	2009	400		VLE	11.04	N/A	Yes	217	TIP4P-QDP-LJ	101
	"----//----"	2009	425		VLE	13.68	N/A	Yes	217	TIP4P-QDP-LJ	101
	"----//----"	2009	450		VLE	16.32	N/A	Yes	217	TIP4P-QDP-LJ	101
	"----//----"	2009	475		VLE	20.60	N/A	Yes	217	TIP4P-QDP-LJ	101
	"----//----"	2009	500		VLE	24.40	N/A	Yes	217	TIP4P-QDP-LJ	101
	"----//----"	2009	525		VLE	28.85	N/A	Yes	217	TIP4P-QDP-LJ	101
	"----//----"	2009	550		VLE	33.79	N/A	Yes	217	TIP4P-QDP-LJ	101
	"----//----"	2009	575		VLE	40.05	N/A	Yes	217	TIP4P-QDP-LJ	101
	"----//----"	2009	600		VLE	49.95	N/A	Yes	217	TIP4P-QDP-LJ	101

106	Molinero & Moore	2009	361.05	1		10.95	N/A	No	4096	mW	106
	"----//----"	2009	341.00	1		9.67	N/A	No	4096	mW	106
	"----//----"	2009	320.42	1		8.12	N/A	No	4096	mW	106
	"----//----"	2009	298.00	1		6.50	N/A	No	4096	mW	106
	"----//----"	2009	280.21	1		5.45	N/A	No	4096	mW	106
	"----//----"	2009	260.52	1		4.04	N/A	No	4096	mW	106
	"----//----"	2009	240.15	1		2.70	N/A	No	4096	mW	106
	"----//----"	2009	219.98	1		1.44	N/A	No	4096	mW	106
107	Pi et al.	2009	224.72	1		0.039	N/A	No	256	TIP4P/2005	80
	"----//----"	2009	233.62	1		0.113	N/A	No	256	TIP4P/2005	80
	"----//----"	2009	242.65	1		0.253	N/A	No	256	TIP4P/2005	80
	"----//----"	2009	252.09	1		0.382	N/A	No	256	TIP4P/2005	80
	"----//----"	2009	261.80	1		0.592	N/A	No	256	TIP4P/2005	80
	"----//----"	2009	272.04	1		0.871	N/A	No	256	TIP4P/2005	80
	"----//----"	2009	282.97	1		1.438	N/A	No	256	TIP4P/2005	80
	"----//----"	2009	215.82	1500		0.058	N/A	No	256	TIP4P/2005	80
	"----//----"	2009	224.58	1500		0.117	N/A	No	256	TIP4P/2005	80
	"----//----"	2009	233.48	1500		0.214	N/A	No	256	TIP4P/2005	80
	"----//----"	2009	242.65	1500		0.368	N/A	No	256	TIP4P/2005	80
	"----//----"	2009	252.09	1500		0.488	N/A	No	256	TIP4P/2005	80
	"----//----"	2009	261.93	1500		0.796	N/A	No	256	TIP4P/2005	80
	"----//----"	2009	272.31	1500		1.126	N/A	No	256	TIP4P/2005	80
	"----//----"	2009	282.97	1500		1.419	N/A	No	256	TIP4P/2005	80
114	Chopra et al.	2010	500		0.85	19.04	N/A	No	368	SPC/E	13
	"----//----"	2010	500		0.90	18.22	N/A	No	368	SPC/E	13
	"----//----"	2010	500		0.95	17.43	N/A	No	368	SPC/E	13
	"----//----"	2010	500		1.00	14.46	N/A	No	368	SPC/E	13
	"----//----"	2010	500		1.10	11.76	N/A	No	368	SPC/E	13
	"----//----"	2010	500		1.20	9.11	N/A	No	368	SPC/E	13
	"----//----"	2010	500		1.30	6.58	N/A	No	368	SPC/E	13

"----//----"	2010	400	0.85	11.30	N/A	No	368	SPC/E	13
"----//----"	2010	400	0.90	9.83	N/A	No	368	SPC/E	13
"----//----"	2010	400	0.95	9.40	N/A	No	368	SPC/E	13
"----//----"	2010	400	1.00	9.21	N/A	No	368	SPC/E	13
"----//----"	2010	400	1.10	7.49	N/A	No	368	SPC/E	13
"----//----"	2010	400	1.20	5.67	N/A	No	368	SPC/E	13
"----//----"	2010	400	1.30	4.09	N/A	No	368	SPC/E	13
"----//----"	2010	350	0.85	6.39	N/A	No	368	SPC/E	13
"----//----"	2010	350	0.90	5.97	N/A	No	368	SPC/E	13
"----//----"	2010	350	0.95	5.85	N/A	No	368	SPC/E	13
"----//----"	2010	350	1.00	5.46	N/A	No	368	SPC/E	13
"----//----"	2010	350	1.10	4.77	N/A	No	368	SPC/E	13
"----//----"	2010	350	1.20	3.88	N/A	No	368	SPC/E	13
"----//----"	2010	350	1.30	2.80	N/A	No	368	SPC/E	13
"----//----"	2010	300	0.85	2.72	N/A	No	368	SPC/E	13
"----//----"	2010	300	0.90	2.86	N/A	No	368	SPC/E	13
"----//----"	2010	300	0.95	2.61	N/A	No	368	SPC/E	13
"----//----"	2010	300	1.00	2.62	N/A	No	368	SPC/E	13
"----//----"	2010	300	1.10	2.40	N/A	No	368	SPC/E	13
"----//----"	2010	300	1.20	2.04	N/A	No	368	SPC/E	13
"----//----"	2010	300	1.30	1.44	N/A	No	368	SPC/E	13
"----//----"	2010	280	0.85	1.61	N/A	No	368	SPC/E	13
"----//----"	2010	280	0.90	1.58	N/A	No	368	SPC/E	13
"----//----"	2010	280	0.95	1.41	N/A	No	368	SPC/E	13
"----//----"	2010	280	1.00	1.63	N/A	No	368	SPC/E	13
"----//----"	2010	280	1.10	1.60	N/A	No	368	SPC/E	13
"----//----"	2010	280	1.20	1.43	N/A	No	368	SPC/E	13
"----//----"	2010	280	1.30	0.94	N/A	No	368	SPC/E	13
"----//----"	2010	260	0.85	0.79	N/A	No	368	SPC/E	13
"----//----"	2010	260	0.90	0.74	N/A	No	368	SPC/E	13

"----//----"	2010	260	0.95	0.78	N/A	No	368	SPC/E	13
"----//----"	2010	260	1.00	0.86	N/A	No	368	SPC/E	13
"----//----"	2010	260	1.10	1.00	N/A	No	368	SPC/E	13
"----//----"	2010	260	1.20	0.89	N/A	No	368	SPC/E	13
"----//----"	2010	260	1.30	0.60	N/A	No	368	SPC/E	13
"----//----"	2010	250	0.85	0.52	N/A	No	368	SPC/E	13
"----//----"	2010	250	0.90	0.43	N/A	No	368	SPC/E	13
"----//----"	2010	250	0.95	0.51	N/A	No	368	SPC/E	13
"----//----"	2010	250	1.00	0.57	N/A	No	368	SPC/E	13
"----//----"	2010	250	1.10	0.77	N/A	No	368	SPC/E	13
"----//----"	2010	250	1.20	0.67	N/A	No	368	SPC/E	13
"----//----"	2010	250	1.30	0.44	N/A	No	368	SPC/E	13
"----//----"	2010	240	0.85	0.27	N/A	No	368	SPC/E	13
"----//----"	2010	240	0.90	0.21	N/A	No	368	SPC/E	13
"----//----"	2010	240	0.95	0.27	N/A	No	368	SPC/E	13
"----//----"	2010	240	1.00	0.35	N/A	No	368	SPC/E	13
"----//----"	2010	240	1.10	0.52	N/A	No	368	SPC/E	13
"----//----"	2010	240	1.20	0.47	N/A	No	368	SPC/E	13
"----//----"	2010	240	1.30	0.30	N/A	No	368	SPC/E	13
"----//----"	2010	230	0.85	0.13	N/A	No	368	SPC/E	13
"----//----"	2010	230	0.90	0.08	N/A	No	368	SPC/E	13
"----//----"	2010	230	0.95	0.13	N/A	No	368	SPC/E	13
"----//----"	2010	230	1.00	0.19	N/A	No	368	SPC/E	13
"----//----"	2010	230	1.10	0.31	N/A	No	368	SPC/E	13
"----//----"	2010	230	1.20	0.31	N/A	No	368	SPC/E	13
"----//----"	2010	230	1.30	0.20	N/A	No	368	SPC/E	13
"----//----"	2010	220	0.85	0.04	N/A	No	368	SPC/E	13
"----//----"	2010	220	0.90	0.03	N/A	No	368	SPC/E	13
"----//----"	2010	220	0.95	0.04	N/A	No	368	SPC/E	13
"----//----"	2010	220	1.00	0.09	N/A	No	368	SPC/E	13

	"----//----"	2010	220		1.10	0.19	N/A	No	368	SPC/E	13
	"----//----"	2010	220		1.20	0.19	N/A	No	368	SPC/E	13
	"----//----"	2010	220		1.30	0.11	N/A	No	368	SPC/E	13
113	Fuhrmans et al.	2010	323	1		1.8	0.11	No	1068	Model 1 Fuhrmans	113
	"----//----"	2010	323	1		1.81	0.1	No	1068	Model 2 Fuhrmans	113
	"----//----"	2010	323	1		6.19	0.29	No	1068	SPC	178
	"----//----"	2010	323	1		1.97	0.04	No	1068	MARTINI W	192
115	Guevara-Carrion et al.	2011	280	1		3.11	0.02	No	2048	SPC	178
	"----//----"	2011	298.15	1		4.34	0.03	No	2048	SPC	178
	"----//----"	2011	328.15	1		6.80	0.04	No	2048	SPC	178
	"----//----"	2011	280	1		1.79	0.01	No	2048	SPC/E	13
	"----//----"	2011	288.15	1		2.17	0.01	No	2048	SPC/E	13
	"----//----"	2011	298.15	1		2.72	0.02	No	2048	SPC/E	13
	"----//----"	2011	313.15	1		3.60	0.02	No	2048	SPC/E	13
	"----//----"	2011	328.15	1		4.66	0.03	No	2048	SPC/E	13
	"----//----"	2011	343.15	1		5.74	0.04	No	2048	SPC/E	13
	"----//----"	2011	363.15	1		7.39	0.04	No	2048	SPC/E	13
	"----//----"	2011	373.15	1		8.21	0.04	No	2048	SPC/E	13
	"----//----"	2011	280	1		2.49	0.02	No	2048	TIP4P	191
	"----//----"	2011	288.15	1		3.00	0.02	No	2048	TIP4P	191
	"----//----"	2011	298.15	1		3.69	0.02	No	2048	TIP4P	191
	"----//----"	2011	313.15	1		4.84	0.02	No	2048	TIP4P	191
	"----//----"	2011	328.15	1		5.72	0.03	No	2048	TIP4P	191
	"----//----"	2011	343.15	1		7.56	0.04	No	2048	TIP4P	191
	"----//----"	2011	363.15	1		9.69	0.05	No	2048	TIP4P	191
	"----//----"	2011	273.15	1		1.11	0.01	No	2048	TIP4P/2005	80
	"----//----"	2011	280	1		1.38	0.01	No	2048	TIP4P/2005	80

