The Journal of Chemical Physics

EDITORIAL | OCTOBER 21 2026

Autobiography of Carlos Vega

Special Collection: Carlos Vega Festschrift

Carlos Vega

Check for updates

J. Chem. Phys. 165, 150401 (2026)
https://doi.org/10.1063/5.0361614

View Online
Export Citation

Articles You May Be Interested In

The discovery of the depletion force
J. Chem. Phys. (June 2021)

Autobiography of Louis E. Brus
J. Chem. Phys. (October 2025)

Autobiography of Y. Ron Shen
J. Chem. Phys. (February 2025)

21 October 2026 13:04:58

AIP Publishing
The Journal of Chemical Physics
Special Topics Open for Submissions
Learn More

AIP Publishing

The Journal of Chemical Physics

EDITORIAL

pubs.aip.org/aip/jcp

Autobiography of Carlos Vega

Cite as: J. Chem. Phys. 165, 150401 (2026); doi: 10.1063/5.0361614
Submitted: 21 September 2026 • Accepted: 25 September 2026 •
Published Online: 21 October 2026

View Online Export Citation CrossMark

Carlos Vega[a)]

AFFILIATIONS

Dpto. Química Fisica, Fac. Ciencias Químicas, Universidad Complutense de Madrid, 28040 Madrid, Spain

Note: This paper is part of the Special Topic, Carlos Vega Festschrift.
[a)]**Author to whom correspondence should be addressed:** cvega@quim.ucm.es

ABSTRACT

I do not believe my biography is particularly interesting, but I hope that it may at least be entertaining, and that anyone reading it may find in it at least one sentence that proves inspiring, especially those researchers who are just beginning their scientific careers. It is only fair to acknowledge that life is an adventure, and that we never quite know what lies ahead.

Published under an exclusive license by AIP Publishing. https://doi.org/10.1063/5.0361614

21 October 2026 13:04:58

I. FIRST STEPS

I was born in Madrid (Spain) in 1964 into a middle-class family. Although for science I signed always as Carlos Vega, my official name in Spain is Carlos Vega de las Heras (where the first name comes from my father and the second one from my mother). I was the elder of two siblings (my sister Myriam was born in 1966). My father (Carlos) was a commercial sales representative in the footwear trade (representing the shoe factories of Elche and Elda in the shoe shops of Madrid), and my mother (Maria del Pilar) was a housewife (during the dictatorship, women were not allowed to work once they married). Neither of my parents held a university degree; in both cases, and despite their outstanding performance at school, they began working at the age of fourteen to sixteen, compelled by the economic hardship of a Spain impoverished by a civil war (1936–1939) that caused around seven hundred thousand deaths, drove many intellectuals and scientists into exile, and left a country devastated by the destruction of war and by the absolute suppression of freedom of expression. The military dictatorship remained in place in Spain between 1939 and 1975, the year in which the dictator died.

The 1960s brought a certain economic revival to Spain, together with a baby boom. My generation was fortunate not to have experienced either the war or the hunger that our parents had endured. My childhood was a happy one; I never went hungry, and I was able to study from the age of six to the age of eighteen at a school in a modest neighborhood of Madrid, Carabanchel, the religious school San Viator. Spain was, by imposition, a Catholic country (until 1975), where the best educational institutions were controlled by the Church. I must say that, in my case, that religious school was fairly liberal and allowed me to develop my love for sports (handball, football, chess and trekking were among my interests) as well as a good number of cultural activities. My academic performance was good, and I remember with affection my chemistry teacher, Marcos Velez. Spain underwent a profound transition and evolved rapidly toward a democratic regime from 1975 onwards; in the 1980s one could breathe in Madrid an air of profound freedom, which coincided with my years as a university student.

II. UNIVERSITY

In 1982, after completing secondary education, the opportunity came to enter university. Spain had at that time (and still has) a system of public universities in which tuition fees are not that big (for instance in 2026 they are of the order of 1200 euros per year which is similar to the minimum wage per month in Spain). My parents encouraged me to continue studying (as did the parents of many of those born in the 1960s), thus making possible a dream that they themselves had not been able to fulfill: "to study at the university." Although I was greatly drawn to philosophy and literature, I finally decided that I would study a scientific discipline, and I chose Chemistry (Physics being my second option). In 1982 I entered to the Faculty of Chemistry of the Complutense University of Madrid, in Spanish named as Universidad Complutense de Madrid (UCM), and it has been my home ever since. In Spain (especially in cities having a University) it was customary to continue living with our parents during the university years, thereby saving the cost of accommodation and board. I completed my degree in Chemistry in 1987. I was not (and am not) particularly fond of honors, but it is only fair to mention that I received the national award for the best academic

Published under an exclusive license by AIP Publishing

record in Chemistry in Spain in 1987 (my father submitted the application, since I had not done so myself, considering it pretentious). I should also mention that in the third year (of five) of my undergraduate studies in Chemistry, in 1985, I came close to abandoning my university education in order to start working, since my family's financial situation was extremely difficult and the company where my mother worked (she had returned to work in 1977) was about to dismiss half of its staff. Fortunately (for my studies), my mother was not among those dismissed, and this allowed me to complete my degree. My parents did everything in their power to enable me to study. Moreover, my father, despite his lack of higher education, possessed enormous culture and a passion for classical music, opera and theater, passions that I have inherited from him and that have enriched my life. He was also very fond of football, and from him I inherited that passion too, along with our unconditional support for our team, Atletico de Madrid.

III. THE WORLD IS NOT JUST MADRID

Once I had completed my degree in June 1987, the summer of that year became a crossroads. I had finished my final-year research project under the supervision of Santiago Lago (who had been my Physical Chemistry lecturer in the third year of the degree), on perturbation theories of liquids. Santiago Lago encouraged me to do two things. Firstly, to apply for a fellowship from the Spanish Ministry of Education (known as FPU) in order to carry out my doctoral thesis under his supervision at the Complutense University (even today, more than half of the doctoral theses in Spain are funded by the Spanish government rather than from research project budgets). Secondly, he encouraged me to apply for a grant to spend four months with Daan Frenkel in Amsterdam in order to learn molecular simulation and thus complement the results of a thesis that was to be theoretical in nature. Besides, the Complutense University offered the possibility of two-month summer stays at other universities with which agreements existed. In my case I was assigned a two-month visit (July and August) to the University of Bratislava in Czechoslovakia, to work on electron spin resonance. In July 1987, at the age of twenty-three, I left Spain for the first time on a long train journey to Bratislava, taking the opportunity to stop and visit every city I found along the way (Nice, Milan, Venice and Vienna). At secondary school I had studied French and was able to speak it with relative fluency. My level of English, however, was very poor (I had taken only a few one-semester courses during my time at university). In Bratislava, the foreign students were housed in a student residence. I must say that their command of English was far superior to mine and this, combined with the fact that I find it impossible to remain silent for long (as it is well known by my friends and colleagues), produced an exponential improvement in my English. I must be one of the few people (if not the only one) who learned English at breakneck speed in a non-Anglo-Saxon country, and on the other side of the Iron Curtain. Beyond the language, those two months represented an ideological shock. After the Spanish Civil War, in 1939, my paternal grandfather was imprisoned for three years and lost all his property (a shoe shop located in Carabanchel) for having defended the Spanish democratic Republic. Although the post-war years were hard for all Spaniards, they were even harder for those who had lost the war. If the Spanish military dictatorship was bad, the summer of 1987 taught me that a dictatorship of another kind was equally atrocious. I have had the good fortune to live in a democratic country (Spain) since 1978, when the constitution was approved, and I regard tolerance and democracy as unquestionable values that must be defended.

