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ABSTRACT

The melting point of water is a fundamental thermodynamic property and a key benchmark for molecular simulations of phase behavior. Here, we estimate the melting temperature of the TIP4P/2005 and TIP4P/Ice models at ambient pressure using the direct coexistence method. We simulate systems containing up to 8640 water molecules and treat long-range interactions with the particle mesh Ewald approach for both electrostatics and dispersion [Lennard-Jones Particle-Mesh Ewald (LJ-PME)], thereby substantially reducing finite-size and cutoff-truncation artifacts. We find that, once these effects are properly accounted for, the melting point of both models increases by nearly 1 K relative to the values obtained from truncating the dispersion interactions at 8.5 Å. The resulting melting temperatures are 250.25 and 270.75 K for the TIP4P/2005 and TIP4P/Ice water models, respectively, thereby bringing the latter significantly closer to experiment. We also evaluate melting enthalpies at coexistence and find them largely insensitive to system size and the long-range treatment. Overall, these results highlight the importance of accurate long-range interactions in phase-coexistence simulations of water.

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The melting point (T_m) of water is a fundamental thermodynamic property that plays a crucial role in understanding its behavior, particularly when simulating phase transitions.^{1–7} Other related properties, such as the densities of the coexistence phases, the solid–fluid interfacial free energy, or the melting enthalpy, could be affected due to a change in the melting point of water.^{8–10} These effects become especially relevant for properties such as freezing point depression or nucleation rates as they strongly depend on the degree of supercooling relative to T_m . Therefore, an accurate determination of the melting point is essential for reliably computing more challenging thermodynamic properties.

In molecular simulation, there are two main factors that can affect the melting point of a model. The first factor is finite-size effects. When having an insufficient number of atoms or molecules in the simulation box, the thermodynamic properties intended to be studied can lead to inaccurate results. Second, a cutoff radius that

is not large enough may not include most dispersive interactions, thereby mapping the system poorly and yielding misleading results. In conclusion, a model could be suitable for exploring given thermodynamic properties, but an inadequate choice of simulation details could result in erroneous values.

For water, two of the most widely used rigid, nonpolarizable models are TIP4P/2005⁸ and TIP4P/Ice,¹¹ which have been employed extensively in the literature.^{5,6,12–17} These models are reparameterizations of the TIP4P water model proposed by Jorgensen *et al.*¹⁸ Both have a Lennard-Jones (LJ) interaction center placed in the oxygen atom of the water model. Positive charges are placed in the position of the hydrogen atoms, and the negative charge from the oxygen is moved a distance d_{OM} along the H–O–H bisector. The H–O–H angle remains the same for both models, with only a slight modification in the distance d_{OM} and in the charge distribution. Regarding the ϵ and σ parameters of the LJ interaction centers, these values are specific to each model.

These models have been widely used to explore fluid and solid phases of water, respectively. To this extent, Conde *et al.*¹⁴ identified the finite-size effect when conducting an extensive analysis of the ice-water melting point using the direct coexistence method. They concluded that this effect ceases to have a meaningful impact for systems with ≥ 4000 water molecules. Enlarging the systems above 4000 molecules only reduces the error bars of the estimation, but does not change the value of the melting point, where the T_m values for TIP4P/2005 and TIP4P/Ice for larger systems converge at 249.5(1) K and 269.8(1) K, respectively. However, Conde *et al.*¹⁴ truncated the Lennard-Jones and Coulombic potential at 8.5 Å, a cutoff rather small but necessary when running a large number of simulations in combination with large systems.

In this work, we calculate the melting points of the TIP4P/2005 and TIP4P/Ice water models, at ambient pressure, avoiding finite-size effects and the cutoff inconvenience. To do this, we simulate systems with $N = 4320$ and 8640 water molecules, with the same initial system length for both simulation boxes in the x and y axes, $L_x = 4.04$ nm and $L_y = 3.74$ nm, but different initial lengths in the z axis, $L_z = 8.96$ nm and $L_z = 18.49$ nm, respectively. We also employ the Particle Mesh Ewald (PME) not only for electrostatic interactions, but also for dispersive ones,^{19,20} an option available in the modern versions of GROMACS, but not in the older ones. When using PME (for both electrostatic and LJ contributions), there is no truncation of the potential, and interactions at all distances are taken into account, for both Coulombic and dispersive interactions. Thus, with PME, the truncation of the potential is gone. Its main drawback, the computational cost compared to the traditional combination of a small cutoff in addition to pressure and energy long-range corrections, is becoming less significant as advances in computing technology make it increasingly affordable.