"----//----"	2011	288.15	1	1.75	0.01	No	2048	TIP4P/2005	80
"----//----"	2011	298.15	1	2.26	0.02	No	2048	TIP4P/2005	80
"----//----"	2011	313.15	1	3.05	0.02	No	2048	TIP4P/2005	80
"----//----"	2011	333.15	1	4.42	0.03	No	2048	TIP4P/2005	80
"----//----"	2011	353.15	1	5.94	0.03	No	2048	TIP4P/2005	80
"----//----"	2011	363.15	1	6.93	0.04	No	2048	TIP4P/2005	80
"----//----"	2011	260.00	500	0.77	0.07	No	2048	TIP4P/2005	80
"----//----"	2011	273.15	500	1.22	0.01	No	2048	TIP4P/2005	80
"----//----"	2011	280.00	500	1.47	0.01	No	2048	TIP4P/2005	80
"----//----"	2011	288.15	500	1.77	0.01	No	2048	TIP4P/2005	80
"----//----"	2011	298.15	500	2.3	0.02	No	2048	TIP4P/2005	80
"----//----"	2011	313.15	500	3.1	0.02	No	2048	TIP4P/2005	80
"----//----"	2011	333.15	500	4.34	0.03	No	2048	TIP4P/2005	80
"----//----"	2011	343.15	500	5.04	0.03	No	2048	TIP4P/2005	80
"----//----"	2011	363.15	500	6.62	0.04	No	2048	TIP4P/2005	80
"----//----"	2011	380.00	500	3.49	0.06	No	2048	TIP4P/2005	80
"----//----"	2011	260.00	1000	0.837	0.07	No	2048	TIP4P/2005	80
"----//----"	2011	273.15	1000	1.261	0.09	No	2048	TIP4P/2005	80
"----//----"	2011	280.00	1000	1.52	0.01	No	2048	TIP4P/2005	80
"----//----"	2011	288.15	1000	1.86	0.01	No	2048	TIP4P/2005	80
"----//----"	2011	298.15	1000	2.3	0.02	No	2048	TIP4P/2005	80
"----//----"	2011	313.15	1000	3.09	0.02	No	2048	TIP4P/2005	80
"----//----"	2011	333.15	1000	4.32	0.03	No	2048	TIP4P/2005	80
"----//----"	2011	343.15	1000	4.97	0.03	No	2048	TIP4P/2005	80
"----//----"	2011	363.15	1000	6.49	0.04	No	2048	TIP4P/2005	80
"----//----"	2011	380.00	1000	7.77	0.04	No	2048	TIP4P/2005	80
"----//----"	2011	400.00	1000	7.77	0.04	No	2048	TIP4P/2005	80
"----//----"	2011	260.00	2000	0.89	0.008	No	2048	TIP4P/2005	80
"----//----"	2011	273.15	2000	1.30	0.009	No	2048	TIP4P/2005	80
"----//----"	2011	280.00	2000	1.55	0.001	No	2048	TIP4P/2005	80
"----//----"	2011	288.15	2000	1.90	0.001	No	2048	TIP4P/2005	80
"----//----"	2011	298.15	2000	2.30	0.001	No	2048	TIP4P/2005	80

	"----//----"	2011	313.15	2000		3.06	0.002	No	2048	TIP4P/2005	80
	"----//----"	2011	333.15	2000		4.20	0.002	No	2048	TIP4P/2005	80
	"----//----"	2011	343.15	2000		4.78	0.003	No	2048	TIP4P/2005	80
	"----//----"	2011	363.15	2000		6.10	0.003	No	2048	TIP4P/2005	80
	"----//----"	2011	380.00	2000		7.38	0.004	No	2048	TIP4P/2005	80
	"----//----"	2011	400.00	2000		8.94	0.004	No	2048	TIP4P/2005	80
	"----//----"	2011	260.00	3000		0.90	0.009	No	2048	TIP4P/2005	80
	"----//----"	2011	273.15	3000		1.30	0.001	No	2048	TIP4P/2005	80
	"----//----"	2011	280.00	3000		1.54	0.001	No	2048	TIP4P/2005	80
	"----//----"	2011	288.15	3000		1.86	0.001	No	2048	TIP4P/2005	80
	"----//----"	2011	298.15	3000		2.28	0.001	No	2048	TIP4P/2005	80
	"----//----"	2011	313.15	3000		2.97	0.002	No	2048	TIP4P/2005	80
	"----//----"	2011	333.15	3000		4.05	0.002	No	2048	TIP4P/2005	80
	"----//----"	2011	343.15	3000		5.86	0.003	No	2048	TIP4P/2005	80
	"----//----"	2011	363.15	3000		6.47	0.004	No	2048	TIP4P/2005	80
	"----//----"	2011	400.00	3000		8.38	0.005	No	2048	TIP4P/2005	80
119	Alejandre et al.	2011	280	1	0.9984	1.27	N/A	No	500	TIP4Q	119
	"----//----"	2011	300	1	0.9984	2.2	N/A	No	500	TIP4Q	119
	"----//----"	2011	320	1	0.9872	3.26	N/A	No	500	TIP4Q	119
	"----//----"	2011	340	1	0.9774	4.67	N/A	No	500	TIP4Q	119
120	Viererblova & Kolafa	2011	263.005	1.01325		0.700	0.004	Yes	360	POL4D	120
	"----//----"	2011	272.995	1.01325		1.089	0.007	Yes	360	POL4D	120
	"----//----"	2011	273.150	1.01325		1.086	0.012	Yes	360	POL4D	120
	"----//----"	2011	273.001	1.01325		1.174	0.006	Yes	360	POL4D	120
	"----//----"	2011	282.998	1.01325		1.547	0.009	Yes	360	POL4D	120
	"----//----"	2011	297.981	1.01325		2.423	0.013	Yes	360	POL4D	120
	"----//----"	2011	298.150	1.01325		2.461	0.015	Yes	360	POL4D	120
	"----//----"	2011	298.116	1.01325		2.458	0.028	Yes	360	POL4D	120
	"----//----"	2011	319.964	1.01325		4.054	0.015	Yes	360	POL4D	120
	"----//----"	2011	349.802	1.01325		6.924	0.022	Yes	360	POL4D	120

121	Orsi & Essex	2011	303	1.01325		2.6	1%	No	4000	ELBA	121
123	Qvist et al.	2011	230.75		0.9756	0.165	0.001	Yes	2048	SPC/E	13
	"----//----"	2011	246.54		0.9935	0.509	0.004	Yes	2048	SPC/E	13
	"----//----"	2011	253.35		0.9963	0.705	0.006	Yes	2048	SPC/E	13
	"----//----"	2011	259.28		0.9982	0.909	0.007	Yes	2048	SPC/E	13
	"----//----"	2011	266.08		0.9998	1.20	0.01	Yes	2048	SPC/E	13
	"----//----"	2011	276.03		0.9997	1.58	0.02	Yes	2048	SPC/E	13
	"----//----"	2011	290.29		0.9982	2.34	0.02	Yes	2048	SPC/E	13
122	Wang & Hou	2011	235.47			1.059	0.001	No	624	TIP3P	6
	"----//----"	2011	247.96			1.374	0.001	No	624	TIP3P	6
	"----//----"	2011	260.49			1.734	0.009	No	624	TIP3P	6
	"----//----"	2011	273.16			2.085	0.014	No	624	TIP3P	6
	"----//----"	2011	285.49			2.717	0.020	No	624	TIP3P	6
	"----//----"	2011	298.13			2.984	0.005	No	624	TIP3P	6
	"----//----"	2011	310.45			3.667	0.016	No	624	TIP3P	6
	"----//----"	2011	322.85			3.667	0.012	No	624	TIP3P	6
	"----//----"	2011	335.42			4.629	0.008	No	624	TIP3P	6
	"----//----"	2011	347.87			5.056	0.014	No	624	TIP3P	6
	"----//----"	2011	360.43			5.527	0.014	No	624	TIP3P	6
	"----//----"	2011	373.04			6.268	0.007	No	624	TIP3P	6
	"----//----"	2011	400.00			8.073	0.056	No	624	TIP3P	6
124	Raabe & Sadus	2012	277.15	1		1.502	0.06	No	400	SPC/E	13
	"----//----"	2012	298.15	1		2.432	0.023	No	400	SPC/E	13
	"----//----"	2012	323.15	1		3.878	0.169	No	400	SPC/E	13
	"----//----"	2012	353.15	1		5.77	0.277	No	400	SPC/E	13
	"----//----"	2012	277.15	1		1.410	0.047	No	400	SPC/Fw	83
	"----//----"	2012	298.15	1		2.359	0.035	No	400	SPC/Fw	83

"----//----"	2012	313.15	1	3.229	0.158	No	400	SPC/Fw	83
"----//----"	2012	318.15	1	3.431	0.134	No	400	SPC/Fw	83
"----//----"	2012	323.15	1	3.797	0.15	No	400	SPC/Fw	83
"----//----"	2012	333.15	1	4.5	0.094	No	400	SPC/Fw	83
"----//----"	2012	343.15	1	5.218	0.302	No	400	SPC/Fw	83
"----//----"	2012	353.15	1	5.927	0.22	No	400	SPC/Fw	83
"----//----"	2012	363.15	1	6.720	0.205	No	400	SPC/Fw	83
"----//----"	2012	277.15	1	2.659	0.103	No	400	SPC	178
"----//----"	2012	298.15	1	3.861	0.03	No	400	SPC	178
"----//----"	2012	333.15	1	6.675	0.275	No	400	SPC	178
"----//----"	2012	353.15	1	8.281	0.276	No	400	SPC	178
"----//----"	2012	298.15	1	2.359	0.035	No	400	SPC/Fw	83
"----//----"	2012	298.15	500	2.378	0.027	No	400	SPC/Fw	83
"----//----"	2012	298.15	1000	2.328	0.045	No	400	SPC/Fw	83
"----//----"	2012	298.15	1500	2.344	0.041	No	400	SPC/Fw	83
"----//----"	2012	298.15	2000	2.269	0.011	No	400	SPC/Fw	83
"----//----"	2012	318.15	1	3.432	0.134	No	400	SPC/Fw	83
"----//----"	2012	318.15	100	3.502	0.160	No	400	SPC/Fw	83
"----//----"	2012	318.15	1000	3.468	0.187	No	400	SPC/Fw	83
"----//----"	2012	333.15	1	4.499	0.094	No	400	SPC/Fw	83
"----//----"	2012	333.15	100	4.584	0.177	No	400	SPC/Fw	83
"----//----"	2012	333.15	500	4.472	0.193	No	400	SPC/Fw	83
"----//----"	2012	333.15	1000	4.29	0.208	No	400	SPC/Fw	83
"----//----"	2012	673.15	500	60.086	1222	No	400	SPC/Fw	83
"----//----"	2012	673.15	1000	47.297	0.531	No	400	SPC/Fw	83
"----//----"	2012	673.15	2000	37.9	0.412	No	400	SPC/Fw	83
"----//----"	2012	298.15	1	1.43	0.06	No	400	SPC/E	13
"----//----"	2012	298.15	500	1.42	N/A	No	400	SPC/E	13
"----//----"	2012	298.15	1000	1.39	N/A	No	400	SPC/E	13