In September 1987 I took my first airplane flight (at the age of twenty-three) and flew to Amsterdam, where I lived from September to December in order to learn molecular simulation under the supervision of Daan Frenkel at the Institute for Atomic and Molecular Physics (AMOLF). Those months shaped my career. Over morning coffee I would assail him with questions about the Monte Carlo program for spherocylinders that he had given me. From him I learned, coffee after coffee, about neighbor lists and periodic boundary conditions, that it is possible to ride a bicycle even in the rain (one of my first questions to him was how to get to AMOLF when it rained), and that one may drink milk with meals. Daan Frenkel was thirty-nine years old at the time. Daan is one of the most intelligent people I have ever met. But not only that: he is also one of the most honest and generous scientists I have known. Only with the passage of time I have been able to appreciate the generosity of a person who taught me to perform simulations selflessly, without seeking anything in return. It is common in life to encounter people whose decisions tend to maximize their own personal benefit. Some even change their principles over the years, in the manner of Groucho Marx, with the curious circumstance that such changes always happen to be the ones most beneficial to themselves. Daan taught me how to simulate, but he also taught me that one of our duties as scientists is to help young people, and to do so even when it is not obvious what benefit we shall derive from that help. At the end, I believe that life is better lived with generosity than with a calculator. Our paths (Daan's and mine) were to cross again later, albeit indirectly. From that stay in Amsterdam we published a paper together.[1] One of the happiest moments of my research life, which I still remember, was when I managed to reproduce with my own code (adapted from Daan's) the simulation results for the Kihara potential previously published by Tomas Boublik and cycled home happily (in the rain) through Amsterdam at two o'clock in the morning (I have always liked to work at night). I believed then, and I still believe now, that having fun doing science is one of the greatest privileges of our profession, and as a reminder I keep on the wall of my office a printed copy of Rabindranath Tagore's poem "Playthings" (one of my mother's favorite poets), whose closing line reads: "In my frail canoe I struggle to cross the sea of desire, and forget that I too am playing a game."

IV. LET US GO BACK TO MADRID

In January 1988 I obtained an FPU fellowship to undertake my doctorate in Spain, which I carried out under the supervision of Santiago Lago (I continued to live with my parents during that period, contributing part of my income). For three years I worked on perturbation theories of liquids and on integral equations, and I also performed simulations to test the theoretical results. The potential I used was the Kihara potential, and the algorithm we proposed in 1994 to determine the minimum distance between rods[2] of different lengths is still in use in a good number of problems, not always related to statistical mechanics.

The Spanish university system was decimated after the civil war, losing its foremost scientific and intellectual figures. The year

21 October 2026 13:04:58

Published under an exclusive license by AIP Publishing

1975 marked, besides the end of the military dictatorship, the beginning of a new era. It may be said that Spain has been climbing steadily in the world scientific rankings over the past forty years. Indeed, Spain currently occupies the tenth to twelfth position worldwide in terms of scientific productivity, which is remarkable. It is often said that Spain lived a silver age of science a century ago, but in my opinion the golden age of Spanish science is the present one. The origin of this change has to do with the baby boom of the 1960s, with the massive arrival of that generation at the public university (unlike the previous generation, whose prospects of higher education had been frustrated by the poverty that followed the Spanish Civil War), and with the policies of the 1980s, when thousands of doctoral fellowships were awarded. Those doctoral fellowships included a magical gift: in each of the four years of the thesis it was possible to choose an international laboratory and to spend up to three months there, with the salary doubled during those months. I am deeply grateful (as are many other young people of my generation) to those who designed this strategy, which transformed the Spanish scientific landscape. Thanks to this unique opportunity, I worked at the Ruhr University in Bochum (Germany) for three months under the supervision of Johann Fischer. In Bochum I learned the technique of Molecular Dynamics (MD) and applied it to refrigerants[3] (and also how to play football on grass alongside a professional such as Ivo Nezbeda). In 1990 I was able to visit Cornell University to work with Keith Gubbins (working on simulations of carbon dioxide[4]). In addition, Tomas Boublik spent a sabbatical year in Madrid, which allowed me to work with him in the development of an equation of state for hard chain molecules.[5] Santiago Lago always advised me on which places to visit, and his advice proved entirely sound. I learned a great deal from being able to work during my thesis with scientists of the stature of Tomas Boublik, Johann Fischer and Keith Gubbins, and I published papers with all of them. Finally, in 1991, I defended my thesis and received the extraordinary doctoral award (this time I did apply for it myself).

In July 1988 my relationship with Mari Carmen began (we met at an adult education center in Carabanchel, the Oporto adult school, where we both worked as volunteers teaching French, English, science and other subjects). Our relationship began then and has lasted to this day, thirty-eight years later. She was a teacher of English to children aged ten and eleven in public schools in Madrid until her recent retirement. It is difficult to convey what her support has meant throughout my entire career. Her infectious cheerfulness, her constant support (taking on far more of the household work than I did), and her unconditional love have made possible everything I have achieved both as a person and as a scientist. We had two sons, Miguel and Carlos (born in 1998 and 2002 respectively) I am enormously proud of them, and I have shared with them some of the best moments of my life. We go mountain biking together (on routes of 50 km), we dance together at family celebrations, they enjoy my paellas, and we go together to the Metropolitano soccer stadium in Madrid (although I have not managed to pass on to them my passion for opera). They studied Physics (Miguel) and Computer Engineering (Carlos), and have chosen to work in the private sector. In July 2026 I had the joy of attending the wedding of the elder one, Miguel, to his wife Meghan.

V. AMHERST, MASSACHUSETTS

After completing my doctorate I obtained a Fulbright fellowship and carried out a postdoctoral stay of a year and a half at the University of Massachusetts (Amherst) under the supervision of Peter Monson. This postdoctoral stay was absolutely critical to my career. Although my postdoctoral work was initially to focus on adsorption problems (in which Peter was a highly regarded expert), on arrival I was offered the study of the phase diagram of hard dumbbells [a linear molecule formed by two hard spheres (HS) rigidly bonded at a distance L]. The office in which I was placed was full of used table tennis balls, employed (once cut and glued) to build hard dumbbells and close-packing models (and also to play table-tennis on the office desk once Peter had left the university in the evening). I agreed, albeit with a certain scepticism, to work on the project, on the condition that I would also work at least partly on adsorption problems and indeed we eventually published an interesting paper[6] on the Madden-Glandt integral equations[7] for adsorption in disordered porous media. Although I was familiar with performing simulations to obtain equations of state, I had never worked on free energy calculations. I had to read Daan Frenkel's papers on the calculation of free energies in solids (the Frenkel-Ladd method[8]) and on the calculation of the phase diagram of ellipsoids that he had published with Bela Mulder in 1985.[9] I found it amusing to be reading now the important papers written by the very person from whom I had learned to perform simulations. I soon implemented the Frenkel-Ladd method, and we calculated the phase equilibria for three reduced elongations, $L = 0.3, 0.6, 0.8$[10] and subsequently determined the length at which the plastic crystal phase disappears[11] (and even demonstrated the possibility of having three phases in equilibrium in a hard-body model, by extending the phase rule to include the potential parameters as possible thermodynamic variables[12]). These papers constituted, without me knowing it at that moment, the foundation upon which I would later build many of the subsequent contributions of my career. If Santiago Lago opened the doors for me (and I am enormously grateful to him for that), and Daan taught me how to simulate, Peter taught me the value of rigor and the importance of choosing interesting problems. With him, calculations were checked again and again, and I have tried to maintain that practice throughout my career. We may make mistakes in our papers, but there are two obligations: to check them exhaustively before submitting them, and to correct them if, once published, we discover an error. On a human level, Peter is a true gentleman: extremely generous with his time, patient with my obstinacy and kind to correct my errors. His influence on my career has been enormous, and the year and a half I spent in the United States (hard from a personal point of view, since Mari Carmen remained in Spain working) was professionally fruitful and marked a point of no return, for by then I unequivocally wanted to devote myself to a scientific career. I always have Peter in mind before submitting a paper, asking myself whether I have performed all the necessary checks and repeated all the calculations as many times as required. This has no doubt reduced my productivity, but it has been to the benefit of credibility, a virtue that in science takes a long time to earn and very little to lose.

