

Role of nonadditive forces on the structure and properties of liquid water

Jianhui Li, Zhongwu Zhou, and Richard J. Sadus^{a)}

Centre for Molecular Simulation, Swinburne University of Technology, P.O. Box 218, Hawthorn, Victoria 3122, Australia

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The role of nonadditive interactions on the structure and dielectric properties of water is investigated at different temperatures using molecular dynamics. A new intermolecular potential is developed which contains an *ab initio* description of two-body additive interactions plus nonadditive contributions from both three-body interactions and polarization. Polarization is the main nonadditive influence, resulting in improved agreement with experiment for the radial distribution function, dielectric constant, and dipole moment. A comparison is also made with other widely used intermolecular potentials. The new potential provides a superior prediction of the dielectric constant and dipole moment. It also predicts the relative contribution of hydrogen bonding better than the SPC/E potential [Berendsen *et al.*, *J. Phys. Chem.* **91**, 6269 (1987)]. © 2007 American Institute of Physics. [DOI: 10.1063/1.2786449]

I. INTRODUCTION

The key role played by water in many important biological, chemical, and physical processes^{1–3} has motivated many theoretical and modeling studies. The engineering approach of developing equations of state⁴ has been of limited success for water. Accurate reference equations⁵ for pure water have been developed, which cannot be easily extended to mixtures. In contrast, theoretical equations of state can often qualitatively predict^{6,7} the properties of aqueous mixtures up to very high pressures but they are not reliable for accurate predictions. A molecular-based approach has been used to formulate improved equations of state for water.^{8,9} Despite such theoretical improvements, many approximations are required to transform the molecular model to an equation of state. This means that it is unrealistic to expect an equation of state to genuinely represent the underlying intermolecular potential.

When used properly, molecular simulation¹⁰ is a useful alternative to the conventional theoretical approach, because it provides unambiguous information regarding the merit of the underlying intermolecular potential used to describe molecular interactions. There are many alternative intermolecular potentials¹¹ for water, which reflects the difficulty¹² of accurately predicting all the diverse properties of water. Currently, fully *ab initio* models do not generally provide accurate predictions and the most widely used models are variants of either the four-site¹³ (TIP4P) or the three-site simple point charge^{14,15} (SPC and SPC/E) models.

Although these simple models for water are of great practical value, the use of simplifying approximations often obscures the role of the various contributions to intermolecular interactions. For example, repulsive and dispersive interactions are often crudely approximated via the Lennard-Jones potential and the explicit contributions of multibody

interactions are ignored. Recent work^{16–20} on three-body interactions in atomic systems indicate that they can have a profound effect on both the vapor-liquid¹⁹ and solid-liquid²⁰ phase behavior of fluids. In view of this, it is reasonable to infer that multibody interactions could be even more important in polarizable molecular fluids such as water. Three-body potentials have been proposed²¹ for water by fitting multibody potentials to the results of quantum chemical calculations. Currently this approach is computationally prohibitive and the results are not reliable. A less computationally demanding alternative is to use polarizable potentials.^{22–25} Polarizable potentials approximate the effect of multibody interactions by using fluctuating charges or flexible geometries. The multibody influence arises because the induced dipole of each molecule generates an electric field that affects all other molecules.

A feature common to many polarizable models of water is that they incorporate either Lennard-Jones²⁶ or exponential-6 interactions.²⁷ The use of such effective multibody terms means that the nonadditive contribution to intermolecular interactions is not clearly identified. The aim of this work is to identify the nonadditive influence of the structure and properties of liquid water.

II. THEORY

A. Intermolecular potential and total energy

We propose that the intermolecular potential [$u(r)$] for water is the sum of two-body additive (u_2) and nonadditive three-body [$u_3(\text{disp})$] and polarizable (u_{pol}) contributions,

$$u(r) = u_2 + u_3(\text{disp}) + u_{\text{pol}}. \quad (1)$$

This means that the total configurational energy (U) for the system on N molecules is obtained from

$$U = \sum_{i < j}^N u_2(\mathbf{r}_i, \mathbf{r}_j) + \sum_{i < j < k}^N u_3(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k) + u^{\text{pol}}. \quad (2)$$

^{a)}Author to whom correspondence should be addressed. Electronic mail: rsadus@swin.edu.au

TABLE I. Intermolecular parameters used in the MCY and MCYna intermolecular potential. Unless otherwise stated, all values are in atomic units.