At present, the Coulombic interactions are treated in all cases with PME so that there is no truncation of the Coulombic interaction. However, for the LJ part of the potential, the common choice was truncating the potential at a certain distance r_c (often the value 8.5 Å was chosen). We shall refer to this approach as truncated. Another possibility is the use of truncation in the LJ part of the potential at r_c and adding a homogeneous long-range correction (LRC) to the LJ contribution. This setup will be denoted as truncated + LRC.

Simulations are carried out using the direct coexistence method,^{21,22} which consists of putting in contact a solid phase with a liquid phase and studying the stability of the system at a given pressure and different temperatures. Simulations above T_m will tend to melt the ice, whereas simulations below T_m will tend to crystallize the liquid water. Near the coexistence temperature, the system's evolution is stochastic; the reported $T_m \pm \sigma_{T_m}$ represents the interval where the probability of melting equals the probability of crystallization. Simulations are performed in the anisotropic isobaric-isothermic or NPT ensemble. This ensemble keeps the pressure constant and allows independent fluctuations of the box lengths along the x , y , and z directions, avoiding any stress buildup in the ice Ih solid structure during the simulations. Strictly speaking, the $NP_z\mathcal{A}T$ ensemble (where the interfacial area, $\mathcal{A}$, is kept constant) is the rigorous choice for inhomogeneous systems. However, the anisotropic NPT ensemble is often preferred to ensure that the solid phase relaxes to its equilibrium structure without internal stress. According to the literature,^{22,23} the results from both

ensembles are mutually consistent for sufficiently large systems, as any error introduced by the NPT ensemble becomes negligible when using elongated simulation boxes with sufficiently long L_z values much larger than the length of the interfacial region. Furthermore, it has been shown that the uncertainty arising from the choice of ensemble is significantly smaller than the error associated with the stochastic nature of the direct coexistence simulations, which is properly accounted for by the number of seeds performed in this study at temperatures near the T_m . The liquid–solid interface is placed along the z axis. If the solid phase grows, the system is freezing, and the fixed temperature, T , is lower than the T_m model value. If the liquid phase grows, the system is melting and $T > T_m$. As a result, the melting point is estimated between the highest temperature that provokes crystallization and the lowest temperature that melts the system.

It is worth noting that many of the earlier estimates of the melting points of TIP4P-family water models were based on free-energy calculations combined with thermodynamic integration. Within that framework, the free energies of the liquid and relevant solid phases are evaluated under selected thermodynamic conditions, extended to other state points by thermodynamic integration, and used to locate coexistence points through the equality of phase free energies. The corresponding coexistence lines can then be propagated using the Gibbs–Duhem method. By contrast, the direct coexistence approach does not rely on an explicit determination of free energies. Rather, solid and liquid phases are placed in contact within the same simulation box, and the evolution of the interface is followed at constant pressure over a range of temperatures. In this case, the melting point is inferred from the temperature at which neither phase systematically advances over the other. Traditionally, free-energy calculations, thermodynamic integration, and Gibbs–Duhem simulations were typically implemented in home-made Monte Carlo codes, whereas direct coexistence simulations are now routinely carried out using parallelized open-source molecular dynamics engines such as GROMACS.

For each system, the initial simulation box is built up with half of the molecules in a liquid water phase and the other half in a solid ice Ih phase. The solid phase in the initial configuration is obtained using the algorithm proposed by Buch *et al.*,²⁴ generating an ice phase with proton disorder and almost zero dipole moment satisfying the Bernal–Fowler rules.²⁵ The TIP4P/2005 and TIP4P/Ice water models are studied for each system size, having four different systems overall. We first sweep a broad range of temperatures, and then, for each temperature, we run a minimum of ten seeds in the region where the T_m could be located, with increments of 0.5 K. Typical simulation times required to determine whether the system melts or crystallizes are on the order of ~ 250 ns for the large systems and around 100 ns for the small ones. Overall, the total simulation time accumulated in this work amounts to ~ 25 μ s.