21 October 2026 13:04:58

Published under an exclusive license by AIP Publishing

VI. MADRID AGAIN. LIFE IS A DREAM (THE GOOD TIMES): WATER AND SEEDING

In 1993 the opportunity arose to return to Spain to the place that was my academic home, the Complutense University of Madrid and with an assistant professor position. There, I started my academic career. Although there were temptations to remain in the United States, I always knew, in one way or another, that I wanted to contribute to the advance of Spanish science to the best of my ability, and to give back in some way everything that the country had invested in me. I was aware that this decision would come at a price, but I accepted it entirely. I have developed my whole career at the Complutense University, with the exception of the three years of my life that I have spent abroad. Madrid is undoubtedly my place in the world (and I have shown it enthusiastically to all who have visited me), and the Complutense is my professional home, from the age of eighteen to the present day, over the past forty-four years, I have gone there every day, first as a student and then as a professor.

Between 1993 and 1999 I worked on various problems related mainly to the equation of state of hard bodies and to polymers with my first doctoral student (Luis G. MacDowell). We published a paper in collaboration with Kurt Binder and Marcus Muller at Mainz on the critical temperature of infinitely long polymers[13] in the light of the theory that Wertheim had developed in the 1980s.[14] We extended Wertheim's theory to the study of the liquid-solid equilibrium of repulsive polymer models[15] and with Carl McBride (a postdoc in our group) in the liquid crystal formation of simple hard linear molecules.[16] Also, in the period 1997–2000, I carried out simulation studies of the restricted primitive models of electrolytes (RPM) in collaboration with Fernando Bresme and with another member of the department, Jose Luis F. Abascal, predicting the existence of a new phase that was later found in experiments with colloidal particles.[17,18] In 1997, having obtained an associate professor position at the Complutense University, I spent the summer once again in Amherst with Peter Monson (this time with Mari Carmen), and we decided to work on a primitive model of water developed by Kolafa and Nezbeda.[19] During that summer I gathered a folder of papers on water, and we calculated the phase diagram of that model using molecular simulation, publishing it in the Journal of Chemical Physics.[20] That summer was the seed of my studies on water, for until 1998 I had not carried out any work related to it.

In 2002, Eduardo Sanz (my second doctoral student) started the PhD under my supervision. The planned topic for his thesis was solubility of amino acids in water determined through computer simulation. Before starting, it was necessary to choose a water model, and we decided to take as the basis for our study one whose melting temperature was reasonable. After consulting Jose Luis F. Abascal, we decided that SPC/E[21] might be a reasonable choice. Jose Luis and I decided to collaborate on that objective, in what was the beginning of a long collaboration that has continued to the present day. Looking back, that collaboration, and the decision to undertake the calculation of the melting point of a realistic water model, changed my career. Using the Monte Carlo code that I had been developing over the years, Eduardo and I incorporated the Einstein crystal method for water, and determined that the melting temperature of ice I_h at 1 bar for the SPC/E model was about 215 K, far from the experimental value (273.15 K). We soon realized how much interest such calculations might hold. On the one hand, water models were being used by a very wide community and their melting points were unknown, so their determination would be of great utility. On the other hand, the phase diagram had not been calculated for any realistic water model (although I had done so with Peter Monson for a primitive model of water in the past[20]). We therefore decided to calculate the melting point of a good number of water models modifying the original Gibbs-Duhem methodology of Kofke[22] to incorporate Hamiltonian changes.[23] We then decided to tackle a more ambitious goal: the calculation of the phase diagram of a water model. Luis G. MacDowell joined the effort, helping us to generate a large number of ice configurations, and after two years of work we obtained the final result. It was somewhat disheartening, since the SPC/E model did not reproduce the phase diagram of water. Having invested two years of our academic lives without publishing a single result, the final outcome was disappointing. At a meeting in July 2003, it was then decided to study a second model, since we estimated that, once the whole methodology had been established, it was worth studying a second water model as this would take only four months. After some hesitation between TIP5P[24] and TIP4P,[25] TIP4P was finally chosen, largely because it was cheaper from a computational point of view. Eduardo Sanz then went off for three months to work with Daan Frenkel (the possibility of visiting other laboratories during the PhD still existed at the time), and in the autumn of 2003 Eduardo, Jose Luis and I tackled with enthusiasm the calculation of the phase diagram of the TIP4P model. Neither Eduardo, nor Jose Luis, nor I have ever, throughout our careers and to this day, given up running our own simulations. At night we would launch the simulations together, with the excitement of seeing how the phase diagram bore a fairly close resemblance to the experimental one. If science is a game, we were playing it and we were having fun. Eduardo presented our first diagram of water in December 2003 in a seminar in Amsterdam at AMOLF having Daan Frenkel in the audience. Finally we prepared a paper in January 2004 and submitted it to Physical Review Letters, with the phase diagrams of the SPC/E and TIP4P models.[26] Despite the rejection of one of the referees (who maintained that he/she would accept the paper only if we presented the phase diagram for a model of water that reproduced the experimental phase diagram), the paper was finally accepted thanks to the more positive view of the other three reviewers.

We soon realized that the melting point of TIP4P, 230 K, although better than that of SPC/E, was still far from the experimental value. The calculation of the temperature of maximum density (TMD) was extremely costly in the late 1990s and was known only for SPC/E[27] and TIP5P.[24] We therefore decided, in 2003 and 2004, to calculate the TMD of SPC, SPC/E and TIP4P. We soon saw that for both models the difference between the TMD and the melting point was about 25 K. This meant that in three-site models (SPC, SPC/E, TIP3P[25]) and in four-site models (TIP4P) it was impossible to reproduce both properties simultaneously.[28] Since TIP4P gave a better prediction of the phase diagram, we decided to develop one model that would reproduce the melting point of ice I_h, namely TIP4P/ICE,[29] and another that would reproduce the value of the TMD, namely TIP4P/2005.[30] Both models were published in 2005 and also the paper on the melting points of water models, thus confirming that 2005 was indeed an important year of my career where besides I was promoted to full professor. What had begun as an adventure in 2002 finally crystallized after three years of hard work.

21 October 2026 13:04:58

Published under an exclusive license by AIP Publishing

In our calculations we already incorporated Ewald sums instead of using a truncation of the Coulombic interaction, because we anticipated that the future of simulation would rely on Ewald sums, and we used the concept of polarization energy in the calculation of the enthalpy of vaporization as proposed by Berendsen *et al.*[21] (in such a way that the model reproduced the experimental enthalpy of vaporization only once that correction was included). In the midst of the development of these models, in May 2004 the paper on the TIP4P-Ew model was published, which shared the philosophy of the TIP4P/2005 model we were developing, since it reproduced the experimental density maximum of water and used Ewald sums. Very often in science, ideas are in the air, and arise spontaneously and simultaneously in different places at once. TIP4P-Ew[31] is undoubtedly an excellent model and shares the spirit and philosophy of our TIP4P/2005. The main difference lay in the fact that the position of the negative charge of the original TIP4P model was moved toward the oxygen in the TIP4P-Ew model and away from it in the TIP4P/2005 model. Although apparently this seems to be a small change, it changes the value of the quadrupole moment of the model[32] and that provokes some differences in the predictions of certain properties (i.e., melting temperature, critical temperature, etc.). We therefore decided to publish the two models, TIP4P/ICE[29] and TIP4P/2005,[30] separately, since we thought they might have different users (as has indeed been the case). The choice of the TIP4P geometry (first proposed by Bernal and Fowler[33] in the Journal of Chemical Physics in 1933 and further developed by Jorgensen *et al.*[25]) instead of the three-site geometry or the five-site TIP5P geometry (which exaggerates the tetrahedral character of water), the use of Ewald sums, the conceptual incorporation of Berendsen's correction to the enthalpy of vaporization,[21] and the importance of reproducing the density maximum of water (implicit in the development of the TIP5P model[24]) led to the TIP4P/2005 model, and this philosophy is shared by the TIP4P-Ew model.[31] Over the past twenty years, most non-polarisable models (being Molinero's mW model[34] an important exception) have been based on this design, and models such as OPC,[35] TIP4P/FB,[36] TIP4P-ϵ[37] and TIP4P-D[38] share this pattern. I am convinced that if Berendsen and Jorgensen had met at a workshop around 2003 they would have developed this approach.