Parameter	Value
a_1	1.731 196
a_2	2.726 696
a_3	1.061 887
a_4	1.460 975
b_1	2.319 395
b_2	1.567 367
b_3	0.436 060
b_4	1.181 792
q^2	0.514 783
R^{OM}	0.505 783
R^{OH}	0.957 200
θ^{HOH} (deg)	104.52
$\alpha\beta$ (\AA^3)	0.802 804
β (dimensionless)	0.557 503
ν	287.9 444

1. Additive two-body terms

The contribution of two-body interactions was obtained from the *ab initio* Matsuoka-Clementi-Yoshimine (MCY) potential.²⁸

$$\begin{aligned}
 u_2 = & q^2 \cdot \left(\frac{1}{r_{13}} + \frac{1}{r_{14}} + \frac{1}{r_{23}} + \frac{1}{r_{24}} \right) + \frac{4q^2}{r_{78}} \\
 & + 2q^2 \left(\frac{1}{r_{18}} + \frac{1}{r_{28}} + \frac{1}{r_{37}} + \frac{1}{r_{47}} \right) + a_1 e^{(-b_1 r_{56})} \\
 & + a_2 [e^{(-b_2 r_{13})} + e^{(-b_2 r_{14})} + e^{(-b_2 r_{23})} + e^{(-b_2 r_{24})}] \\
 & + a_3 [e^{(-b_3 r_{16})} + e^{(-b_3 r_{26})} + e^{(-b_3 r_{35})} + e^{(-b_3 r_{45})}] \\
 & - a_4 [e^{(-b_4 r_{16})} + e^{(-b_4 r_{26})} + e^{(-b_4 r_{35})} + e^{(-b_4 r_{45})}]. \quad (3)
 \end{aligned}$$

The meaning of the parameters is the same as given in the literature²⁸ and their values are summarized in Table I. The benefit of an *ab initio* potential is that it should avoid many of the theoretical uncertainties of empirical intermolecular potentials, such as the need to fit the parameters of the potential to experimental data for various properties. Other *ab initio* potentials for water are available^{29–31} but some of these alternative potentials could not be used because they implicitly include multibody influences that would have led to double counting some contributions to intermolecular interactions.

2. Nonadditive terms

In general, nonadditive contributions to intermolecular interactions arise for induction interactions, resulting from molecular polarizability, short-range repulsion, and dispersion interactions. The theoretical treatment³² of three-body repulsion is much less certain than three-body dispersion and as such it has been omitted from our model. In contrast, it is well documented^{16–20} that multibody dispersion interactions can be adequately described using the Axilrod-Teller³³ triple dipole term,

$$u_3(i, j, k) = \frac{\nu(1 + 3 \cos \theta_i \cos \theta_j \cos \theta_k)}{(r_{ij} r_{ik} r_{jk})^3}, \quad (4)$$

where θ_i , θ_j , and θ_k are inside angles of the triangle formed by three atoms denoted by i , j , and k , and r_{ij} , r_{ik} , and r_{jk} are the three side lengths of the triangle. The parameter ν is the nonadditive coefficient, which can be determined from experiment.³⁴ Equation (4) is only valid for triplets of neutral atoms. For polyatomic molecules, the dispersion interaction depends on both molecular geometry and electron density. MacDowell³⁵ extended the Axilrod-Teller term for the H_2 trimer, in which both the geometry formed by the center of mass and the orientation of the molecule are considered. There is no equivalent molecular reformulation of Eq. (4) for water. Nonetheless, Eq. (4) can be used to calculate the three-body interactions between the constituent atoms of the water molecule. Furthermore, the electron-poor feature of hydrogen means that calculating interactions only between oxygen triplets is likely to be a good approximation for the total three-body contribution. Accurate values of ν are only available for the noble gas atoms.³⁴ In the absence of a known value for the oxygen atom, we have assumed a value of 5/9 of the value of argon (Table I), which reflects the relative difference in size and number of electrons between the two atoms.