	"----//----"	2012	298.15	1500		1.35	N/A	No	400	SPC/E	13
	"----//----"	2012	673.15	500		6.06	N/A	No	400	SPC/E	13
	"----//----"	2012	673.15	1000		4.67	N/A	No	400	SPC/E	13
129	Gallo & Rovere	2012	300		1.00	3.77	N/A	No	256 (?)	TIP4P	191
	"----//----"	2012	280		1.00	2.13	N/A	No	256 (?)	TIP4P	191
	"----//----"	2012	260		1.00	1.22	N/A	No	256 (?)	TIP4P	191
	"----//----"	2012	250		1.00	0.797	N/A	No	256 (?)	TIP4P	191
	"----//----"	2012	240		1.00	0.539	N/A	No	256 (?)	TIP4P	191
	"----//----"	2012	230		1.00	0.337	N/A	No	256 (?)	TIP4P	191
	"----//----"	2012	220		1.00	0.169	N/A	No	256 (?)	TIP4P	191
	"----//----"	2012	210		1.00	7.10E-02	N/A	No	256 (?)	TIP4P	191
	"----//----"	2012	200		1.00	2.60E-02	N/A	No	256 (?)	TIP4P	191
	"----//----"	2012	195		1.00	1.20E-02	N/A	No	256 (?)	TIP4P	191
	"----//----"	2012	190		1.00	6.40E-03	N/A	No	256 (?)	TIP4P	191
130	Rozmanov & Kusalik	2012	210			2.52E-03	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	215			7.90E-03	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	220			1.99E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	225			4.19E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	230			7.70E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	235			1.28E-01	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	240			1.95E-01	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	245			2.81E-01	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	250			3.84E-01	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	255			5.05E-01	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	260			6.43E-01	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	265			7.96E-01	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	270			9.64E-01	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	275			1.14E+00	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	280			1.34E+00	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	285			1.54E+00	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	290			1.75E+00	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	295			1.96E+00	N/A	No	1000	TIP4P/2005	80

	"----//----"	2012	298			2.10E+00	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	300			2.19E+00	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	305			2.42E+00	N/A	No	1000	TIP4P/2005	80
	"----//----"	2012	310			2.65E+00	N/A	No	1000	TIP4P/2005	80
131	Zlenko	2012	273.15	-14.12		1.00	N/A	No	11337	TIP4P	191
	"----//----"	2012	277.15	14.63		1.02	N/A	No	11337	TIP4P	191
	"----//----"	2012	283.15	53.89		1.20	N/A	No	11337	TIP4P	191
	"----//----"	2012	293.15	119.46		1.48	N/A	No	11337	TIP4P	191
	"----//----"	2012	298.15	143.68		1.59	N/A	No	11337	TIP4P	191
	"----//----"	2012	303.15	176.10		1.73	N/A	No	11337	TIP4P	191
	"----//----"	2012	313.15	233.86		2.02	N/A	No	11337	TIP4P	191
	"----//----"	2012	323.15	287.26		2.28	N/A	No	11337	TIP4P	191
	"----//----"	2012	333.15	341.97		2.57	N/A	No	11337	TIP4P	191
	"----//----"	2012	343.15	391.72		2.86	N/A	No	11337	TIP4P	191
	"----//----"	2012	348.15	416.65		3.06	N/A	No	11337	TIP4P	191
	"----//----"	2012	353.15	441.47		3.10	N/A	No	11337	TIP4P	191
	"----//----"	2012	363.15	487.07		3.50	N/A	No	11337	TIP4P	191
	"----//----"	2012	373.15	529.42		3.79	N/A	No	11337	TIP4P	191
132	Lee	2013	300		0.9965	2.78	0.06	No	1024	SPC/E	13
	"----//----"	2013	350		0.9737	6.02	0.09	No	1024	SPC/E	13
	"----//----"	2013	400		0.9375	10.3	0.02	No	1024	SPC/E	13
	"----//----"	2013	450		0.8903	15.3	0.01	No	1024	SPC/E	13
	"----//----"	2013	500		0.8313	21.8	0.03	No	1024	SPC/E	13
	"----//----"	2013	550		0.7558	30.1	0.03	No	1024	SPC/E	13
143	Wang et al.	2013	260	1.01325		0.74	N/A	Yes	216/512/1000	iAMOEBA	143
	"----//----"	2013	273	1.01325		1.23	N/A	Yes	216/512/1000	iAMOEBA	143
	"----//----"	2013	285	1.01325		1.79	N/A	Yes	216/512/1000	iAMOEBA	143
	"----//----"	2013	298	1.01325		2.54	N/A	Yes	216/512/1000	iAMOEBA	143
	"----//----"	2013	310	1.01325		3.25	N/A	Yes	216/512/1000	iAMOEBA	143
	"----//----"	2013	323	1.01325		4.03	N/A	Yes	216/512/1000	iAMOEBA	143

	"----//----"	2013	255	1.01325		0.2	N/A	Yes	216/512/1000	AMOEBA	78
	"----//----"	2013	260	1.01325		0.31	N/A	Yes	216/512/1000	AMOEBA	78
	"----//----"	2013	265	1.01325		0.51	N/A	Yes	216/512/1000	AMOEBA	78
	"----//----"	2013	273	1.01325		0.78	N/A	Yes	216/512/1000	AMOEBA	78
	"----//----"	2013	278	1.01325		0.84	N/A	Yes	216/512/1000	AMOEBA	78
	"----//----"	2013	285	1.01325		1.26	N/A	Yes	216/512/1000	AMOEBA	78
	"----//----"	2013	298	1.01325		1.92	N/A	Yes	216/512/1000	AMOEBA	78
	"----//----"	2013	323	1.01325		3.38	N/A	Yes	216/512/1000	AMOEBA	78
141	Stukan et al.	2013	298.15	1.01325		2.4	N/A	No	1024	SWM4-NDP	82
	"----//----"	2013	323	1.01325		4	N/A	No	1024	SWM4-NDP	82
	"----//----"	2013	348	1.01325		6.1	N/A	No	1024	SWM4-NDP	82
	"----//----"	2013	363	1.01325		7.2	N/A	No	1024	SWM4-NDP	82
137	Corsetti et al.	2013	300		1	1.92	Yes (Fig. 12)	No	200	TIP4P	191
	"----//----"	2013	300		1.05	2.09	Yes (Fig. 12)	No	200	TIP4P	191
	"----//----"	2013	300		1.1	1.54	Yes (Fig. 12)	No	200	TIP4P	191
	"----//----"	2013	300		1.15	1.21	Yes (Fig. 12)	No	200	TIP4P	191
	"----//----"	2013	300		1.2	1.06	Yes (Fig. 12)	No	200	TIP4P	191
144	Arismendi-Arrieta et al.	2014	273			1.34	N/A	No	256	NCC(Q)	144
	"----//----"	2014	283			1.67	N/A	No	256	NCC(Q)	144
	"----//----"	2014	303			2.5	N/A	No	256	NCC(Q)	144
	"----//----"	2014	333			3.8	N/A	No	256	NCC(Q)	144
	"----//----"	2014	373			5.93	N/A	No	256	NCC(Q)	144
150	Kiss & Baranyai	2014	225	1		0.0615	N/A	Yes	432	BK3	136
	"----//----"	2014	230	1		0.0954	N/A	Yes	432	BK3	136
	"----//----"	2014	235	1		0.1417	N/A	Yes	432	BK3	136
	"----//----"	2014	238	1		0.1750	N/A	Yes	432	BK3	136
	"----//----"	2014	243	1		0.2472	N/A	Yes	432	BK3	136

"----//----"	2014	248	1	0.3434	N/A	Yes	432	BK3	136
"----//----"	2014	253	1	0.4498	N/A	Yes	432	BK3	136
"----//----"	2014	258	1	0.5841	N/A	Yes	432	BK3	136
"----//----"	2014	263	1	0.7210	N/A	Yes	432	BK3	136
"----//----"	2014	268	1	0.8902	N/A	Yes	432	BK3	136
"----//----"	2014	273	1	1.0806	N/A	Yes	432	BK3	136
"----//----"	2014	278	1	1.2898	N/A	Yes	432	BK3	136
"----//----"	2014	283	1	1.4885	N/A	Yes	432	BK3	136
"----//----"	2014	288	1	1.7470	N/A	Yes	432	BK3	136
"----//----"	2014	293	1	2.0332	N/A	Yes	432	BK3	136
"----//----"	2014	298	1	2.3268	N/A	Yes	432	BK3	136
"----//----"	2014	303	1	2.6627	N/A	Yes	432	BK3	136
"----//----"	2014	308	1	2.9962	N/A	Yes	432	BK3	136
"----//----"	2014	313	1	3.2872	N/A	Yes	432	BK3	136
"----//----"	2014	323	1	4.0583	N/A	Yes	432	BK3	136
"----//----"	2014	333	1	4.7631	N/A	Yes	432	BK3	136
"----//----"	2014	343	1	5.5903	N/A	Yes	432	BK3	136
"----//----"	2014	353	1	6.5612	N/A	Yes	432	BK3	136
"----//----"	2014	363	1	7.3829	N/A	Yes	432	BK3	136
"----//----"	2014	373	1	8.3075	N/A	Yes	432	BK3	136
"----//----"	2014	223	1500	0.13821	N/A	Yes	432	BK3	136
"----//----"	2014	228	1500	0.18563	N/A	Yes	432	BK3	136
"----//----"	2014	233	1500	0.24309	N/A	Yes	432	BK3	136
"----//----"	2014	238	1500	0.31303	N/A	Yes	432	BK3	136
"----//----"	2014	243	1500	0.39302	N/A	Yes	432	BK3	136
"----//----"	2014	248	1500	0.48931	N/A	Yes	432	BK3	136
"----//----"	2014	253	1500	0.60408	N/A	Yes	432	BK3	136
"----//----"	2014	258	1500	0.71499	N/A	Yes	432	BK3	136
"----//----"	2014	263	1500	0.86794	N/A	Yes	432	BK3	136
"----//----"	2014	268	1500	1.01868	N/A	Yes	432	BK3	136
"----//----"	2014	273	1500	1.18556	N/A	Yes	432	BK3	136
"----//----"	2014	283	1500	1.57898	N/A	Yes	432	BK3	136