Eduardo Sanz defended his PhD in January 2006. We never computed the solubility of amino acids in water (science is never a bureaucratic work as sometimes discoveries drive your research rather than the opposite). The period 2006–2013 was devoted to the calculation of the properties of the two water models TIP4P/2005 and TIP4P/ICE. We began to make extensive use of molecular dynamics and, in particular, of GROMACS[39] (from 2004 onwards, when a first version of the code was installed on our machines). We evaluated the critical temperature in collaboration with Ivo Nezbeda,[40] the degree of association (from simulation and from theory) in collaboration with the group of George Jackson,[41] the surface tension,[42] the viscosity,[43] the diffusion coefficients, and recalculated the phase diagram[44] of TIP4P/2005 (to account for the fact that the partial proton disorder of ice III from experiment was found to be different to that of the model[45]). Overall the results of the TIP4P/2005 model far exceeded our expectations. It is common at conferences to hear it said that, since no water model is perfect, all of them are similar. Motivated by this claim, in 2009 we performed a preliminary qualitative comparison of the performance of different water models.[46] Later in 2011 we proposed a more quantitative test[47] (the Vega-Abascal test) which may continue to be very useful in the future, in order to discriminate the ability of water models (including machine learning models) to describe the properties of water. Always concerned with rigor, we decided to recalculate the melting temperature (which we had obtained through free energy calculations) using the direct coexistence method, which had been proposed many years earlier by Ladd and Woodcock[48] but whose practical value for the calculation of the melting temperatures of ices had not previously been clearly demonstrated. We then published a paper showing that the melting points obtained from both types of calculation were consistent,[49] and we contributed to showing that the technique was powerful, fast and efficient. Slowly, our group began to abandon the Monte Carlo method and the original code in favor of MD calculations with GROMACS. In 2004 Poland joined the European Union, and my friend (we shared an office in Bochum in 1989) Stefan Sokolowski (who unfortunately passed away recently) applied for a European project. Thanks to this project I spent the summer of 2006 in Lublin (Poland) with my family (one of the best summers of my life) and was able to work in collaboration with Andrzej Patrykiejew and my PhD student Maria M. Conde on two interesting projects using GROMACS. One on the determination of the thickness of the liquid layer at the free surface of ice,[50] and another on a new method to estimate the melting temperature of water models (including TIP4P/2005 and TIP4P/ICE) by taking advantage of the absence of super-heating of ice I_h in the presence of a free surface.[51] The melting point obtained by this method[51] was again consistent with that obtained from free energy calculations and from the direct coexistence method.

We also began the study of the properties of supercooled water using the TIP4P/2005 model,[52] determining the Widom line and estimating the location of the second critical point.[53] The possible existence of a second critical point in water was proposed by Poole, Essmann, Sciortino and Stanley in 1992.[54] Although Jose Luis and I were initially sceptical about the existence of such a second critical point, the results of the TIP4P/2005 model gradually led us to become firm supporters of the idea.[53] Indeed, in 2020, Zerze, Sciortino and Debenedetti demonstrated its existence for the TIP4P/2005 and TIP4P/ICE models.[55] At a memorable conference on water, held in Stockholm in 2014 (organized by Lars G.M. Pettersson and Anders Nilsson), several review articles on water were prepared, and one of them, "Water: A Tale of Two Liquids," lead by Paola Gallo and Lars Pettersson sets out the viewpoint to which we subscribe.[56]

In the period 2008–2012 I had two excellent doctoral students, Maria M. Conde and Juan Luis Aragones. In both theses the existence of two new solid phases of water was predicted, using simulations with the TIP4P/2005 model. In María's thesis it was discovered (in collaboration with Ben Slater and Gareth Tribello in UCL in London) that the sII hydrate structure was stable at negative pressures (similar results were found simultaneously in Molinero's group[57]) even in the absence of guest molecules,[58] and this phase (ice XVI) was found experimentally by Kuhs and co-workers in 2014.[59] In Juan Luis' thesis, on the other hand, the existence of a plastic crystal phase in the region of ice VII was predicted,[60,61] (found also independently[62] by the group of Hideki Tanaka and Kenichiro Koga

21 October 2026 13:04:58

Published under an exclusive license by AIP Publishing

in Japan) and it was discovered experimentally by Livia Bove and coworkers in 2025.[63] I have always believed that the aim of simulation does not lie in reproducing experimental behavior exactly, but rather in helping to interpret and understand it and, in the best of cases, in suggesting new experiments based on computational predictions. Caution is always necessary in any case, because potential models are not, and never will be, experimental reality. In María's thesis we also proposed a molecular dynamics method to determine the three-phase line T_3 (hydrate-water-gas), which is still widely used today,[64] and we showed that reproducing the T_3 line in good agreement with experiment requires a model with a good melting point for ice I_h.[65] Maybe for this reason the TIP4P/ICE model has gained popularity in the community simulating hydrates. That reproducing melting temperatures is a good idea when developing force fields was further shown in the development of a force field for methanol[66] (OPLS/2016) in collaboration with Diego Gonzalez Salgado from the University of Vigo. The calculation of the dielectric constant for the solid phases of water (ices) is far from trivial (due to the presence of proton disorder) and for this reason is rarely calculated (in contrast with the dielectric constant of liquid water which is obtained trivially). For this reason Juan Luis, Luis and I decided to calculate the dielectric constant of ices,[45] showing that many models that describe the dielectric constant of liquid water do not describe that of ices, and suggesting the idea (on which I have insisted in several publications) that the charges used in empirical models describe only the potential energy surface (PES) and not the dipole moment surface (DMS).[67]

From the year 2000 I began a collaboration with the University of Huelva. During my stay at Cornell in 1990 I met Enrique de Miguel, from the University of Seville. We soon became friends, in a friendship that endures to this day. In the 1990s we collaborated on several publications implementing Gibbs ensemble simulations[68] to study the effect of quadrupoles and dipoles on the critical point of linear molecules, in collaboration with Santiago Lago and Luis F. Rull.[69] From the year 2000 onwards we decided to collaborate more closely and to apply for research projects jointly. As a result of these collaborations, I began to visit the University of Huelva regularly (where Enrique de Miguel had settled), and I eventually fell in love with a small town in that province, Moguer, where I have spent my summers for the past thirty years (riding the bicycle with my friends from Moguer in the morning and going to the beach in the late afternoon). Through Enrique de Miguel first, and subsequently with Felipe Blas, I have maintained scientific and personal contact with this university, and both are today good friends with whom I have collaborated on a good number of projects. With Enrique de Miguel we determined the phase diagram of the Gay-Berne model,[70] and implemented the direct coexistence method for HS.[71] We also calculated the surface tension of water[42] using both MC and the test-area method[72] and MD simulations. This was crucial because for a year the results of the two methodologies did not agree, and at the end it turned out that the Monte Carlo results from our code and the test-area results were correct, whereas those of GROMACS were incorrect owing to a bug in the calculation of the pressure tensor in GROMACS, which was corrected in a new version released in 2006. Enrique de Miguel has been all along his career an extremely careful scientist (also when changing the research topic from statistical mechanics to astronomy in 2010) and suggested not to publish our results until both methods agreed. Even though our results disagreed with those published a few months earlier by another group who was using LAMMPS,[73] we were confident that our results were correct, and time has proved us right. Using GROMACS or LAMMPS is very useful, but it does not absolve the user of responsibility: one must verify by every possible means that one's results are correct. The lessons learned during my postdoctoral stay with Peter Monson were tremendously useful. Even now, nothing gives me greater pleasure than to know that someone has reproduced the numbers I published twenty years ago, and I continue to express my admiration for the great simulators of the 1960s and 1970s – Hoover, Ree, Alder, Verlet, Rahman, Stillinger, Hansen – whose results I have reproduced every time I have compared against them. A solid result withstands the passage of time better than passing fashions.