The contribution of multibody nonadditive from polarization interactions was obtained from^{32,36}

$$u^{\text{pol}} = -\frac{1}{2} \sum_{i=1}^N \boldsymbol{\mu}_i^{\text{ind}} \cdot \mathbf{E}_i^0, \quad (5)$$

where \mathbf{E}_i^0 is the electrostatic field of surrounding charges, and $\boldsymbol{\mu}_i^{\text{ind}}$ is the induced dipole at site i given by

$$\boldsymbol{\mu}_i^{\text{ind}} = \alpha\beta \cdot \mathbf{E}_i = \alpha\beta \left[\mathbf{E}_i^0 + \sum_{j=1, j \neq i}^N \mathbf{T}_{ij} \boldsymbol{\mu}_j^{\text{ind}} \right]. \quad (6)$$

In Eq. (6), α is the polarizability and \mathbf{T}_{ij} is the dipole tensor given by

$$\mathbf{T}_{ij} = \frac{1}{4\pi\epsilon_0 r_{ij}^5} [3\mathbf{r}_{ij} \mathbf{r}'_{ij} - \mathbf{r}_{ij}^2]. \quad (7)$$

In our model, one polarizable site is added to the negative charge center on each water molecule. To simplify the calculation, intramolecular interactions are not considered, which means that the induced dipole has no interaction with the partial charges on the same water molecule.

Using a gas phase polarizability coefficient of 1.44 \AA^3 obtained from the literature,³⁶ we obtained a dipole moment that significantly exceeded the 2.95–3 D range reported from *ab initio* molecular dynamics³⁷ and experiment³⁸ for water. This suggests that the experimental value of the polarizability coefficient for water in the gas phase is incompatible with the polarization term in liquid water. To improve the calculation of the induced dipole, we scaled the polarizability coefficient by a factor of $\beta=0.557 503$. This means that the actual polarizability term is $\alpha\beta=0.802 804 \text{ \AA}^3$. This resulted in a dipole moment of 2.9 D, with 0.9 D attributed to induction interactions. The contribution of induction to the overall energy is 30%, which is consistent with estimates in

the literature.²⁹ In contrast to this simple change, Niesar *et al.*²⁹ reparametrized both the partial charges and well depth of the MCY potential to properly include the induction in the reformulated Niesar-Corongiu-Clementi (NCC) potential. The total potential obtained from the sum of all of the above terms will be denoted as MCYna, where “na” indicates non-additive. The parameters for the MCYna potential are summarized in Table I.

B. Properties calculated

1. Structural properties

The structure of water was investigated by calculating the radial distribution function (RDF) [$g(r)$] from the following formula:³⁶

$$g(r) = \frac{V}{4\pi r^2 N(N-1)} \left\langle \sum_i n_i(r) \Delta r \right\rangle, \quad (8)$$

where V is the system volume, and $n(r)\Delta r$ is the number of particles which exist in the region between r and $r+\Delta r$. For polyatomic molecules, all the different combinations of RDFs give relative positions of molecules as well as the intermolecular bonding information. We also calculated the first and second oxygen-oxygen coordination numbers,

$$N_{oo} = 4\pi\rho \int_0^{\min} g_{oo}(r)r^2 dr, \quad (9)$$

where ρ is the density.