	"----//----"	2014	298	1500		2.24964	N/A	Yes	432	BK3	136
	"----//----"	2014	313	1500		3.04710	N/A	Yes	432	BK3	136
	"----//----"	2014	333	1500		4.26876	N/A	Yes	432	BK3	136
	"----//----"	2014	353	1500		5.63760	N/A	Yes	432	BK3	136
	"----//----"	2014	373	1500		7.19855	N/A	Yes	432	BK3	136
147	Fuentes-Azcatl & Alejandre	2014	240	1	0.9851	0.1852	N/A	No	500	TIP4P/2005	80
	"----//----"	2014	250	1	0.9929	0.3423	N/A	No	500	TIP4P/2005	80
	"----//----"	2014	260	1	0.9978	0.601	N/A	No	500	TIP4P/2005	80
	"----//----"	2014	270	1	1	0.8644	N/A	No	500	TIP4P/2005	80
	"----//----"	2014	280	1	1.0002	1.1682	N/A	No	500	TIP4P/2005	80
	"----//----"	2014	290	1	0.999	1.643	N/A	No	500	TIP4P/2005	80
	"----//----"	2014	300	1	0.9967	2.1048	N/A	No	500	TIP4P/2005	80
	"----//----"	2014	310	1	0.9935	2.8515	N/A	No	500	TIP4P/2005	80
	"----//----"	2014	320	1	0.9894	3.3919	N/A	No	500	TIP4P/2005	80
	"----//----"	2014	330	1	0.9843	3.9504	N/A	No	500	TIP4P/2005	80
	"----//----"	2014	340	1	0.9789	4.7134	N/A	No	500	TIP4P/2005	80
	"----//----"	2014	240	1	0.9867	0.2141	N/A	No	500	TIP4P/ε	147
	"----//----"	2014	250	1	0.9945	0.3739	N/A	No	500	TIP4P/ε	147
	"----//----"	2014	260	1	0.998	0.6578	N/A	No	500	TIP4P/ε	147
	"----//----"	2014	270	1	0.9997	0.9235	N/A	No	500	TIP4P/ε	147
	"----//----"	2014	280	1	0.9993	1.1939	N/A	No	500	TIP4P/ε	147
	"----//----"	2014	290	1	0 0.998	1.7265	N/A	No	500	TIP4P/ε	147
	"----//----"	2014	300	1	0.9958	2.0963	N/A	No	500	TIP4P/ε	147
	"----//----"	2014	310	1	0.9926	2.6428	N/A	No	500	TIP4P/ε	147
	"----//----"	2014	320	1	0.9885	3.3458	N/A	No	500	TIP4P/ε	147
	"----//----"	2014	330	1	0.9837	3.7811	N/A	No	500	TIP4P/ε	147
	"----//----"	2014	340	1	0.9786	4.3345	N/A	No	500	TIP4P/ε	147
149	Moultos et al.	2014	298.15	1		3.6	0.5	No	2000	SPC	178
	"----//----"	2014	323.15	1		6.2	0.5	No	2000	SPC	178

"----//----"	2014	348.15	1	8.8	0.3	No	2000	SPC	178
"----//----"	2014	373.15	480	10.7	0.2	No	2000	SPC	178
"----//----"	2014	298.15	1	2.6	0.1	No	2000	SPC/E	13
"----//----"	2014	323.15	1	4.3	0.2	No	2000	SPC/E	13
"----//----"	2014	323.15	200	4.2	0.1	No	2000	SPC/E	13
"----//----"	2014	323.15	480	4.2	0.2	No	2000	SPC/E	13
"----//----"	2014	348.15	1	6.2	0.2	No	2000	SPC/E	13
"----//----"	2014	348.15	200	6.2	0.2	No	2000	SPC/E	13
"----//----"	2014	373.15	15	8.4	0.2	No	2000	SPC/E	13
"----//----"	2014	373.15	200	8.2	0.1	No	2000	SPC/E	13
"----//----"	2014	373.15	480	7.8	0.3	No	2000	SPC/E	13
"----//----"	2014	398.15	200	10.8	0.3	No	2000	SPC/E	13
"----//----"	2014	423.15	200	13.6	0.5	No	2000	SPC/E	13
"----//----"	2014	448.15	200	16.7	0.5	No	2000	SPC/E	13
"----//----"	2014	473.15	200	19.9	0.4	No	2000	SPC/E	13
"----//----"	2014	473.15	480	19.4	0.4	No	2000	SPC/E	13
"----//----"	2014	473.15	1000	17.8	0.3	No	2000	SPC/E	13
"----//----"	2014	523.15	200	28.2	0.8	No	2000	SPC/E	13
"----//----"	2014	523.15	480	26.4	0.5	No	2000	SPC/E	13
"----//----"	2014	523.15	1000	24.2	0.7	No	2000	SPC/E	13
"----//----"	2014	573.15	480	35.7	0.8	No	2000	SPC/E	13
"----//----"	2014	623.15	200	60	2	No	2000	SPC/E	13
"----//----"	2014	623.15	480	48	2	No	2000	SPC/E	13
"----//----"	2014	623.15	1000	39.9	0.8	No	2000	SPC/E	13
"----//----"	2014	298.15	1	2.1	0.1	No	2000	TIP4P/2005	80
"----//----"	2014	323.15	1	3.6	0.1	No	2000	TIP4P/2005	80
"----//----"	2014	323.15	200	3.6	0.1	No	2000	TIP4P/2005	80
"----//----"	2014	323.15	480	3.6	0.1	No	2000	TIP4P/2005	80
"----//----"	2014	348.15	1	5.4	0.2	No	2000	TIP4P/2005	80
"----//----"	2014	348.15	200	5.3	0.1	No	2000	TIP4P/2005	80

	"----//----"	2014	373.15	15	7.5	0.1	No	2000	TIP4P/2005	80
	"----//----"	2014	373.15	200	7.4	0.2	No	2000	TIP4P/2005	80
	"----//----"	2014	373.15	480	7.4	0.2	No	2000	TIP4P/2005	80
	"----//----"	2014	398.15	200	9.7	0.2	No	2000	TIP4P/2005	80
	"----//----"	2014	423.15	200	12.6	0.3	No	2000	TIP4P/2005	80
	"----//----"	2014	448.15	200	15.4	0.3	No	2000	TIP4P/2005	80
	"----//----"	2014	473.15	200	18.7	0.6	No	2000	TIP4P/2005	80
	"----//----"	2014	473.15	480	17.6	0.5	No	2000	TIP4P/2005	80
	"----//----"	2014	473.15	1000	17	0.5	No	2000	TIP4P/2005	80
	"----//----"	2014	523.15	200	25.9	0.9	No	2000	TIP4P/2005	80
	"----//----"	2014	523.15	480	24.9	0.8	No	2000	TIP4P/2005	80
	"----//----"	2014	523.15	1000	22.7	0.5	No	2000	TIP4P/2005	80
	"----//----"	2014	573.15	480	32.3	0.7	No	2000	TIP4P/2005	80
	"----//----"	2014	623.15	200	51	2	No	2000	TIP4P/2005	80
	"----//----"	2014	623.15	480	43	1	No	2000	TIP4P/2005	80
	"----//----"	2014	623.15	1000	38	3	No	2000	TIP4P/2005	80
156	Espinosa et al.	2014	170		0.00035	N/A	No		TIP4P	191
	"----//----"	2014	180		0.00059	N/A	No		TIP4P	191
	"----//----"	2014	190		0.00237	N/A	No		TIP4P	191
	"----//----"	2014	200		0.01032	N/A	No		TIP4P	191
	"----//----"	2014	210		0.04893	N/A	No		TIP4P	191
	"----//----"	2014	220		0.15063	N/A	No		TIP4P	191
	"----//----"	2014	230		0.30088	N/A	No		TIP4P	191
	"----//----"	2014	191		0.00040	N/A	No		TIP4P/2005	80
	"----//----"	2014	199		0.00062	N/A	No		TIP4P/2005	80
	"----//----"	2014	207		0.00129	N/A	No		TIP4P/2005	80
	"----//----"	2014	216		0.00796	N/A	No		TIP4P/2005	80
	"----//----"	2014	225		0.03942	N/A	No		TIP4P/2005	80
	"----//----"	2014	234		0.11620	N/A	No		TIP4P/2005	80
	"----//----"	2014	243		0.27595	N/A	No		TIP4P/2005	80

	"----//----"	2014	252			0.39000	N/A	No		TIP4P/2005	80
	"----//----"	2014	202			0.00080	N/A	No		TIP4P/ICE	204
	"----//----"	2014	212			0.00119	N/A	No		TIP4P/ICE	204
	"----//----"	2014	232			0.01032	N/A	No		TIP4P/ICE	204
	"----//----"	2014	242			0.04298	N/A	No		TIP4P/ICE	204
	"----//----"	2014	252			0.08222	N/A	No		TIP4P/ICE	204
	"----//----"	2014	252			0.09775	N/A	No		TIP4P/ICE	204
	"----//----"	2014	258			0.17907	N/A	No		TIP4P/ICE	204
	"----//----"	2014	210			0.71448	N/A	No		mW	106
	"----//----"	2014	220			1.30893	N/A	No		mW	106
	"----//----"	2014	230			1.84995	N/A	No		mW	106
	"----//----"	2014	240			2.61458	N/A	No		mW	106
	"----//----"	2014	254			3.38910	N/A	No		mW	106
	"----//----"	2014	260			4.39304	N/A	No		mW	106
157	Shvab & Sadus	2014	277.70		0.998	1.63	N/A	No	500	SPC/E	13
	"----//----"	2014	296.91		0.998	2.45	N/A	No	500	SPC/E	13
	"----//----"	2014	323.82		0.998	4.02	N/A	No	500	SPC/E	13
	"----//----"	2014	343.04		0.998	5.28	N/A	No	500	SPC/E	13
	"----//----"	2014	379.96		0.998	8.06	N/A	No	500	SPC/E	13
	"----//----"	2014	399.95		0.998	9.38	N/A	No	500	SPC/E	13
	"----//----"	2014	420.71		0.998	10.77	N/A	No	500	SPC/E	13
	"----//----"	2014	450.69		0.998	12.34	N/A	No	500	SPC/E	13
	"----//----"	2014	500.65		0.998	14.99	N/A	No	500	SPC/E	13
	"----//----"	2014	550.61		0.998	17.26	N/A	No	500	SPC/E	13
	"----//----"	2014	600.58		0.998	20.09	N/A	No	500	SPC/E	13
	"----//----"	2014	649.79		0.998	23.31	N/A	No	500	SPC/E	13
158	Gallo et al.	2014	SC	SC	SC	see Fig. 1b	N/A	No	4096	TIP4P/2005	80
161	Park et al.	2015	550			29.67148	N/A	No	1024	SPC/E	13