With Felipe Blas and Amparo Galindo we extended Wertheim's theory to the liquid-solid equilibrium of flexible Lennard-Jones chains,[74] and with Felipe Blas I have been collaborating continuously on hydrate simulations over the past ten years.[75] On one of my visits to Huelva I gave a seminar. At the end of the lecture I encouraged some of those present (members of the Physics department) to attempt to develop a curriculum for a degree in Physics at Huelva. After many years of effort, that degree finally became a reality in the 2025–2026 academic year. If the Complutense University has been my home, the University of Huelva has been my second home, for I have published a total of twenty papers in collaboration with Enrique de Miguel and Felipe Blas, professors at that university. To be proposed recently as honorary doctor of this University has been for me a joy and an honor.

For three years (2007–2010), Eva G. Noya carried out a postdoctoral stay with me. We evaluated the phase diagram of patchy models in collaboration with John P. K. Doye and Ard A. Louis.[76,77] In addition, we slightly modified the Einstein crystal method[8] of Frenkel and Ladd that fixed the center of mass of the system so as to fix the position of one of the particles of the system and the new method was denoted as the Einstein Molecule method.[75] We also demonstrated how the direct coexistence method reproduces the coexistence pressure of hard spheres.[71] Together with the British postdoctoral researcher Carl McBride (who ultimately stayed on to live in Spain), we worked on the incorporation of nuclear quantum effects into rigid water models. We developed the propagator (a task that was far from straightforward[78]), proposed a rigid TIP4P-type model incorporating nuclear quantum effects, TIP4PQ/2005,[79] demonstrated that the heat capacity of water is strongly dominated by nuclear quantum effects,[80] and calculated (how could we not) a phase diagram for the rigid non-polarisable quantum model.[81] Without the collaboration of Luis Sese and Rafael Merino we could not have carried out these studies. Eva now holds an independent position at the CSIC and we have keep collaborating along these years. She is a modest, hard worker and absolutely bright researcher.

The year 2012 brought the return of Eduardo Sanz after five years in the Netherlands and the United Kingdom, and the incorporation of Chantal Valeriani into the group as a postdoctoral researcher. Eduardo and Chantal had met in 2003 during the three months Eduardo spent in the Netherlands with Daan Frenkel during his doctorate, where they began to work together on nucleation problems.[82] Both brought the field of nucleation into the group.

21 October 2026 13:04:58

Published under an exclusive license by AIP Publishing

It was the perfect moment to tackle the study of nucleation problems using the potential models developed in Madrid, TIP4P/2005 and TIP4P/Ice. After some unsuccessful attempts with the umbrella sampling technique (probably owing to an incorrect choice of order parameter[83]), the idea of using a simple technique to evaluate nucleation rates gradually emerged. We denoted the technique as "seeding," and it was applied first to studies of ice,[84,85] and later to simple hard-sphere and Lennard-Jones models.[86] At the same time we developed the mold integration technique[87,88] (to evaluate the solid-liquid interfacial energy of the planar interface) and the lattice mold[89,90] technique to evaluate nucleation rates. During this time Jorge Reñe carried out his thesis in our group, under the joint supervision of Eduardo Sanz and myself, and contributed decisively, through his great capacity for hard work and his creativity, to the achievement of important results. The period 2012–2017 was one of great creative intensity, thanks to the impetus of Eduardo and Chantal, who brought great enthusiasm, boundless energy (who can stop Chantal's energy and organizational power?!) and remarkable creativity. This line of work on nucleation is undoubtedly their responsibility. It was a pleasure to take part in this second golden age of the group (2012–2016), which linked up almost seamlessly with the first (2004–2010). At the end of the day, Frenkel's papers were always very much present in our phase diagram studies and now in our nucleation studies. One never knows what the person one taught to simulate in three months may end up doing.

In March 2014, during the ACS Meeting in Dallas, Marsha Lester (the Editor in Chief at that time) invited me to become Associate Editor of the Journal of Chemical Physics. Many of the best papers I had read throughout my career had been published in JCP, and for me it was an honor to be part of this journal, so it was impossible for me to decline the invitation. I humbly believe that some of my best papers have also been published in this journal. In these times in which science has in many cases become a marketing exercise, I personally feel a certain sympathy for what I would call Community Journals: journals with a long tradition, which have gradually forged a community and in which important results have historically been published. In any case, we should not forget that in at the end the quality of a paper lies in the paper itself and not in the place where it is published. Being part of this journal (founded in 1933) is a source of great pride to me, all the more so if one considers that the first paper published in this journal from Spain appeared only in the late 1960s, and that the first paper submitted from my department to this journal was in the 1970s. I believe this illustrates how effective Spanish science policy has been since the country returned to the path of democracy in 1978.

In September 2014, Ana Laura Benavides (from the University of Guanajuato, Mexico) visited me for a sabbatical year (which at the end became two). Panagiotopoulos and co-workers had just published a paper[91] (and there was another of the group of Nezbeda[92]) questioning the value of the solubility of a NaCl model in water that we had recently published.[93] In Eduardo's thesis we never did get around to calculating the solubility of amino acids in water (our water studies became the main topic). However, at the end of his thesis we calculated the solubility of a NaCl model in water,[94] and in 2012 we continued to develop those calculations.[93] Using GROMACS (which allowed longer runs) and to the hard and patient work of Ana Laura we recalculated the solubility in 2016 by means of free energy calculations and obtained a value in agreement with those of Panagiotopoulos and Nezbeda.[95] This value (3.7 m) of the solubility of NaCl Joung-Cheatham[96] force field in SPC/E water is currently the benchmark value for testing new methodologies for determining solubility. This value was also confirmed by direct coexistence calculations by Jorge Reñe *et al.*[97] in collaboration with the Princeton group of Panagiotopoulos and Debenedetti. Once this difficulty had been overcome, Ana Laura and I decided to develop a model of electrolytes for the TIP4P/2005 model, in collaboration with Jose Luis F. Abascal.[98] After several attempts with unit-charge models, we were not satisfied with the results, and we decided to adopt scaled charges (an idea pioneered by Leontyev and Stuchebrukhov,[99] and embraced with youthful enthusiasm by Pavel Jungwirth, who tragically passed away in July 2026, just two months after a conference held in Prague in May 2026 to celebrate his sixtieth birthday). To Pavel we owe his committed advocacy of the usefulness of scaled charges for electrolytes.[100] One advantage of using scaled charges is that we were able to recover the experimental coefficient of the Debye-Hückel law when using the TIP4P/2005 model of water.[101] In March 2017 we submitted the paper with the corresponding model (for NaCl), named Madrid.[98] A few days after submitting this paper my life would be turned upside down.

VII. LIFE IS A DREAM: THE DIFFICULT TIMES

In February 2017, my father underwent emergency surgery and was diagnosed with advanced colon cancer. His life expectancy was one year. For this reason I requested my sabbatical year in order to care for him during the course of his chemotherapy, and so that he could live with my family (and with the family of my sister Myriam) during that time. At a visit to the oncologist of my father in March 2017, she recommended that I have a test for colon cancer and for prostate cancer. I did not pay much attention to the recommendation, but my father's insistence led me finally to agree to a blood test. To my surprise, the analysis (PSA level 27.5) and the subsequent biopsy confirmed an advanced prostate cancer (T3b) of a very aggressive tumor. After some further tests, fortunately it had not yet reached the bones, which meant that a treatment could be attempted (I still remember the grave expression of the oncologist as she looked at the bone scintigraphy to determine whether the cancer had affected the bones, and her smile as she looked up at me). The sabbatical year became eighteen months of oncological treatment, including surgery, radiotherapy and hormone therapy. During that time I did not go in to work at my university, although the members of my group visited me regularly and we discussed science at my house. During that period I limited myself to finish the research already under way, to continuing my work as an editor of JCP (I was on the point of giving it up, although my wife wisely encouraged me not to, since the only happy moment of the day, when my mind was able to escape, was the time I spent working as an editor), and to reading dozens of papers on prostate cancer (to choose among the options offered by my doctors). Thanks to the good decisions of my doctors (Dr. Mario Alvarez and Dr. Aurora Rodriguez), that literally saved my life, I returned to the University in September 2018 and to this day I have passed all the relevant medical check-ups. My life is certainly divided into two halves, and 2017 (when I was fifty-three years old) marks the boundary.