2. Dielectric constant and dipole moment

The dielectric constant ϵ_r is directly related to the orientation of the dipole. To investigate the influence of nonadditive interactions, the dielectric constant was calculated in this simulation from the total dipole moment fluctuation,^{10,36}

$$\epsilon_r = 1 + \frac{4\pi\rho\mu^2}{3k_B T} g_k. \quad (10)$$

In Eq. (10), k_B is the Boltzmann constant, ϵ_0 is the vacuum permittivity, and g_k is the Kirkwood factor, which can be obtained from the fluctuation of the total dipole moment [$\mathbf{M} = \sum(\boldsymbol{\mu} + \boldsymbol{\mu}^{\text{ind}})$] of the ensemble,

$$g_k = \frac{\langle M^2 \rangle}{N\mu^2}. \quad (11)$$

The evaluation of ϵ_r depends on the treatment of the long-range electrostatic interactions. The Ewald sum was used for long-range electrostatic interactions in the dielectric constant calculation, which is equivalent to “tin-foil” boundary conditions in the reaction field method.^{39–41} As discussed elsewhere⁴² this approximation introduces an additional uncertainty in the results. However, in practice the reported errors^{43,44} are negligible.

The total molecular dipole moment μ_m which has contributions from both the partial charge (permanent electric dipole) and the induction interactions, is averaged over the entire ensemble,

$$\mu_m = \frac{1}{N} \sum_{i=1}^N (\mu_i + \mu_i^{\text{ind}}). \quad (12)$$

C. Simulation details

N - V - T molecular dynamics simulations using the Shake algorithm¹⁰ were performed for 500 water molecules at a density of 0.997 g/cm³ and temperatures of 278, 298, 323, and 343 K. The long-range Coulombic interactions were calculated using an Ewald sum.¹⁰ The convergence parameter for the Ewald sum was $\alpha=5.0/L$, with summation over $5 \times 5 \times 5$ reciprocal lattice vectors, where L is the box length. The three-body interactions were truncated at $L/4$, 6.15 Å,¹⁶ and a cutoff of $L/2$, 12.3 Å, is applied to the additive two-body interaction. During the preequilibration stage, the temperature was held constant by rescaling the velocities every ten steps, which we found to be equivalent to results obtained using a Gaussian thermostat. The simulations were commenced from an initial face centered cubic (fcc) lattice with a time step of 2 fs. The system was equilibrated for 500 ps before any ensemble averages were determined. At each temperature, the total simulation time was at least 2 ns, which corresponds to 1×10^6 time steps. The equations of motion were integrated using a leap-frog algorithm.¹⁰ To determine the induced dipole moment, a direct solver, namely, the conjugate gradient method,⁴⁵ was used.

To speed up the calculations of the dielectric constant, which is slow to converge, the first 500 ps of the simulation was performed without the Axilrod-Teller term. In this case, the total simulation time was 2 ns. Ensemble averages were obtained by analyzing postequilibrium configurations at intervals of 100 time steps and standard deviations were determined. The introduction of the inducted dipole calculation and the Axilrod-Teller term significantly increases the computation load, requiring the implementation of a modified force decomposition algorithm⁴⁶ to parallelize the calculation. It was implemented with the MPI library, with more than 98% computation load distributed among 32 processors.

III. RESULTS AND DISCUSSION

To obtain an insight into the effect of nonadditivity on the properties of water, simulations were performed for both the MCY and MCYna potentials. In all cases, matching calculations were also obtained for the SPC/E potential¹⁵ to compare the results with a widely used empirical model.

The $g_{HH}(r)$, $g_{OH}(r)$, and $g_{OO}(r)$ radial distribution functions obtained from the MCY, MCYna, and SPC/E intermolecular potentials at various temperatures are illustrated in Figs. 1–4. It is apparent from these comparisons that there are considerable quantitative differences in the $g(r)$ data obtained for the various models. In terms of the position of the $g(r)$ peaks, the following order is observed: SPC/E < MCYna < MCY. In most cases, the height of the second peak is similar for the three potentials. However, significant differences are observed for both the height and breadth of the first peak. The first $g_{HH}(r)$ peak is of similar height for all three potentials, however, the SPC/E potential results in a noticeably broader peak than either the MCY and MCYna