	"----//----"	2015	499			21.56	N/A	No	1024	SPC/E	13
	"----//----"	2015	449			15.33	N/A	No	1024	SPC/E	13
	"----//----"	2015	399			10.20	N/A	No	1024	SPC/E	13
	"----//----"	2015	350			5.95	N/A	No	1024	SPC/E	13
	"----//----"	2015	300			2.80	N/A	No	1024	SPC/E	13
	"----//----"	2015	273		0.9980	1.53	N/A	No	1024	SPC/E	13
	"----//----"	2015	268		0.9993	1.33	N/A	No	1024	SPC/E	13
	"----//----"	2015	263		0.9981	1.13	N/A	No	1024	SPC/E	13
	"----//----"	2015	258		0.9963	0.94	N/A	No	1024	SPC/E	13
	"----//----"	2015	253		0.9935	0.79	N/A	No	1024	SPC/E	13
	"----//----"	2015	248		0.9896	0.65	N/A	No	1024	SPC/E	13
	"----//----"	2015	243		0.9839	0.50	N/A	No	1024	SPC/E	13
159	Tainter et al.	2015	673		0.0995	284.70	Yes (Fig. 13)	Yes	500	E3B3	159
	"----//----"	2015	673		0.1990	154.99	Yes (Fig. 13)	Yes	500	E3B3	159
	"----//----"	2015	673		0.2998	118.40	Yes (Fig. 13)	Yes	500	E3B3	159
	"----//----"	2015	673		0.4006	88.47	Yes (Fig. 13)	Yes	500	E3B3	159
	"----//----"	2015	673		0.5002	69.84	Yes (Fig. 13)	Yes	500	E3B3	159
	"----//----"	2015	673		0.5997	58.54	Yes (Fig. 13)	Yes	500	E3B3	159
	"----//----"	2015	673		0.7005	47.89	Yes (Fig. 13)	Yes	500	E3B3	159
	"----//----"	2015	673		0.0995	280.04	Yes (Fig. 13)	Yes	500	TIP4P/2005	80
	"----//----"	2015	673		0.1990	143.02	Yes (Fig. 13)	Yes	500	TIP4P/2005	80
	"----//----"	2015	673		0.2998	108.43	Yes (Fig. 13)	Yes	500	TIP4P/2005	80
	"----//----"	2015	673		0.4006	89.80	Yes (Fig. 13)	Yes	500	TIP4P/2005	80
	"----//----"	2015	673		0.5002	73.17	Yes (Fig. 13)	Yes	500	TIP4P/2005	80
	"----//----"	2015	673		0.5997	57.87	Yes (Fig. 13)	Yes	500	TIP4P/2005	80
	"----//----"	2015	673		0.7005	49.22	Yes (Fig. 13)	Yes	500	TIP4P/2005	80
160	Lobanova et al.	2015	432.9	VLE		8.65	N/A	No		Mie (8-6) CGW1-vle	160
	"----//----"	2015	412.9	VLE		7.29	N/A	No		Mie (8-6) CGW1-vle	160
	"----//----"	2015	392.9	VLE		6.02	N/A	No		Mie (8-6) CGW1-vle	160
	"----//----"	2015	362.9	VLE		4.56	N/A	No		Mie (8-6) CGW1-vle	160
	"----//----"	2015	343.0	VLE		3.50	N/A	No		Mie (8-6) CGW1-vle	160

	"----//----"	2015	432.9	VLE	14.19	N/A	No		Mie (8-6) CGW1-ift	160
	"----//----"	2015	392.9	VLE	13.91	N/A	No		Mie (8-6) CGW1-ift	160
	"----//----"	2015	372.8	VLE	12.11	N/A	No		Mie (8-6) CGW1-ift	160
	"----//----"	2015	343.0	VLE	11.34	N/A	No		Mie (8-6) CGW1-ift	160
	"----//----"	2015	313.0	VLE	8.82	N/A	No		Mie (8-6) CGW1-ift	160
	"----//----"	2015	298.0	VLE	7.53	N/A	No		Mie (8-6) CGW1-ift	160
	"----//----"	2015	293.0	VLE	7.38	N/A	No		Mie (8-6) CGW1-ift	160
162	Fuentes-Azcatl et al.	2015	240		0.10	N/A	No	500	SPC/ε	162
	"----//----"	2015	250		0.21	N/A	No	500	SPC/ε	162
	"----//----"	2015	260		0.38	N/A	No	500	SPC/ε	162
	"----//----"	2015	270		0.56	N/A	No	500	SPC/ε	162
	"----//----"	2015	280		0.82	N/A	No	500	SPC/ε	162
	"----//----"	2015	290		1.12	N/A	No	500	SPC/ε	162
	"----//----"	2015	300		1.62	N/A	No	500	SPC/ε	162
	"----//----"	2015	310		1.91	N/A	No	500	SPC/ε	162
	"----//----"	2015	320		2.31	N/A	No	500	SPC/ε	162
	"----//----"	2015	330		3.12	N/A	No	500	SPC/ε	162
	"----//----"	2015	340		3.68	N/A	No	500	SPC/ε	162
	"----//----"	2015	350		4.71	N/A	No	500	SPC/ε	162
	"----//----"	2015	240		0.28	N/A	No	500	SPC/ε1	162
	"----//----"	2015	250		0.44	N/A	No	500	SPC/ε1	162
	"----//----"	2015	260		0.70	N/A	No	500	SPC/ε1	162
	"----//----"	2015	270		1.03	N/A	No	500	SPC/ε1	162
	"----//----"	2015	280		1.25	N/A	No	500	SPC/ε1	162
	"----//----"	2015	290		1.60	N/A	No	500	SPC/ε1	162
	"----//----"	2015	300		2.01	N/A	No	500	SPC/ε1	162
	"----//----"	2015	310		2.56	N/A	No	500	SPC/ε1	162
	"----//----"	2015	320		2.95	N/A	No	500	SPC/ε1	162
	"----//----"	2015	330		3.74	N/A	No	500	SPC/ε1	162
	"----//----"	2015	340		4.24	N/A	No	500	SPC/ε1	162
	"----//----"	2015	350		5.09	N/A	No	500	SPC/ε1	162

	"----//----"	2015	240		0.21	N/A	No	500	TIP4P/ε	147
	"----//----"	2015	250		0.37	N/A	No	500	TIP4P/ε	147
	"----//----"	2015	260		0.65	N/A	No	500	TIP4P/ε	147
	"----//----"	2015	270		0.91	N/A	No	500	TIP4P/ε	147
	"----//----"	2015	280		1.18	N/A	No	500	TIP4P/ε	147
	"----//----"	2015	290		1.73	N/A	No	500	TIP4P/ε	147
	"----//----"	2015	300		2.12	N/A	No	500	TIP4P/ε	147
	"----//----"	2015	310		2.66	N/A	No	500	TIP4P/ε	147
	"----//----"	2015	320		3.36	N/A	No	500	TIP4P/ε	147
	"----//----"	2015	330		3.80	N/A	No	500	TIP4P/ε	147
	"----//----"	2015	340		4.36	N/A	No	500	TIP4P/ε	147
	"----//----"	2015	350		5.15	N/A	No	500	TIP4P/ε	147
	"----//----"	2015	240		0.20	N/A	No	500	SPC/E	13
	"----//----"	2015	250		0.36	N/A	No	500	SPC/E	13
	"----//----"	2015	260		0.88	N/A	No	500	SPC/E	13
	"----//----"	2015	270		1.18	N/A	No	500	SPC/E	13
	"----//----"	2015	280		1.57	N/A	No	500	SPC/E	13
	"----//----"	2015	290		2.03	N/A	No	500	SPC/E	13
	"----//----"	2015	300		2.44	N/A	No	500	SPC/E	13
	"----//----"	2015	310		3.22	N/A	No	500	SPC/E	13
	"----//----"	2015	320		3.87	N/A	No	500	SPC/E	13
	"----//----"	2015	330		4.33	N/A	No	500	SPC/E	13
163	Shvab & Sadus	2015	670	0.100	289.47	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670	0.152	200.00	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670	0.203	152.05	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670	0.247	125.15	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670	0.298	112.57	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670	0.322	101.75	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670	0.333	101.75	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670	0.346	98.25	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670	0.400	86.26	N/A	No	1728	TIP4P/2005f	117

	"----//----"	2015	670		0.450	76.61	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670		0.500	67.84	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670		0.550	59.94	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670		0.600	55.85	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670		0.700	45.61	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670		0.800	35.96	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670		0.900	28.65	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670		1.000	23.39	N/A	No	1728	TIP4P/2005f	117
	"----//----"	2015	670		0.100	274.27	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		0.152	183.04	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		0.203	144.44	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		0.247	118.13	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		0.298	104.68	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		0.322	100.58	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		0.333	97.95	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		0.346	95.32	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		0.400	81.87	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		0.450	74.56	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		0.500	65.50	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		0.550	61.70	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		0.600	53.22	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		0.700	45.32	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		0.800	37.13	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		0.900	29.53	N/A	No	1728	TIP4P/2005	80
	"----//----"	2015	670		1.000	23.10	N/A	No	1728	TIP4P/2005	80
164	Corradini et al.	2015	SC	SC	SC	see Fig. 6	N/A	No	4096	TIP4P/2005	80
	"----//----"	2015	SC	SC	SC	see Fig. 6	N/A	No	4096	TIP4P	191
	"----//----"	2015	SC	SC	SC	see Fig. 6	N/A	No	4096	SPC/E	13
	"----//----"	2015	SC	SC	SC	see Fig. 6	N/A	No	4096	TIP5P	183
	"----//----"	2015	SC	SC	SC	see Fig. 6	N/A	No	4096	TIP3P	6

165	Tran et al.	2016	238	1.01325	0.09	Yes (Fig. 5)	Yes	512	SSMP	165
	"----//----"	2016	258	1.01325	0.53	Yes (Fig. 5)	Yes	512	SSMP	165
	"----//----"	2016	268	1.01325	0.85	Yes (Fig. 5)	Yes	512	SSMP	165
	"----//----"	2016	278	1.01325	1.22	Yes (Fig. 5)	Yes	512	SSMP	165
	"----//----"	2016	298	1.01325	2.24	Yes (Fig. 5)	Yes	512	SSMP	165
	"----//----"	2016	318	1.01325	3.49	Yes (Fig. 5)	Yes	512	SSMP	165
	"----//----"	2016	338	1.01325	4.95	Yes (Fig. 5)	Yes	512	SSMP	165
	"----//----"	2016	298	1.01325	2.60	Yes (Fig. 9)	Yes	512	TIP4P-Ew	75
	"----//----"	2016	298	506.625	2.66	Yes (Fig. 9)	Yes	512	TIP4P-Ew	75
	"----//----"	2016	298	1013.25	2.70	Yes (Fig. 9)	Yes	512	TIP4P-Ew	75
	"----//----"	2016	298	5066.25	2.57	Yes (Fig. 9)	Yes	512	TIP4P-Ew	75
	"----//----"	2016	298	10132.5	2.09	Yes (Fig. 9)	Yes	512	TIP4P-Ew	75
	"----//----"	2016	298	1.01325	2.24	Yes (Fig. 9)	Yes	512	SSMP	165
	"----//----"	2016	298	506.625	2.24	Yes (Fig. 9)	Yes	512	SSMP	165
	"----//----"	2016	298	1013.25	2.27	Yes (Fig. 9)	Yes	512	SSMP	165
	"----//----"	2016	298	5066.25	1.83	Yes (Fig. 9)	Yes	512	SSMP	165
	"----//----"	2016	298	10132.5	1.26	Yes (Fig. 9)	Yes	512	SSMP	165
167	Franco et al.	2016	288	1	2.05	Yes (Fig. 1)	No	1000	SPC/E	13
	"----//----"	2016	298	1	2.44	Yes (Fig. 1)	No	1000	SPC/E	13
	"----//----"	2016	308	1	3.02	Yes (Fig. 1)	No	1000	SPC/E	13
	"----//----"	2016	318	1	3.54	Yes (Fig. 1)	No	1000	SPC/E	13
	"----//----"	2016	329	1	4.26	Yes (Fig. 1)	No	1000	SPC/E	13
	"----//----"	2016	288	1	2.03	Yes (Fig. 1)	No	1000	SPC/E	13
	"----//----"	2016	298	1	2.49	Yes (Fig. 1)	No	1000	SPC/E	13
	"----//----"	2016	308	1	3.05	Yes (Fig. 1)	No	1000	SPC/E	13
	"----//----"	2016	318	1	3.65	Yes (Fig. 1)	No	1000	SPC/E	13
	"----//----"	2016	329	1	4.37	Yes (Fig. 1)	No	1000	SPC/E	13
166	Jiang et al.	2016	298.15	1	2.42	0.01	Yes	512	HBP	166