21 October 2026 13:04:58

Published under an exclusive license by AIP Publishing

I learned many things during the year and a half of treatment. The first lesson is how important the love and affection of those closest to us is. Mari Carmen sustained my family, and my depressed spirits, during that time. I shall never be able to thank her enough. I am grateful to have found such a good and cheerful person on my path, because neither professionally nor personally could I have come this far without her. My mother was another great source of support, and remains so to this day, for I speak with her every day and consult her and ask her advice on countless matters; nor could I have achieved anything without her and without the sacrifice of my parents. She had to cope with her husband's cancer and her son's at the same time. The second lesson is that we are not as important as we believe ourselves to be, and life goes on smoothly in our institutes and universities in our absence as well. My scientific family (Eduardo, Jose Luis, Maria, Eva, Jorge and Chantal) were an immense support during that difficult period. I am tremendously grateful to them for their visits and for their support. The third lesson is that chance and caprice govern our lives (even if our will may slightly shape their course). My father's cancer and a casual advice to me from his oncologist had changed my destiny. My father (who finally passed away in 2021) had, in a sense, given me life twice. I was able to verify how capricious chance can be even more clearly when, as my medical treatment was drawing to a close, I traveled to Iceland in June 2018 with my younger son Carlos to celebrate the end of the treatment, and on the return flight to Madrid from Reykjavík we experienced an emergency landing in Birmingham. Since then I have accepted that life flows on, and that one must enjoy every moment as if it were the last (since 2018 I have held season tickets to the opera in Madrid, to the theater and to the football). If one reads carefully the acknowledgments of some of my papers, one will find thanks to the doctors who treated me and to the Virgen del Rocío, who represents the caprices of destiny (I do not quite recall now, but I believe that at some point I may even have thanked a manager of my football team).

VIII. THE EXTRA TIME: EACH DAY CAN BE THE LAST

In September 2018 I returned to the University, and began supervising the thesis of Pablo Montero de Hijes (being Eduardo Sanz the co-advisor). His thesis brought an enormous dose of positive energy for me. Once again I felt the curiosity and the passion of doing research. During this time we studied the variation of the interfacial energy with the radius of curvature.[102] The methodology proposed by Binder and co-workers[103] showed that it was possible to have spherical clusters in equilibrium in the NVT ensemble.[104] In collaboration with Kaihang Shi, Erik Santiso, Keith Gubbins, Eva G. Noya and Eduardo Sanz we showed that the pressure inside a solid cluster of hard spheres is lower than the external pressure of the fluid phase, in clear contradiction with the Young-Laplace equation.[105] Using arguments already outlined by Gibbs,[106,107] we resolved this apparent paradox by showing that it is the thermodynamic pressure (and not the mechanical one) that must be used in the Young-Laplace equation[105] and further work on this problem was done in collaboration with Laura Filion and Frank Smallenburg.[108] The liquid-solid interfacial energy (both for the planar and for the curved interface) has been a topic of interest in our group.[87] In the thesis of Pablo Rosales (also from that period and co-supervised by Eduardo Sanz and Chantal Valeriani) it was shown that clusters that are stable at fluid-fluid interfaces in the NVT ensemble become critical in the NpT ensemble.[109] In Pablo Montero's thesis it was shown that the same occurs for solid-fluid interfaces.[104] As a consequence of this, the seeding technique (originally conceived in the NpT ensemble) was extended to the NVT ensemble. As the free energy barrier obtained via seeding depends significantly on the choice of the order parameter (whereas the dependence is much smaller when using umbrella sampling) we combined both techniques, and proposed the variational umbrella-seeding method[110] in collaboration with Willem Gispen and Marjolein Dijkstra. In collaboration with Daan Frenkel we compared the homogeneous and heterogeneous nucleation rates for hard spheres and suggested a possible hypothesis to explain the discrepancy between experiments and simulations for the observed nucleation rates in this system[111] and also determined with Jorge Reñe and Rosana Collepardo-Guevara via MD the vapor-liquid equilibria of patchy models of colloidal particles.[112] Finally in 2025 in collaboration with leading experts in the field, we published a review setting out our view of the current state of the solid-liquid interfacial energy.[113]

In September 2018, Valentino Bianco joined us as a postdoctoral researcher, with whom we worked on the study of ice nucleation at negative pressures.[114] Our interest in the behavior of water at negative pressure continued in the following years and Pablo Montero de Hijes in collaboration with Cristoph Dellago found the existence of a minimum in the value of the interfacial energy of the planar ice I_h-water interface at negative pressures.[115] Also in 2018, Ivan M. Zeron joined our group as a postdoctoral researcher for the study of electrolytes. Already in 2017 we had proposed a model of NaCl in water (TIP4P/2005) with scaled charges.[98] In 2019 we extended this concept to many other ions (mainly the most abundant ions in seawater) and published a new force field for electrolytes in water described by the TIP4P/2005 model, named Madrid-2019.[116] The name is not very original, but given my strong connection with this city it seemed to me a fitting tribute. The model can be used to describe the properties of seawater,[117] and in the thesis of Samuel Blázquez (co-supervised by Maria M. Conde who is now full professor at UPM) it was extended to many more ions,[118] to the TIP4P/ICE water model,[119] and to values of the charge other than 0.85 (the original value).[120] The Madrid-2019 model of electrolytes in water has continued to grow, extending to many other ions (nitrates,[121,122] perchlorates,[123] acids, bases[124,125]) in collaboration with Victor M. Trejos (University UAM-Izt Mexico), Paola Gallo (University of Roma Tre), Francisco Gamez (Universidad Complutense de Madrid) and Othonas A. Moultos and Thijs J. H. Vlugt (TU Delft, Netherlands). It is obvious that such a simple model cannot reproduce all the properties of electrolytes in water, but it is interesting to explore the benefits and improvements brought by the scaling of charges (common in the ionic liquids community) in the description of electrolyte solutions. In collaboration with Othonas A. Moultos and Thijs J. H. Vlugt we showed that the use of scaled charges for the description of the PES and of unscaled charges for the DMS can reproduce the electrical conductivity of certain electrolyte solutions.[126] During these years we proposed the TMD as an important target property for fitting potential parameters[127] (in collaboration with experimental measurements carried out by Jacobo Troncoso), the determination of the freezing point depression of

21 October 2026 13:04:58

Published under an exclusive license by AIP Publishing

electrolytes[128] (in the thesis of Cintia P. Lamas), and the relationship between the Jones-Dole dynamic coefficient B and the energetic changes in water[129] (in the thesis of Lucia F. Sedano, co-supervised by Eva G. Noya, and in collaboration with Luis Carlos Pardo and Gustavo Madrigal in Barcelona).

In the period 2020–2025, a close collaboration with the group of Felipe J. Blas (University of Huelva), together with the help of Joanna Grabowska, a professor at the University of Gdansk who spent a year in our group (during which she learned both to simulate hydrates and following my advice also learned to swim), has enabled us to deepen our study of hydrates, both as regards new routes for determining the three-phase line T_3 (the solubility route[130,131]) and as regards the application of seeding to estimate nucleation rates in hydrates, in both homogeneous[132] and heterogeneous nucleation.[133] Hydrates have remained a topic of interest in our group since 2010 when we started during the thesis of Maria M. Conde and it has been the main reason for a nice collaboration initiated in 2015 with the group of Felipe in the University of Huelva.[75,134]

Looking back, my interests have oscillated between simple models of a physical character (hard spheres, hard dumbbells, the restricted primitive model, Lennard-Jones) and more complex systems of chemical interest such as water, electrolytes and hydrates. The determination of the phase diagram was always of the greatest interest to me, in both simple and complex systems. In 2008 we wrote a review describing the methodology we have used throughout all these years for the determination of phase diagrams.[71] That methodology could in principle also be applied to polarisable models, or to potentials obtained from *ab initio* calculations via machine learning.