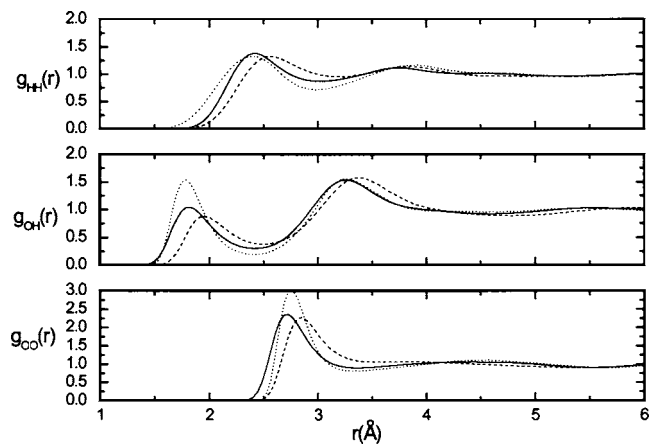


FIG. 1. Radial distribution functions at a temperature of 278 K and a density of 0.997 g/cm^3 predicted by the MCYna (—), MCY (---), and SPC/E (····) intermolecular potentials.

potentials. Arguably, the main difference in the potentials is evident from the height of the first peak in both $g_{\text{OH}}(r)$ and $g_{\text{OO}}(r)$. In these cases, both the peak height and breadth increase in the following sequence: SPC/E > MCYna > MCY.

The differences in the $g(r)$ behavior of the MCY and MCYna potentials quantify the important role of nonadditive interactions on the structure of water. We also performed simulations with the polarization term in the absence of the Axilrod-Teller term. The results were almost indistinguishable which indicates that three-body dispersion interactions do not noticeably affect the structure of water. This means that the differences between the MCY and MCYna potentials can be mainly attributed to the effect of polarization. Polarization greatly increases the ordered structure of liquid water, bringing water molecules closer together and facilitating hydrogen bonding.

For 298 K (Fig. 2), we are able to compare our calculations directly with experimental data⁴⁷ obtained from neutron diffraction studies. In all cases, the MCY potential yields inadequate agreement with experiment. The positions of the peaks are shifted to greater distances; the heights of the peaks are too low and they are broader than observed experi-

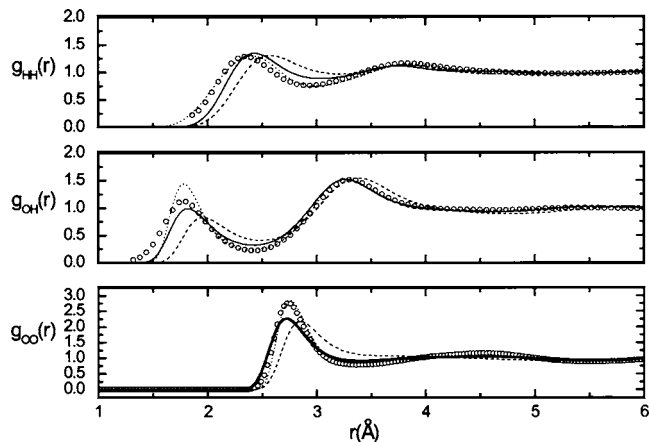


FIG. 2. Radial distribution functions at a temperature of 298 K and a density of 0.997 g/cm^3 predicted by the MCYna (—), MCY (---), and SPC/E (····) intermolecular potentials. A comparison is also made with experiment (○) (Ref. 47).

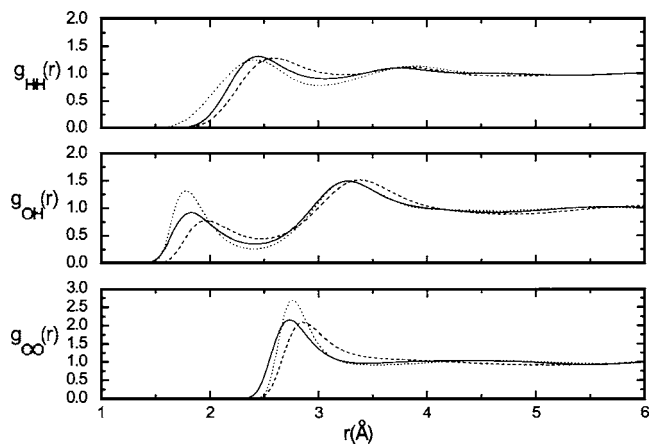


FIG. 3. Radial distribution functions at a temperature of 323 K and a density of 0.997 g/cm^3 predicted by the MCYna (—), MCY (---), and SPC/E (····) intermolecular potentials.