	"----//----"	2016	298.15	200	2.45	0.04	Yes	512	HBP	166
	"----//----"	2016	298.15	480	2.47	0.02	Yes	512	HBP	166
	"----//----"	2016	298.15	1000	2.55	0.04	Yes	512	HBP	166
	"----//----"	2016	373.15	15	7.74	0.01	Yes	512	HBP	166
	"----//----"	2016	373.15	200	7.32	0.04	Yes	512	HBP	166
	"----//----"	2016	373.15	480	7.52	0.02	Yes	512	HBP	166
	"----//----"	2016	373.15	1000	7.17	0.04	Yes	512	HBP	166
	"----//----"	2016	523.15	200	25.1	0.6	Yes	512	HBP	166
	"----//----"	2016	523.15	480	25.3	0.3	Yes	512	HBP	166
	"----//----"	2016	523.15	1000	24.2	0.6	Yes	512	HBP	166
	"----//----"	2016	298.15	1	2.04	0.05	Yes	512	BK3	136
	"----//----"	2016	298.15	200	1.91	0.06	Yes	512	BK3	136
	"----//----"	2016	298.15	480	1.93	0.05	Yes	512	BK3	136
	"----//----"	2016	298.15	1000	1.9	0.1	Yes	512	BK3	136
	"----//----"	2016	373.15	15	7.2	0.1	Yes	512	BK3	136
	"----//----"	2016	373.15	200	7.1	0.1	Yes	512	BK3	136
	"----//----"	2016	373.15	480	6.9	0.2	Yes	512	BK3	136
	"----//----"	2016	373.15	1000	6.8	0.2	Yes	512	BK3	136
	"----//----"	2016	523.15	200	28	2	Yes	512	BK3	136
	"----//----"	2016	523.15	480	24.8	0.08	Yes	512	BK3	136
	"----//----"	2016	523.15	1000	22.8	0.04	Yes	512	BK3	136
	"----//----"	2016	298.15	1	2.1	0.1	Yes	512	TIP4P/2005	80
	"----//----"	2016	373.15	15	7.5	0.1	Yes	512	TIP4P/2005	80
	"----//----"	2016	373.15	200	7.4	0.2	Yes	512	TIP4P/2005	80
	"----//----"	2016	373.15	480	7.4	0.2	Yes	512	TIP4P/2005	80
	"----//----"	2016	523.15	200	25.9	0.9	Yes	512	TIP4P/2005	80
	"----//----"	2016	523.15	480	24.9	0.8	Yes	512	TIP4P/2005	80
	"----//----"	2016	523.15	1000	22.7	0.5	Yes	512	TIP4P/2005	80
168	Ding et al.	2016	268	1.01325	1.38	No	No		ELBA	121

	"----//----"	2016	278	1.01325	1.65	No	No		ELBA	121
	"----//----"	2016	288	1.01325	1.89	No	No		ELBA	121
	"----//----"	2016	298	1.01325	2.21	No	No		ELBA	121
	"----//----"	2016	308	1.01325	2.50	No	No		ELBA	121
	"----//----"	2016	318	1.01325	2.77	No	No		ELBA	121
	"----//----"	2016	328	1.01325	3.13	No	No		ELBA	121
	"----//----"	2016	338	1.01325	3.47	No	No		ELBA	121
	"----//----"	2016	348	1.01325	3.81	No	No		ELBA	121
	"----//----"	2016	358	1.01325	4.32	No	No		ELBA	121
	"----//----"	2016	368	1.01325	4.66	No	No		ELBA	121
	"----//----"	2016	378	1.01325	5.17	No	No		ELBA	121
169	Koster et al.	2016	280	1	1.36	No	No	3000	TIP4P/2005	80
	"----//----"	2016	300	1	2.33	No	No	3000	TIP4P/2005	80
	"----//----"	2016	320	1	3.46	No	No	3000	TIP4P/2005	80
	"----//----"	2016	340	1	4.85	No	No	3000	TIP4P/2005	80
	"----//----"	2016	280	1	2.28	No	No	3000	TIP4P-TPSS	151
	"----//----"	2016	300	1	3.70	No	No	3000	TIP4P-TPSS	151
	"----//----"	2016	320	1	5.47	No	No	3000	TIP4P-TPSS	151
	"----//----"	2016	340	1	7.54	No	No	3000	TIP4P-TPSS	151
	"----//----"	2016	280	1	2.92	No	No	3000	TIP4P-TPSS-D3	151
	"----//----"	2016	300	1	4.37	No	No	3000	TIP4P-TPSS-D3	151
	"----//----"	2016	320	1	6.11	No	No	3000	TIP4P-TPSS-D3	151
	"----//----"	2016	340	1	8.11	No	No	3000	TIP4P-TPSS-D3	151
	"----//----"	2016	280	1	2.97	No	No	3000	Huang et al.	205
	"----//----"	2016	300	1	4.00	No	No	3000	Huang et al.	205
	"----//----"	2016	320	1	5.19	No	No	3000	Huang et al.	205
	"----//----"	2016	340	1	6.48	No	No	3000	Huang et al.	205

170	Dhabal et al.	2016	see Fig. 4a		see Fig. 4a	see Fig. 4a	N/A	No	4096	mW	106
171	Guillaud et al.	2017	228	1.01325		0.065	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	231	1.01325		0.077	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	234	1.01325		0.083	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	237	1.01325		0.13	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	240	1.01325		0.181	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	243	1.01325		0.211	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	246	1.01325		0.277	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	249	1.01325		0.327	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	252	1.01325		0.454	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	255	1.01325		0.443	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	258	1.01325		0.536	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	261	1.01325		0.644	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	264	1.01325		0.715	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	267	1.01325		0.836	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	270	1.01325		0.896	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	273	1.01325		1.094	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	276	1.01325		1.215	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	279	1.01325		1.384	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	282	1.01325		1.471	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	285	1.01325		1.55	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	288	1.01325		1.706	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	291	1.01325		1.927	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	294	1.01325		2.103	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	297	1.01325		2.216	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	300	1.01325		2.481	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	303	1.01325		2.683	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	306	1.01325		2.979	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	309	1.01325		2.903	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	312	1.01325		3.032	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	315	1.01325		3.485	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117

	"----//----"	2017	318	1.01325	3.704	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	321	1.01325	3.803	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	324	1.01325	4.149	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	327	1.01325	4.487	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	330	1.01325	4.566	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	333	1.01325	4.812	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	336	1.01325	5.026	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	339	1.01325	5.205	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	342	1.01325	5.629	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	345	1.01325	5.83	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	348	1.01325	6.25	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	351	1.01325	6.251	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	354	1.01325	6.474	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	357	1.01325	7.063	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
	"----//----"	2017	360	1.01325	7.378	Yes (Fig. 4)	Yes	512 - 10648	TIP4P/2005f	117
173	Gabrieli et al.	2018	251.154734	1	0.5029	N/A	No	343	OPC	150
	"----//----"	2018	258.62069	1	0.7076	N/A	No	343	OPC	150
	"----//----"	2018	270.354257	1	1.0295	N/A	No	343	OPC	150
	"----//----"	2018	278.31094	1	1.2841	N/A	No	343	OPC	150
	"----//----"	2018	289.421158	1	1.7357	N/A	No	343	OPC	150
	"----//----"	2018	299.793246	1	2.1941	N/A	No	343	OPC	150
	"----//----"	2018	310.714286	1	2.7003	N/A	No	343	OPC	150
	"----//----"	2018	319.38326	1	3.1289	N/A	No	343	OPC	150
	"----//----"	2018	329.295988	1	3.6991	N/A	No	343	OPC	150
	"----//----"	2018	340.109461	1	4.4026	N/A	No	343	OPC	150
	"----//----"	2018	220.073598	1	0.0289	N/A	No	343	TIP4P-Ew	75
	"----//----"	2018	230.08449	1	0.0886	N/A	No	343	TIP4P-Ew	75
	"----//----"	2018	233.895706	1	0.1394	N/A	No	343	TIP4P-Ew	75
	"----//----"	2018	254.060808	1	0.4568	N/A	No	343	TIP4P-Ew	75
	"----//----"	2018	261.914985	1	0.7383	N/A	No	343	TIP4P-Ew	75

	"----//----"	2018	272.662256	1		1.1014	N/A	No	343	TIP4P-Ew	75
	"----//----"	2018	281.963576	1		1.4380	N/A	No	343	TIP4P-Ew	75
	"----//----"	2018	293.947571	1		2.0612	N/A	No	343	TIP4P-Ew	75
	"----//----"	2018	307.832055	1		2.7638	N/A	No	343	TIP4P-Ew	75
	"----//----"	2018	311.510571	1		2.8766	N/A	No	343	TIP4P-Ew	75
	"----//----"	2018	318.537859	1		3.5606	N/A	No	343	TIP4P-Ew	75
	"----//----"	2018	324.952056	1		3.6568	N/A	No	343	TIP4P-Ew	75
	"----//----"	2018	338.249972	1		4.7744	N/A	No	343	TIP4P-Ew	75
	"----//----"	2018	347.261756	1		5.5286	N/A	No	343	TIP4P-Ew	75
174	Handle & Sciortino	2018	270		0.90	5.87E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	270		0.94	7.51E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	270		0.98	8.60E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	270		1.02	9.85E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	270		1.06	1.13E-01	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	270		1.10	1.13E-01	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	270		1.14	1.16E-01	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	270		1.18	1.04E-01	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	270		1.22	9.29E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	270		1.26	7.79E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	270		1.30	6.53E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	270		1.34	4.79E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	270		1.38	3.43E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	270		1.42	1.97E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	250		0.90	1.18E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	250		0.94	2.21E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	250		0.98	3.23E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	250		1.02	4.62E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	250		1.06	5.29E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	250		1.10	5.66E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	250		1.14	5.93E-02	N/A	No	1000	TIP4P/2005	80
	"----//----"	2018	250		1.18	5.55E-02	N/A	No	1000	TIP4P/2005	80