Simulations are run in the GROMACS software package²⁶ (version 2016.6 in double precision, since previous versions do not support PME for the LJ potential). Although PME is applied in both electrostatic and dispersive interactions, a given cutoff is needed for GROMACS to calculate the direct and reciprocal space contributions. In this work, $r_c = 1.2$ nm is chosen. However, this value is a technicality and does not affect the final result, since the LJ potential is effectively not truncated. The pressure selected for all simulations is the ambient pressure, 1 bar. Parrinello–Rahman²⁷

and Nosé–Hoover²⁸ are the barostat and thermostat, respectively, applied to stabilize pressure and temperature, both with a coupling time of 2.0 ps. The barostat compressibility is fixed at $5 \times 10^{-5} \text{ bar}^{-1}$. We refer the reader to the [supplementary material](#) to see the files used to run these simulations in GROMACS, as well as tables summarizing the behavior (crystallization or melting) of every simulation performed in this work.

A comparison between different T_m values estimated in the literature is presented in [Tables I](#) and [II](#) for the TIP4P/Ice and TIP4P/2005 water models, respectively. Here, we can differentiate three scenarios: (I) simulations where both system and cutoff radius are rather small, (II) simulations where the system is large enough, but the small radius persists, and (III) simulations where both system and cutoff radius are large, avoiding both finite-size and cutoff truncation effects. In scenario I, the estimated melting temperatures at ambient pressure are systematically underestimated due to these two aforementioned issues. In scenario II, the melting point gradually shifts toward higher values, despite the cutoff effect that these systems present. In this scenario, it is worth mentioning that some studies use homogeneous long-range corrections^{29,30} to assess the tail of the LJ potential, as an analytic solution to solve the cutoff truncation problem. This is a good approximation when having homogeneous systems, since the last part of the LJ potential is calculated analytically and added to the interactions of the system. However, using LRC is only advisable when having purely

homogeneous systems, since the simulation program assumes that the density is homogeneous along all the simulation box. In solid–liquid water simulations, applying LRC is not strictly correct since the density is spatially heterogeneous: the two distinct phases have slightly different bulk densities, and the density also varies continuously across the interfacial region. That said, as the bulk densities of water and ice are similar (although not identical), the use of LRC for the LJ part of the potential seems reasonable. Still, this approach cannot be used when applying the direct coexistence method to a case where one of the phases is liquid/solid and the other is a gas.

Finally, scenario III, which corresponds to the results obtained in this study, is reached. It is noticeable that the liquid water–ice Ih melting point does not change considerably when systems have more than 4000 molecules, as stated in the literature.¹⁴ However, when no cutoff is used for the LJ part of the potential (i.e., PME), the melting point is shifted to higher temperatures, nearly 1 K with respect to the values found by Conde *et al.*¹⁴ for a truncated potential of 8.5 Å. Thus, the actual melting points, once after the finite-size effect and potential truncations are removed, for TIP4P/2005 and TIP4P/Ice are 250.25(25) and 270.75(25) K, respectively. Notice that the refined value of the melting point of TIP4P/Ice is now closer to the experimental melting temperature of water at ambient pressure, 273.15 K. Since the results for $N = 4320$ and $N = 8640$ are identical within the statistical error, and following the convergence

TABLE I. Melting point of solid ice Ih–liquid water at different numbers of molecules N and cutoff r_c for the TIP4P/Ice water model. In all cases, simulations were carried out taking explicitly into account the ice Ih–water interface. Numbers in parentheses correspond to the uncertainty in the estimation. PME stands for particle mesh Ewald, PPPM stands for particle–particle particle–mesh, and LRC stands for homogeneous long-range correction.

T_m (K)	N	r_c (nm)	Coulombic	LJ
270.75(25) (this work)	8 640	...	PME	PME
270.75(25) (this work)	4 320	...	PME	PME
270(1) ³¹	3072	...	PME	PME
270(1) ³²	4 000	0.9	PME	Truncated + LRC
270(2) ³³	1 154	0.85	PME	Truncated
269.8(1) ¹⁴	16 000	0.85	PME	Truncated
268(2) ³⁴	870	0.85	PME	Truncated
269.1 ³	576	0.85	PPPM	Truncated + LRC

TABLE II. Melting point of solid ice Ih–liquid water at different numbers of molecules N and cutoff r_c for the TIP4P/2005 water model. In all cases, simulations were carried out taking explicitly into account the ice Ih–water interface. The numbers in parentheses correspond to the uncertainty in the estimation. PME stands for particle mesh Ewald, and LRC stands for homogeneous long-range correction.