mentally. The introduction of polarization in the MCYna potential largely compensates for these deficiencies, resulting in an improved agreement with experiment. For both $g_{\text{HH}}(r)$ and $g_{\text{OO}}(r)$, the SPC/E potential yields the best overall agreement with experiment. However, for $g_{\text{OH}}(r)$, the SPC/E potential significantly overestimates the first peak whereas better agreement is obtained from the MCYna potential.

The first peak of $g_{\text{OH}}(r)$ can be attributed to hydrogen bonding. The fact that the SPC/E potential overestimates the first peak indicates that it overestimates the role of hydrogen bonding relative to nonbonded interaction. The differences in the first peak height between the SPC/E and MCYna potentials are also apparent at 278 K (Fig. 1), 323 K (Fig. 3), and 343 K (Fig. 4). In view of this, it is reasonable to infer that the MCYna potential might possibly provide a better overall description of the relative importance of hydrogen bonding in water compared with conventional nonbonded interactions between hydrogen and oxygen. In particular, Figs. 1–4 show that the MCYna potential predicts that the relative importance of hydrogen bonding declines with increasing temperature, whereas the SPC/E results are much less sensitive to temperature.

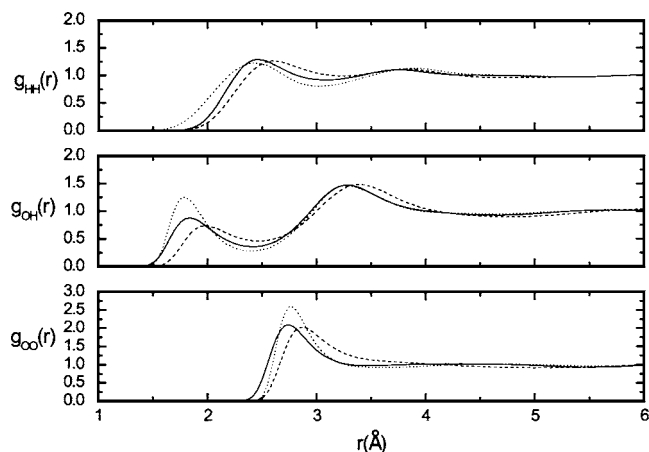


FIG. 4. Radial distribution functions at a temperature of 343 K and a density of 0.997 g/cm^3 predicted by the MCYna (—), MCY (---), and SPC/E (····) intermolecular potentials.

TABLE II. Comparison of the first and second oxygen-oxygen coordination numbers predicted for the SPCE, MCY, and MCYna potentials.

Model	First coordination number				Second coordination number			
	278 K	298 K	323 K	343 K	278 K	298 K	323 K	343 K
Expt. ^a		4.42				23.07		
SPC/E	4.51	4.66	5.33	5.76	24.33	24.06	23.74	24.79
MCY	4.41	4.60	4.91	5.15	21.45	20.27	20.25	22.77
MCYna	4.43	4.55	4.81	5.02	22.65	21.91	22.57	22.07

^aFrom Ref. 47.

The first and second oxygen-oxygen coordination numbers for the SPCE, MCY, and MCYna potentials at various temperatures are compared in Table II. It is apparent that the first coordination number increases noticeably with increasing temperature whereas the value of the second coordination number is less sensitive to temperature. Experimental data⁴⁷ are only available at 298 K. The comparison for 298 K indicates that including nonadditive interactions significantly improves the predicted oxygen-oxygen coordination in liquid water.