"----//----"	2018	250	1.22	5.09E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	250	1.26	4.27E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	250	1.30	3.13E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	250	1.34	2.24E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	250	1.38	1.23E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	250	1.42	6.46E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	240	0.90	4.33E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	240	0.94	9.67E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	240	0.98	1.73E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	240	1.02	2.83E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	240	1.06	3.54E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	240	1.10	3.79E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	240	1.14	3.71E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	240	1.18	3.72E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	240	1.22	3.26E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	240	1.26	2.56E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	240	1.30	1.87E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	240	1.34	1.29E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	240	1.38	6.75E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	240	1.42	2.59E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	230	0.90	1.09E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	230	0.94	3.63E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	230	0.98	8.86E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	230	1.02	1.48E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	230	1.06	2.07E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	230	1.10	2.43E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	230	1.14	2.43E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	230	1.18	2.28E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	230	1.22	2.13E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	230	1.26	1.53E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	230	1.30	1.10E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	230	1.34	6.44E-03	N/A	No	1000	TIP4P/2005	80

"----//----"	2018	230	1.38	2.71E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	220	0.90	1.79E-04	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	220	0.94	1.11E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	220	0.98	3.18E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	220	1.02	7.43E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	220	1.06	1.11E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	220	1.10	1.27E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	220	1.14	1.27E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	220	1.18	1.28E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	220	1.22	1.12E-02	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	220	1.26	8.20E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	220	1.30	4.81E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	220	1.34	2.42E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	220	1.38	8.88E-04	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	210	0.94	2.92E-04	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	210	0.98	1.17E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	210	1.02	3.05E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	210	1.06	4.98E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	210	1.10	6.38E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	210	1.14	6.68E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	210	1.18	6.69E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	210	1.22	4.59E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	210	1.26	3.44E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	210	1.30	1.77E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	210	1.34	5.19E-04	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	200	0.98	2.86E-04	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	200	1.02	1.17E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	200	1.06	1.91E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	200	1.10	2.50E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	200	1.14	2.45E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	200	1.18	2.30E-03	N/A	No	1000	TIP4P/2005	80

"----//----"	2018	200		1.22	1.80E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	200		1.26	1.06E-03	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	200		1.30	4.85E-04	N/A	No	1000	TIP4P/2005	80
"----//----"	2018	200		1.34	7.31E-05	N/A	No	1000	TIP4P/2005	80

TABLE SI-3. Studies in which the self-diffusion coefficient of water confined by various materials has been calculated using MD simulations. ***D_{par}*** stands for the parallel component of the self-diffusion coefficient, ***D_{perp}*** stands for the perpendicular component of the self-diffusion coefficient, ***D_{eff}*** stands for the effective self-diffusion coefficient, ***D_{bulk}*** stands for the bulk self-diffusion coefficient, and ***η*** stands for viscosity.

	References	Year	Journal	vol.	First page	T / K	D_{par}	D_{perp}	D_{eff}	D_{bulk}	η	Confining material	H_2O force field	Method
1	Bellissent-Funel et al.	1995	*Phys. Rev. E*	51	4558	238-298	-	-	Yes	No	No	vycor glass	Lee & Rossky, 1994	EISF
2	Smirnov & Bougeard	1999	*J. Phys. Chem. B*	103	5266	300	-	-	Yes	Yes	No	kaolinite (clay)	SPC (Toukan & Rahman, 1985)	Green-Kubo
3	Spohr et al.	1999	*J. Mol. Liquids*	80	165	298	Yes	No	No	Yes	No	silica	SPC/E	Einstein
4	Ricci et al.	2000	*J. Phys. Condens. Matter*	12	A345	298	Yes	No	No	No	No	vycor glass	SPC/E	MSD
5	Martí & Gordillo	2002	*Chem. Phys. Lett.*	354	227	573, 673, 773	No	No	Yes	Yes	No	carbon nanotubes	Flex. SPC (Martí et al., 2004)	VACF
6	Beckstein & Samsom	2003	*Proc. Nac. Acad. Sci.*	100	7063	300	Yes	Yes	No	Yes	No	L-J	SPC	Einstein
7	Brovchenko et al.	2003	*Eur. Phys. J. E*	12	69	300 – 533	Yes	Yes	Yes	Yes	No	hydrophobic & hydrophilic cylinders	TIP4P	MSD
8	Marañón Di Leo & Marañón	2003	*J. Mol. Structure (Theochem)*	623	159	300	Yes	Yes	No	Yes	No	hydrophobic & hydrophilic nanotubes	SPC/E	MSD
9	Mashl et al.	2003	*Nano Lett.*	3	589	300	Yes	No	No	Yes	No	carbon nanotubes	SPC/E	MSD
10	Liu et al.	2004	*J. Phys. Chem. B*	108	6595	-	Yes	Yes	No	Yes	No	-	-	Liu et al. (2004)
11	Patsahan & Holovko	2004	*Condens. Matter Phys.*	7	3	300, 350	-	-	Yes	-	No	silica gel	SPC/E	Einstein
12	Zangi	2004	*J. Phys. Condens. Matter*	16	55388	300	Yes	No	No	Yes	No	quartz	TIP5P	Zangi, 2003
13	Jensen et al.	2004	*J. Chem. Phys.*	120	9729	300	Yes	No	No	Yes	No	hydrophobic & hydrophilic crystalline structures	TIP3	MSD
14	Choudhury & Pettitt	2005	*J. Phys. Chem. B*	109	6422	298	-	-	Yes	Yes	No	graphite	SPC/E	Green-Kubo/Einstein
15	Liu & Wang	2005	*Phys. Rev. B*	72	85420	298	Yes	Yes	No	Yes	Yes	single-walled carbon nanotube	SPC	Einstein
16	Sega et al.	2005	*Phys. Rev. E*	72	41201	333	Yes	Yes	-	-	No	GME ganglioside bilayers	SPC	Sega et al., 2005
17	Ju et al.	2005	*J. Chem. Phys.*	122	154707	400	Yes	Yes	No	No	No	Au plates	F3C	Green-Kubo
18	Cui	2005	*J. Chem. Phys.*	123	54706	298.15	Yes	Yes	No	Yes	No	cylindrical pores	TIP3P	Einstein
19	Kośmider et al.	2005	*Mat. Sci.-Poland*	23	475	233, 309, 344	No	No	Yes	Yes	No	single-walled carbon nanotube	flexible SPC	Green-Kubo
20	Kumar et al.	2005	*Phys. Rev. E*	72	51503	220-300	Yes	No	No	Yes	No	hydrophobic plates (paraffin)	TIP5P	Einstein
21	Martí et al.	2006	*J. Phys. Chem. B*	110	23987	298	Yes	Yes	-	Yes	No	highly oriented pyrolitc graphite	SPC	Green-Kubo/Einstein
22	Striolo	2006	*Nano Lett.*	6	633	298	Yes	-	-	No	No	carbon nanotubes	SPC/E	-

23	Shirono & Daiguji	2006	*Chem. Phys. Lett.*	417	251	300	No	No	Yes	No	No	Na-LSX zeolites	SPC-FQ	MSD
24	Leng & Cummings	2006	*J. Chem. Phys.*	124	74711	298	No	No	Yes	Yes	No	mica	TIP4P	-
25	Hua et al.	2006	*J. Phys. Chem. B*	110	3704	-	No	Yes	No	Yes	No	BphC enzyme	SPC	Einstein
26	Hirunsit & Balbuena	2007	*J. Phys. Chem. C*	111	1709	298	-	-	Yes	-	No	graphite	SPC/E	Einstein
27	Prědota et al.	2007	*J. Phys. Chem. C*	111	3071	298, 448, 523	Yes	Yes	-	Yes	Yes	Rutile (a-TiO2)	SPC/E	Prědota et al. (2004)
28	Striolo	2007	*Nanotechnol.*	18	475704	300	Yes	-	-	No	No	carbon nanotubes	SPC/E	-
29	Porion et al.	2007	*J. Phys. Chem. C*	111	5441	298	No	No	Yes	No	No	natural clay (montmorillonite)	SPC	Einstein
30	Michot et al.	2007	*J. Phys. Chem. C*	111	9819	298	No	No	Yes	Yes	No	Na saponite clay	SPC	MSD
31	Gordillo & Martí	2007	*Phys. Rev. B*	75	85406	323-398	Yes	Yes	Yes	Yes	No	graphite	flexible SPC	VACF
32	Li et al.	2007	*Phys. Rev. B*	75	115415	300	No	No	Yes	Yes	Yes	mica, glass and graphite	SPC/E	-
33	Lane et al.	2008	*Langmuir*	24	5209	300	-	-	Yes	Yes	No	SAM layers of alkanethiol on Au	SPC/E	Einstein
34	Thomas & McGaughey	2008	*Nano Lett.*	8	2788	298	No	No	No	Yes	Yes	carbon nanotubes	TIP5P	Green-Kubo
35	Stanley et al.	2008	*AIP Conference Proceedings*	982	251	200-300	No	No	Yes	No	No	Protein and DNA	ST2, Jagla, TIP5P	MSD
36	Won & Aluru	2008	*J. Phys. Chem. C*	112	1812	300	Yes	No	No	Yes	No	boron nitride nanotube	SPC/E	Einstein
37	Kerisit & Liu	2009	*Environ. Sci. Technol.*	43	777	300	Yes	Yes	-	Yes	No	Feldspar	SPC/E	Einstein
38	Sendner et al.	2009	*Langmuir*	25	10768	300	No	Yes	-	Yes	Yes	diamond	SPC/E	Time correlation function
39	Zhang et al.	2009	*Mol. Sim.*	5	1215	298.15	-	-	Yes	Yes	No	amorphous silica	SPC/E	Einstein
40	Kumar et al.	2009	*J. Phys. Condens. Matter*	21	504108	220-300	Yes	Yes	No	Yes	No	solid paraffin	TIP5P	MSD
41	Di Napoli & Gamba	2009	*Physica B*	404	2883	300	Yes	No	No	Yes	No	Newton black films	TIP5P	MSD
42	Martí et al.	2009	*Phys. Rev. E*	79	31606	673	No	No	Yes	Yes	No	graphene	flexible SPC	VACF
43	Bonnaud et al.	2010	*J. Phys. Condens. Matter*	22	284110	300	Yes	Yes	No	Yes	No	hydroxylated silica	SPC	Einstein
44	Martí et al.	2010	*J. Mol. Liquids*	153	72	298-673	-	-	Yes	Yes	No	graphene	SPC	Green-Kubo
45	Park & Aluru	2010	*J. Phys. Chem. C*	114	2595	300	Yes	No	-	Yes	No	graphene	SPC/E	Einstein
46	Han et al.	2010	*Nature Phys.*	6	685	240, 250, 270, 300	Yes	No	No	No	No	hydrophobic plates	TIP5P	MSD
47	Farimani & Aluru	2011	*J. Phys. Chem. B*	115	12145	300	Yes	Yes	-	Yes	No	carbon nanotubes	SPC/E	Einstein
48	Lerbret et al.	2011	*Food Biophys.*	6	233	300	-	Yes	Yes	Yes	No	silica (cylindrical pores)	SPC/E	Einstein
49	Wei et al.	2011	*Fluid Phase Equilib.*	302	316	300	Yes	No	No	Yes	No	rutile (TiO2) and graphite	SPC/E	-
50	Boțan et al.	2011	*J. Phys. Chem. C*	115	16109	300	Yes	Yes	No	Yes	Yes	clay (montmorillonite)	SPC/E	Liu et al. (2004)
51	Nguyen & Bhatia	2012	*J. Phys. Chem. C*	116	3667	298	-	-	Yes	Yes	No	disordered carbons	SPC/E	-