IX. WE ARE NOT ISOLATED PARTICLES

I have supervised ten theses (not that many), but I have devoted all my attention and interest to them. I have never regarded doctoral students as a means but always as an end. It fills me with pride that three of them (Eduardo Sanz, Luis G. MacDowell, Maria M. Conde) already hold Full Professor positions in Spain, and I am confident that there will soon be more on this list. All of them have received from my hand, on completing their doctorate, the book written by Santiago Ramon y Cajal, "Advice for a Young Investigator" (Los tonicos de la voluntad: reglas y consejos sobre la investigacion cientifica). Spain has only two Nobel Prizes in science, but Cajal is the only one who obtained it for research carried out in Spain. Perhaps what the gift concealed was the wish (or the dream) that some of them, or someone else, might achieve it once again. We already have as many football World Cups as Nobel Prizes in science. Moreover, for reasons unknown to me, this book was available at my parents' home (one of those things that come from the Virgen del Rocío). It also fills me with pride to have helped a good number of women along their doctoral and postdoctoral paths (Lucia F. Sedano, Maria M. Conde, Cintia P. Lamas, Eva G. Noya, Chantal Valeriani, Joanna Grabowska). Women have undoubtedly had a far more difficult path in research, and I believe we must continue to fight for their inclusion.

Besides the people I have already mentioned explicitly, I have had the immense good fortune to collaborate (through common publications), or to cross paths at conferences, with a long list of extraordinary scientists (I apologize if I have omitted anyone), to whom I should like to express my gratitude for the good times we have shared at conferences and/or in our joint publications (some of the persons on the list, sadly, are no longer with us):

Jesus Algaba, Jose Manuel Miguez, Cristobal Romero-Guzman, Paula Gomez-Alvarez, Elvira M. del Rio, Ignacio S. Burgos, Jorge Ramirez, Andres R. Tejedor, Malgorzata Borowko, Erik Lascaris, Jonas A. Sellberg, Austen Angell, Charusita Chakravarty, Hajime Tanaka, Harry E. Stanley, Frederic Caupin, Thomas Loerting, Mikhail A. Anisimov, John Russo, Limei Xu, Katrin Amann-Winkel, Parsa Habibi, Poulumi Dey, Husamettin Mert Polat, Marjolein de Jager, Paolo la Francesca, Manuel M. Piñeiro, Jose Ramon Solana, Julio Largo, Maria Jesus Maeso, Jose Maria Labaig, Alejandro Gil-Villegas, Fernando del Río, Guadalupe Jimenez-Serratos, Orest Pizio, Mario Cruz-Sanchez, Ard A. Louis, Andrew J. Haslam, Gary Clark, Erich A. Muller, Jadran Vrabec, Rolf Lustig, Bertold Saager, Juan J. Freire, Antonio Lopez-Rodriguez, Briesta Gonzalez, Guiomar D. Soria, Miguel Fuentes-Cabrera, Jonathan B. Boreyko, Charles Patrick Collier, Baron Peters, Nils E. R. Zimmermann, William R. Smith, Jose Antonio Cobos, Ruth Caballero-Bernal, Carolina Navarro, Alberto Zaragoza, Regina Ramos, Marcos de Lucas, Paz Padilla, Xavier Cottin, Eleanor P.A. Paras, Robert D. Kaminsky, Anthony-Malanoski, Andrij Trokhymchuk, Alex Reinhardt, Francesco Paesani, Victor Cruces Chamorro, Miguel A. Portillo, Helena L. Pi, Nicodemo Di Pasquale, Stephen R. Yeandel, Ruslan L. Davidchack, Colin L. Freeman, John H. Harding, Brian Laird, Lorenzo Rovigatti, Benito Garzon, Marcelo A. Carignano, David Quigley, Bart Vorselaars, Jorn Ilja Siepmann, Jean-Philippe Torre, Pablo Sampedro, Jeffrey Young, Ahmadreza Rahbari, Anatol Malijevsky, Patrick J Merkling, Sofia Calero, Hugh Docherty, Laura Jimenez Bonales, Mauro Rovere, Vladimir Jelle Lagerweij, German Perez-Sanchez, Charlie R. Wand, Pablo Llombart, Ian Bourg, Hannes Jonsson, Amrita Goswami, Miguel Angel Gonzalez, Sri Sastry, Kenichiro Koga, Hideki Tanaka, David Carrasco-Busturia, Pavel Jungwirth, Valeria Molinero and Peter Bolhuis.

On a local basis I would like to thank my colleagues in Statistical Mechanics in Madrid, Eduardo Enciso, Noe G. Almarza, Manuel Lombardero (the grandfather of the statistical mechanics at UCM), Enrique Lomba, Pedro Tarazona and in Spain Claudio Cerdeiriña, Elvira Guardia, David Reguera, Josep Bonet Avalos, Jose Manuel Romero Enrique, Alejandro Cuetos, Luis Rull, Giancarlo Franzese and Lourdes F. Vega and to the very nice community doing research on water, where the seeding method (applied to humans) of Sotiris Xantheas, Paola Gallo, Livia Bove, Fabio Bruni, Francesco Sciortino (the man with the special glasses who saw a second critical point in water[54]), Anders Nilsson (the man who saw evidence of it in the laboratory[135]) and Lars G. M. Pettersson worked very well shaping up a nice community. I shared many good moments during my academic life at the department of Physical Chemistry at UCM with many good colleagues (with some of them I also published some papers together) but I would like to mention specially to Valentin G. Baonza, Elena Junquera, Enrique Verdasco, Javier Aoiz, Antonio Rey, Carlos Menduiña, Francisco Ortega, Ramon G. Rubio, Andres Guerrero, Ana Rubio, Emilio Aicart, Alfredo Lainez, Concha Pando, Jesus Santamaria, Jose Antonio R. Cheda, Javier

21 October 2026 13:04:58

Published under an exclusive license by AIP Publishing

Nuñez, Gloria Tardajos, Mercedes Taravillo, Jose Tortajada, Mateo Diaz-Peña (the leader responsible of the growth of the Department), Francisco Monroy, and Ignacio Sola. On the other hand I enjoyed working together with the editorial staff and a long list of Associate Editors of JCP during the last twelve years with special thanks to David Manolopoulos, Francesco Sciortino, John Straub, Angelos Michaelides, Jim L. Skinner, Patricia Thiel, Mark Ediger, and the two Editors in Chief Marsha Lester and Tim Lian.

Among all the many collaborators I have had, I should like to single out two of them. The first is Jose Luis F. Abascal (who retired in December 2021). With Jose Luis I have shared a good number of scientific adventures (the RPM, water models, phase diagrams, supercooled water and electrolytes). With him I also shared lunch every day for the past thirty years, until his retirement. Modest by nature, Jose Luis is an excellent person and an extraordinary scientist. He and I have proved complementary as scientists. Meticulous to the utmost, intelligent, and a scientist who has always felt that doing research (rather than administration, traveling, and so forth) was the most enjoyable part of the job. I do not recall a single argument between us over these thirty years. I believe that having him as a colleague and friend in the department has been a stroke of good fortune for me, and that our careers could not be explained without our collaboration. Jose Luis, thank you for everything. You are missed now that you have retired. The second is Eduardo Sanz. A doctoral student at first, but subsequently a collaborator and friend over more than twenty-five years. Eduardo possesses great creativity and intelligence, an excellent sense of humor, and great scientific honesty. He was the one who carried out most of the initial calculations on water and the development of the TIP4P/Ice model. Moreover, Eduardo, together with Chantal Valeriani, are the principal architects of the seeding technique that we developed in the group ten years ago. With Eduardo I have spent extraordinary times: doing research, drinking, dancing on a boat, enjoying Atletico's matches, cycling our favorite route (Hoya de San Blas) and laughing. With Jose Luis and Eduardo I would go to the ends of the Earth: my heartfelt thanks to them both. They are the two people with whom I have published most papers. Both are tremendously brilliant and modest people, and they probably deserve a large share of the credit for everything we have achieved over these years. Doing research with them has been fun and a privilege. I believe that scientific collaboration, if one finds good traveling companions, brings enormous satisfaction. I have had the privilege of working with many exceptional PhD students and postdocs, with whom I have shared the joy of discovery. I am deeply indebted to all of them.