The calculation of the dielectric constant is computationally challenging, normally requiring simulations of at least a nanosecond to obtain reliable results. The results are also very sensitive to the nature of the calculation,⁴⁸ and discrepancies are commonly observed between the Ewald sum and reaction field methods for highly polar liquids. For water, variations of more than 50% in the dielectric constant have been observed.⁴⁹ Using the reaction field method, Neumann⁵⁰ reported a dielectric constant of 53 for the TIP4P model at 293 K, whereas values of 61 and 72 were observed by Watanabe and Klein⁵¹ and Ferrario and Tani,⁵² respectively, at 300 K with the Ewald sum. At a temperature of 300 K, using the reaction field method, Smith and van Gunsteren⁵³ reported dielectric constants of 62.3 and 54.0 for the SPC/E and SPC models, respectively. Alper and Levy⁵⁴ also used the reaction field but obtained values of 68 and 59 for the two different models. In contrast, values of 72 and 70, respectively, were reported by Watanabe and Klein⁵¹ from an Ewald sum. For the MCY potential, Neumann⁵⁵ reported a dielectric constant of 35 at 293 K with the reaction field method, whereas Impey *et al.*⁵⁶ reported a value of 50 from an Ewald sum. We note that the internal energy reported by Neumann⁵⁵ for the MCY potential (-35.7 kJ/mol) is substantially lower than the commonly accepted value [-28.42 kJ/mol (Ref. 57)], which may help to partly explain the low value of the dielectric constant.

Although many explanations for these discrepancies have been proposed, the exact reasons have not been resolved fully. Neumann⁴² has argued that a correction should be applied to an infinite system in order to achieve a realistic dielectric constant because Eq. (10) only applies to spherical rather than toroidal symmetry boundaries, which is the reality in water simulations. However, the correction term is very small. For example, the correction term determined by Watanabe and Klein⁵¹ (0.75) is smaller than the numerical uncertainty for the simulation. It has been argued⁵⁸ that the Ewald sum is the most suitable method of simulating a polar

fluid to avoid obtaining an unrealistically low dielectric constant. Although a correction term is theoretically required for Ewald sum calculations, in practice the correction term is negligible, and the results obtained will be closer to experiment than reaction field calculations.

We calculated the dielectric constant for various temperatures using the MCY, MCYna, and SPC/E and these data are illustrated in Fig. 5 and compared with experimental data.⁵⁹ Figure 5 also includes a comparison for the SPC potential⁵⁴ and a continuum calculation reported by Nir.⁶⁰ As discussed above, there are significant differences in the values of the dielectric constant reported in the literature^{54,61,62} for the SPC/E potential, which can be at least partly attributed to the handling of the long-range cut-off and inadequate simulation lengths. Our values fall within the reported range of values (61–71). It is apparent from this comparison that the MCY potential yields poor agreement with experiment, whereas a considerable improvement is achieved using the MCYna potential. Indeed, the results for MCYna significantly outperform the SPC/E potential. Clearly, nonadditive interactions have an important influence on the dielectric constant. Numerical values of the dielectric constant are summarized in Table III.

The dipole moment calculated from Eq. (12) contains the contribution from both the permanent dipole plus the

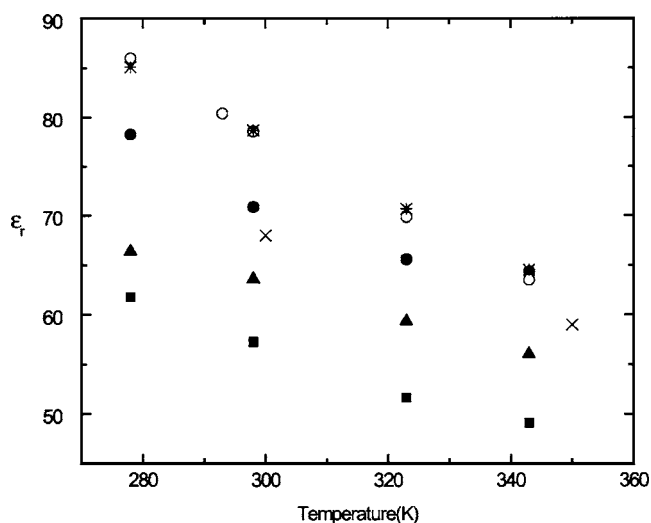


FIG. 5. Comparison of experimental dielectric constant (○) (Ref. 59) as a function of temperature with values predicted by the MCYna (●), MCY (■), SPC/E (▲), and SPC (×) (Ref. 57) potentials and a continuum calculation (*) (Ref. 60).