52	Zheng et al.	2012	*Phys. Chem. Chem. Phys.*	14	964	298, 325, 350	Yes	-	-	Yes	No	carbon nanotubes	TIP4P-EW	Einstein
53	Mosaddeghi et al.	2012	*J. Chem. Phys.*	137	184703	300	Yes	Yes	Yes	Yes	No	graphite plates	SPC/E	Green-Kubo/Einstein
54	Michot et al.	2012	*J. Phys. Chem. C*	116	16619	300	Yes	Yes	No	Yes	No	clay (synthetic saponite)	SPC/E	MSD/VACF
55	Bai & Zeng	2012	*PNAS*	109	21240	250	No	No	Yes	Yes	No	hydrophobic nanopore	TIP5P	-
56	Bauer et al.	2012	*Phys. Rev. E*	85	51506	300	Yes	Yes	Yes	Yes	No	hydrophobic plates	TIP3P, TIP4P, SPC/E, SWM4-NDP, TIP4P-FQ	Green-Kubo
57	Dickey & Stevens	2012	*Phys. Rev. E*	86	51601	300	Yes	No	No	Yes	No	SiO2	TIP4P/2005	Einstein
58	Choudhury	2013	*Chem. Phys.*	421	68	298	Yes	No	No	Yes	No	paraffin	SPC/E	Einstein
59	Sanghi & Aluru	2013	*J. Chem. Phys.*	138	124109	300	No	No	Yes	Yes	No	graphite	SPC/E	MSD
60	Solveyra et al.	2013	*J. Phys. Chem. C*	117	3330	300	Yes	No	Yes	Yes	No	TiO2	SPC/E	MSD (Lounnas et al. 1994)
61	Rao et al.	2013	*J. Phys. Chem. C*	117	14061	460	Yes	No	No	Yes	No	clay	SPC	MSD
62	Siboulet et al.	2013	*Mol. Phys.*	111	22	300	Yes	Yes	No	Yes	No	amorphous silica	SPC/E	Smoluchowski
63	Xu et al.	2013	*Nanotechnol.*	24	505504	300, 400, 600	Yes	No	No	Yes	No	graphene	SPC/F	MSD
64	Kim et al.	2013	*Scientific Reports*	3	2309	300	No	No	Yes	Yes	No	graphene and mica	SPC/E	Einstein
65	Silva	2014	*J. Nanostruct. Chem.*	4	104	300	Yes	-	-	Yes	No	carbon nanotubes	SPC/E	Einstein
66	Qomi et al.	2014	*J. Chem. Phys.*	140	54515	300	Yes	No	No	Yes	No	Calcium-silicate	SPC/E	Einstein
67	Ding et al.	2014	*J. Membr. Sci.*	458	236	300	No	No	Yes	Yes	No	polyamide RO membrane	TIP4P/2005	MSD
68	Ou et al.	2014	*J. Phys. Chem. C*	118	29887	300	Yes	Yes	Yes	Yes	No	Mg(OH)2	flexible SPC	Einstein
69	Boek	2014	*Mol. Phys.*	112	1472	298	No	No	Yes	Yes	No	clay (montmorillonite)	TIP4P	Einstein
70	Renou et al.	2014	*Mol. Phys.*	112	2275	300	Yes	No	Yes	Yes	No	silica (cylindrical pores)	TIP4P/2005	Einstein
71	Pham et al.	2015	*Theor. Chem. Acc.*	134	59	293-323	-	-	Yes	Yes	Yes	hydroxyapatite	Polarizable core-shell	Einstein
72	Yang et al.	2015	*Chin. J. Chem. Eng.*	23	1587	298.15	Yes	No	No	Yes	No	graphene	SPC/E	MSD
73	Kolokathis et al.	2015	*J. Phys. Chem. C*	119	20074	300	No	No	Yes	Yes	No	iron carboxylate sorbent	SPC/E	Einstein
74	Hou et al.	2015	*Microfluid Nanofluid*	19	1309	300	No	No	Yes	Yes	No	Calcium-silicate	-	Einstein
75	Chiavazzo et al.	2015	*Nature Comm.*	5	3565	300	No	No	Yes	Yes	No	protein, CNT, Fe3O4 & SiO2	SPC/E	Einstein
76	Hou et al.	2015	*Phys. Chem. Chem. Phys.*	17	1411	300	Yes	Yes	Yes	Yes	No	Calcium-silicate	ReaxFF	MSD
77	Diallo et al.	2015	*Phys. Rev. E*	91	22124	220-280	No	No	Yes	Yes	No	activated carbon fibers nanopores	SPC/E	EISF
78	Tahat & Martí	2015	*Phys. Rev. E*	92	32402	298	No	No		Yes	Yes	graphene	TIP3P	MSD
79	Hanot et al.	2016	*Nanoscale*	8	3314	300	-	-	Yes	No	No	ionic surfactant	SPC/E	Einstein
80	Ishikawa et al.	2016	*J. Mineral. Petrol. Sci.*	111	297	298-573	Yes	No	-	Yes	No	quartz	Kawamura, 2008	Green-Kubo

81	Muscatello et al.	2016	*ACS Appl. Mater. Interfaces*	8	12330	300	Yes	No	No	No	No	graphene membranes	SPC/E	Green-Kubo
82	Shahbabei & Kim	2016	*Coll. & Surf. A*	507	190	300	Yes	No	No	No	No	aquaporin-like pores	SPC/E	MSD
83	Chen et al.	2016	*J. Phys. Chem. C*	120	12924	300	Yes	No	No	No	No	layered double hydroxides	SPC	Einstein/jump model
84	Futera & English	2016	*J. Phys. Chem. C*	120	19603	300	Yes	No	No	Yes	No	TiO2	flexible SPC	Green-Kubo/Einstein
85	Yamashita & Daiguji	2016	*Mol. Phys.*	114	884	350	No	No	Yes	Yes	No	hydrophilic nanopores	ELBA	MSD
86	Zhou et al.	2016	*Amer. Mineralog.*	101	713	298	No	No	Yes	Yes	No	sepiolite (clay mineral)	ClayFF	MSD
87	Nie et al.	2016	*Front. Phys.*	11	114702	300	Yes	No	No	Yes	No	carbon nanochannels	SPC/E	-
88	Cao et al.	2016	*J. Chem. Eng. Data*	61	4131	300	Yes	No	No	Yes	No	TiO2 nanotubes & carbon nanotubes	SPC/E	-
89	Hou et al.	2016	*Langmuir*	32	4153	300 – 1500	No	No	Yes	Yes	No	Calcium-silicate	SPC/E	MSD
90	Köhler & Silva	2016	*Chem. Phys. Lett.*	645	38	300	Yes	No	No	Yes	Yes	carbon nanotubes	TIP4P/2005	MSD
91	McDonnell et al.	2016	*J. Phys. Chem. B*	120	8997	300	Yes	No	No	No	No	chitin/chitosan	TIP4P	MSD
92	Mozaffari	2016	*Mol. Sim.*	42	1475	285 – 390	Yes	No	No	Yes	No	graphene	SPC/E	Einstein
93	Ishikawa et al.	2017	*Proc. Earth and Plan. Sci.*	17	853	298-573	Yes	No	-	Yes	No	quartz	Kawamura, 2008	Green-Kubo
94	Prakash et al.	2017	*Appl. Surf. Sci.*	418	296	310	-	-	Yes	Yes	No	hydroxyapatite	CS and SPC/E	Einstein
95	Prakash et al.	2017	*Phys. Chem. Miner.*	44	509	310	Yes	Yes	-	Yes	No	hydroxyapatite	SPC/E	Green-Kubo
96	Zubeltzu & Artacho	2017	*J. Chem. Phys.*	147	194509	-	Yes	No	No	No	No	L-J parallel walls	TIP4P/2005	Einstein
97	Han et al.	2017	*J. Phys. Chem. C*	121	381	300	Yes	Yes	Yes	No	No	zeolites	TIP4P/Ew	Einstein
98	Mutisya et al.	2017	*J. Phys. Chem. C*	121	6674	300	Yes	No	Yes	Yes	No	calcite slit pore	SPC/Fw (Raiteri et al. 2010)	Liu et al. (2004)
99	Chen et al.	2017	*J. Phys. Chem. C*	121	23752	300-425	Yes	No	No	No	No	layered double hydroxides	SPC	Einstein/jump model
100	Köhler et al.	2017	*Phys. Chem. Chem. Phys.*	19	12921	300	Yes	No	No	No	Yes	hydrophobic & hydrophilic nanotubes	TIP4P/2005	Einstein
101	Li et al.	2017	*Construction & Building materials*	151	563	300	No	No	Yes	Yes	No	Calcium-silicate	ClayFF	MSD
102	Martí et al.	2017	*Entropy*	19	135	298	Yes	Yes	Yes	Yes	No	carbon nanotube & graphene	Martí & Gordillo, 2001	MSD
103	Sahu & Ali	2017	*J. Chem. Eng. Data*	62	2307	298-573	Yes	No	No	No	No	carbon nanotubes	SPC	MSD
104	Gavazzoni et al.	2017	*J. Chem. Phys.*	146	234509	173, 235, 293	Yes	No	No	Yes	No	AlPO4-54 nanotubes	TIP4P/2005	Einstein
105	Jeddi & Castrillón	2017	*J. Phys. Chem. B*	121	9666	301	Yes	No	No	Yes	No	silica	SPC/E	MSD
106	Bucior et al.	2017	*Langmuir*	33	11834	298	No	No	Yes	Yes	No	carbon nanotubes	TIP3P	Einstein
107	Jiao et al.	2017	*Scientific Reports*	7	2646	300	Yes	No	No	Yes	No	graphene	TIP4P/Ew, SPC/E	Einstein
108	Berrod et al.	2017	*Scientific Reports*	7	8326	-	No	No	Yes	No	No	ionomers and surfactant	Savage & Voth, 2014	MSD
109	Abbaspour et al.	2018	*J. Mol. Liquids*	250	26	300	-	-	Yes	No	No	graphene, graphite, boron nitride, silicon carbide	SPC/E	Einstein

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