T_m (K)	N	r_c (nm)	Coulombic	LJ
250.25(25) (this work)	8 640	...	PME	PME
250.50(50) (this work)	4 320	...	PME	PME
250(1) ³⁵	4 000	1.0	PME	Truncated + LRC
249.5(1) ¹⁴	16 000	0.85	PME	Truncated
249(2) ¹⁴	864	0.85	PME	Truncated
249(2) ³⁴	870	0.85	PME	Truncated
249(3) ³⁶	864	0.85	PME	Truncated

criteria established by Conde *et al.*,¹⁴ finite-size extrapolation was deemed unnecessary.

In Table I the results obtained by Weidmann *et al.*³¹ are also presented. In their study, the melting point of water was estimated using a direct coexistence setup within the *NPH* (isenthalpic–isobaric) ensemble. Their reported values of T_m are, within the associated uncertainty, in agreement with the results obtained in the present work. It is, nevertheless, worth noting some methodological differences between the two studies. In particular, Weidmann *et al.* employed smaller system sizes, below the 4000 molecules that Conde recommended to avoid finite-size effects,¹⁴ and typically performed two simulation runs of ~ 100 ns, whereas in this work, we carry out around 20 independent simulations per model in the vicinity of the melting point, with typical simulation lengths ranging from 100 to 400 ns. These differences likely contribute to the larger error bars reported in the work of Weidmann and colleagues.³¹ In any case, both sets of results are mutually consistent within their respective error estimates.

As an illustration of the results obtained for the TIP4P/2005 model, Fig. 1 shows the time evolution of the potential energy, U , during the simulations for a set of independent seeds at 250.0 and 250.5 K. The trajectories exhibit a clear temperature dependence: all simulations at 250.0 K evolve toward lower potential energies, consistent with progressive crystallization, whereas those at 250.5 K tend to increase with time, indicating melting of the ice phase. In agreement with this behavior, direct coexistence simulations yield a melting point of 250.25(25) K for the TIP4P/2005 model. The corresponding results for the TIP4P/Ice model are also presented in the [supplementary material](#).

Once the T_m is estimated, another interesting property that can be obtained is the melting enthalpy. This is defined as the amount of energy needed to change a substance from solid to liquid under its melting point conditions of temperature and pressure,

$$\Delta H_m = H_S - H_L, \quad (1)$$

where

$$H = U + PV, \quad (2)$$

ΔH_m is the melting enthalpy, and H_S and H_L are the corresponding enthalpies of the solid and fluid phases. For a given enthalpy H , U is the internal energy, P is the pressure, and V is the volume of the simulation box. At low pressures (i.e., atmospheric pressure), the term PV becomes negligible ($PV \approx 0$), and then, $H \approx U$.

To estimate the melting enthalpy, we independently simulate pure bulk liquid and Ih solid phases of water. For liquid, $N = 2220$ and 4440 molecules are simulated; for Ih ice, $N = 2048$ and 4096, resembling these bulk phases to the ones studied through direct coexistence to obtain the T_m (systems with ~ 4000 and ~ 8000 molecules overall). The simulations are conducted in the *NPT* ensemble for 15 ns, with the first 5 ns considered the equilibration period and the final 10 ns considered the production period.

Originally, the melting enthalpies for TIP4P/Ice and TIP4P/2005 were estimated at 1.29 and 1.16 kcal/mol, respectively.⁸ The discrepancy between the first results and the ones proposed in this study is due to two factors. First, the original results were studied with the LJ part of the potential truncated at