TABLE III. Comparison of experiment with the predictions of various intermolecular potentials for the internal energy, dielectric constant, and dipole moment of water at 298 K and a density of 0.997 g/cm³. Values in brackets represent standard deviations.

	Expt.	MCYna	MCY	SPC/E	TIP3P ^a	TIP4P/2005 ^b
Energy (kJ/mol)	-41.67 ^c	-36.98	-29.0	-44.9	-38.5	
Dielectric constant	78.5 ^d	70.98(4.2)	57.30(3.42)	63.73(0.29)	96.9	60
Dipole moment (D)	2.95 ^e	2.92	2.19	2.35	2.347	2.3

^aFrom Ref. 64.

^bFrom Ref. 65.

^cFrom Ref. 13.

^dFrom Ref. 59.

^eFrom Ref. 63.

induced dipole. Figure 6 shows the variation of the dipole moment as a function of temperature. In Table III, the dipole moments at 298 K obtained from various models are compared with experiment. We observe that the dipole moment of 2.92 D calculated from Eq. (12) does not match the initially imposed value of 2.9 D, which reflects the relaxation of the system during the simulation. In contrast, the other models significantly underestimate the dipole moment. This can be partly explained by the absence of an induced dipole contribution. For example, at 298 K, the induced dipole obtained for the MCYna potential contributes 0.9 D to the total dipole moment of 2.92 D. An accurate dipole moment is likely to improve the predicted phase behavior of water.⁶⁶

Values of the energy obtained at 298 K for the various models are compared to experiment in Table III. It is evident from this comparison that the MCY potential significantly overestimates the energy. The introduction of nonadditive interactions in the MCYna potentials reduces this discrepancy to approximately 11%. The contributions of polarization and three-body interactions to the total energy are -9.14 and 0.64 kJ/mol, respectively. In contrast, the SPC/E potential without a polarization correction¹⁴ underestimates the energy by approximately 8%.

IV. CONCLUSIONS

Polarization is the main contribution to nonadditive interactions in liquid water. In contrast, three-body dispersion

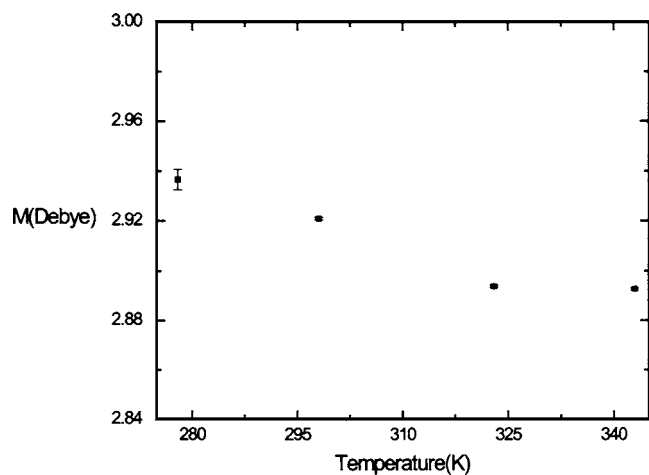


FIG. 6. The dipole moment predicted from the MCYna potential at different temperatures.

interactions have only a minor role. The addition of a polarization term has a significant effect on the structure of water. In particular, it appears to more accurately predict the relative contribution of hydrogen-bond interactions compared with conventional nonbonded interactions. The MCYna potential also results in an improvement in the quality of agreement for the dipole moment and the dielectric constant. The results are superior to those that can be obtained using the SPC/E potential.

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