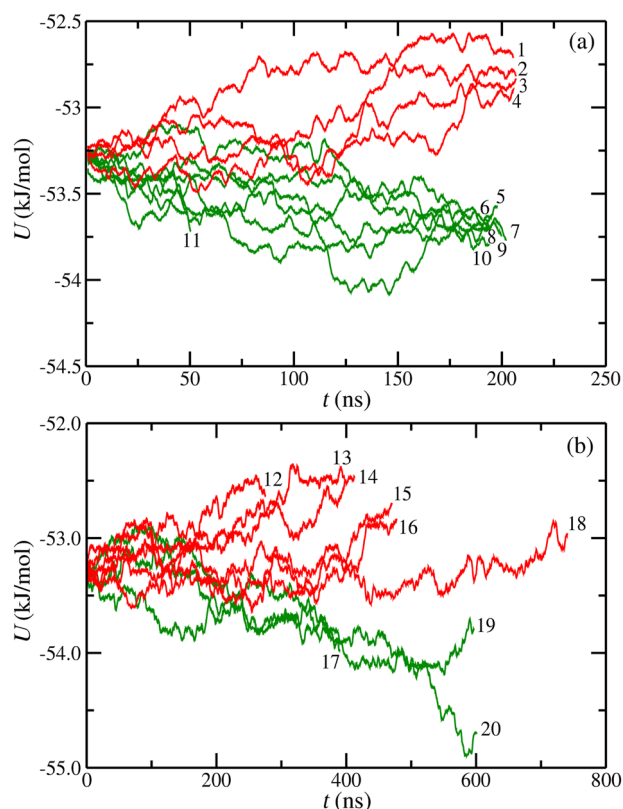


FIG. 1. Evolution of the potential energy as a function of time for independent-seed simulations of the TIP4P/2005 water model with run times below 200 ns (a) and above 200 ns (b). Green curves correspond to simulations at 250 K, and red curves correspond to simulations performed at 250.5 K. Simulations are performed with $N = 8640$ water molecules.

0.85 nm, and then, LRCs were applied. Here, long-range corrections are a better fit for this type of simulation, as the simulations are independent bulk phases, and hence, the density does not change significantly throughout the simulation box. However, the cutoff chosen was insufficient for a proper estimation of these properties, and the LRC is an approximation of the last part of the LJ tail. Second, and more importantly, the bulk liquid water was probably not fully equilibrated in the original simulations.

Table III shows the resulting melting enthalpy for each water model and system size studied. At the new T_m , the melting enthalpy vaguely changes even when increasing the number of bulk molecules in each phase. The results are in good agreement with the ones recently found in the literature, where Blazquez and Vega recalculated the melting enthalpy of the TIP4P/Ice and TIP4P/2005 models, giving 1.22 and 1.13 kcal/mol, respectively.³⁵ These values were obtained with a cutoff of 1.0 nm and homogeneous long-range corrections. However, as stated earlier, long-range corrections are good approximations when applied to homogeneous bulk phases. Therefore, the values of Table III are recommended for the melting enthalpy of these two water models.

To summarize, the melting point and the melting enthalpy are calculated for the TIP4P/2005 and TIP4P/Ice water models.

TABLE III. Melting enthalpy of solid ice Ih–liquid water at different numbers of molecules N for the two water models used.

Water model	N_S	N_L	ΔH_m (kcal/mol)
TIP4P/Ice	4096	4440	1.223
TIP4P/Ice	2048	2220	1.225
TIP4P/2005	4096	4440	1.127
TIP4P/2005	2048	2220	1.127

Although these properties may appear straightforward to estimate and are routinely calculated in the literature, they are essential for nucleation studies.³⁷ We apply PME corrections not only to electrostatic interactions but also to dispersive interactions and to systems whose number of molecules is sufficiently large to avoid finite-size effects. This allows the system to overcome the typical inconveniences that may arise, such as the finite-size effects and the truncation of the potential.

The melting point of both water models increases around ~ 0.5 K (0.25–0.5 K for TIP4P/2005 and 0.5–0.75 K for TIP4P/Ice) with respect to the latest estimates,³⁵ and the melting enthalpies are not significantly modified with respect to the latest estimates.³⁵ Notice that the values reported in 2005 for TIP4P/2005 and TIP4P/Ice for the melting temperature (252 and 272 K, respectively) obtained from free energy calculations are not correct for our modern standard, and the same is true for the melting enthalpies reported in the original papers. We strongly recommend using the values 250.25 and 270.75 K for the melting points of TIP4P/2005 and TIP4P/Ice, respectively, and 1.127 and 1.223 kcal/mol for the melting enthalpies of these models from now on.

The [supplementary material](#) includes detailed tables summarizing the behavior (crystallization or melting) observed for each independent seed at every temperature studied. It also provides the GROMACS configuration files (`topol.top` and `grompp.mdp`) to ensure full reproducibility of our LJ-PME setup, as well as a figure showing the time evolution of the potential energy during the simulations for a set of independent seeds of the TIP4P/Ice water model.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

C. Romero-Guzmán: Investigation (equal); Writing – original draft (equal); Writing – review & editing (equal). **J. Algaba:** Conceptualization (equal); Methodology (equal); Writing – review & editing (equal). **C. Vega:** Funding acquisition (equal); Methodology (equal); Writing – review & editing (equal). **F. J. Blas:** Funding acquisition (equal); Methodology (equal); Writing – review & editing (equal).

DATA AVAILABILITY

The data that support the findings of this study are available within the article.

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