X. LIFE IS A DREAM: FIND YOUR PATH

A final reflection on scientific research. There are researchers who have large groups, others medium-sized ones, others small ones, and others who work alone. There are those who publish dozens of papers, and those who publish only a few. There are those who publish in certain kinds of journals, and those who publish in others (by the way, the best papers of the list of references included here are those of Gibbs and I leave the reader to analyze his/her own conclusions about impact factors, immediacy index, etc.). There is no recipe for how a scientific career ought to unfold. Each scientist must find their own path. In my case the answer is simple: I believe that everyone should have fun doing science and, if possible, find the way to ensure (or at least attempt to ensure) that perhaps a couple of their ideas or contributions withstand the passage of time reasonably well. Mozart died at the age of thirty-five and would throw up his hands in astonishment if he knew the impact he has had upon us. We owe him a great deal, and I believe that we have not repaid him, and cannot repay him, for what he has given us. The same is true for so many scientists who have gone before us. I do not believe there is a nobler task than science (with the possible exception of music).

The reader should take my opinions with caution. After all, nobody is in possession of any absolute truth. Although I take science as seriously as I possibly can, since 2017 (for obvious reasons) I have become considerably more relaxed in matters of form, as will be evident from reading these lines. I must also acknowledge that my recent conference presentations have been rather more entertaining than they were some years ago. After all, one should not take life too seriously. The leitmotiv "life is a dream" has been repeated several times in this text. The Spanish writer Calderon de la Barca (who died in Madrid in 1681) wrote the play: "Life is a dream" that includes the following text:

> "the one who strives and pretends dreams,
> the one who offends and insults dreams,
> and in the world, in conclusion,
> everyone dreams what they are,
> although no one understands it.
> What is life? A frenzy.
> What is life? An illusion,
> a shadow, a fiction,
> and the greatest good is small;
> so all of life is a dream,
> and dreams, dreams are."

In my case, I could not be happier with how the dream has been thus far including the surprise of being honored with this Festschrift, which features numerous contributions from friends, colleagues, and former collaborators. I am deeply grateful to all of them for their generosity, support, and for being part of this project and also to Eva G. Noya, Maria M. Conde, Eduardo Sanz, Jorge R. Espinosa and Chantal Valeriani for making this special issue possible. Recently, while walking through a cemetery, I came across a phrase on a gravestone that struck me as most apt: "No me he ido, me han echado" – "I didn't leave, I was kicked out." Until that moment comes, one must carry on living (even if it is a dream).

AUTHOR DECLARATIONS

Author Contributions

Carlos Vega: Writing – original draft (equal); Writing – review & editing (equal).

21 October 2026 13:04:58

Published under an exclusive license by AIP Publishing

DATA AVAILABILITY

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

REFERENCES

[1] C. Vega and D. Frenkel, "Monte Carlo study of rod like molecules. A test of perturbation theory for the Kihara model," Mol. Phys. **67**, 633 (1989).
[2] C. Vega and S. Lago, "A fast algorithm to evaluate the shortest distance between rods," Comput. Chem. **18**, 55 (1994).
[3] C. Vega, B. Saager, and J. Fischer, "Molecular dynamics studies for the new refrigerant R152a with simple model potentials," Mol. Phys. **68**, 1079 (1989).
[4] C. Vega and K. E. Gubbins, "Monte Carlo study of quadrupolar Kihara fluids," Mol. Phys. **75**, 881 (1992).
[5] T. Boublik, C. Vega, and M. D. Pena, "Equation of state of chain molecules," J. Chem. Phys. **93**, 730 (1990).
[6] C. Vega, R. D. Kaminsky, and P. A. Monson, "Adsorption of fluids in disordered porous media from integral equation theory," J. Chem. Phys. **99**, 3003 (1993).
[7] W. G. Madden and E. D. Glandt, "Distribution functions for fluids in random media," J. Stat. Phys. **51**, 537 (1988).
[8] D. Frenkel and A. J. C. Ladd, "New Monte Carlo method to compute the free energy of arbitrary solids. Application to the FCC and HCP phases of hard spheres," J. Chem. Phys. **81**, 3188–3193 (1984).
[9] D. Frenkel and B. M. Mulder, "The hard ellipsoid-of-revolution fluid I. Monte Carlo simulations," Mol. Phys. **55**, 1171 (1985).
[10] C. Vega, E. P. A. Paras, and P. A. Monson, "Solid-fluid equilibria for hard dumbbells via Monte Carlo simulation," J. Chem. Phys. **96**, 9060–9072 (1992).
[11] C. Vega, E. P. A. Paras, and P. A. Monson, "On the stability limit of the plastic crystal phase of hard dumbbell solids," J. Chem. Phys. **97**, 8543–8548 (1992).
[12] C. Vega and P. A. Monson, "Plastic crystal phases of hard dumbbells and hard spherocylinders," J. Chem. Phys. **107**, 2696 (1997).
[13] L. G. MacDowell, M. Müller, C. Vega, and K. Binder, "Equation of state and critical behavior of polymer models: A quantitative comparison between Wertheim's thermodynamic perturbation theory and computer simulations," J. Chem. Phys. **113**, 419 (2000).
[14] M. S. Wertheim, "Fluids with highly directional attractive forces. II. Thermodynamic perturbation theory and integral equations," J. Stat. Phys. **35**, 35 (1984).
[15] C. Vega and L. G. MacDowell, "Extending Wertheim's perturbation theory to the solid phase: The freezing of the pearl-necklace model," J. Chem. Phys. **114**, 10411 (2001).
[16] C. Vega, C. McBride, and L. G. MacDowell, "Liquid crystal phase formation for the linear tangent hard sphere model from Monte Carlo simulations," J. Chem. Phys. **115**, 4203 (2001).
[17] F. Bresme, C. Vega, and J. L. F. Abascal, "Order-disorder transition in the solid phase of a charged hard sphere model," Phys. Rev. Lett. **85**, 3217–3220 (2000).
[18] C. Vega, J. L. F. Abascal, C. McBride, and F. Bresme, "The fluid-solid equilibrium of a charged hard sphere model revisited," J. Chem. Phys. **119**, 964–971 (2003).
[19] J. Kolafa and I. Nezbeda, "Monte Carlo simulations on primitive models of water and methanol," Mol. Phys. **61**, 161 (1987).
[20] C. Vega and P. A. Monson, "Solid-fluid equilibrium for a molecular model with short ranged directional forces," J. Chem. Phys. **109**, 9938–9949 (1998).
[21] H. J. C. Berendsen, J. R. Grigera, and T. P. Straatsma, "The missing term in effective pair potentials," J. Phys. Chem. **91**, 6269–6271 (1987).
[22] D. A. Kofke, "Direct evaluation of phase coexistence by molecular simulation via integration along the saturation line," J. Chem. Phys. **98**, 4149–4162 (1993).
[23] C. Vega, E. Sanz, and J. L. F. Abascal, "The melting temperature of the most common models of water," J. Chem. Phys. **122**, 114507 (2005).
[24] M. W. Mahoney and W. L. Jorgensen, "A five-site model for liquid water and the reproduction of the density anomaly by rigid, nonpolarizable potential functions," J. Chem. Phys. **112**, 8910–8922 (2000).
[25] W. L. Jorgensen, J. Chandrasekhar, J. D. Madura, R. W. Impey, and M. L. Klein, "Comparison of simple potential functions for simulating liquid water," J. Chem. Phys. **79**, 926–935 (1983).
[26] E. Sanz, C. Vega, J. L. F. Abascal, and L. G. MacDowell, "Phase diagram of water from computer simulation," Phys. Rev. Lett. **92**, 255701 (2004).
[27] L. A. Báez and P. Clancy, "Existence of a density maximum in extended simple point charge water," J. Chem. Phys. **101**, 9837–9840 (1994).
[28] C. Vega and J. L. F. Abascal, "Relation between melting temperature and temperature of maximum density for the most common models of water," J. Chem. Phys. **123**, 144504 (2005).
[29] J. L. F. Abascal, E. Sanz, R. García Fernández, and C. Vega, "A potential model for the study of ices and amorphous water: TIP4P/ICE," J. Chem. Phys. **122**, 234511 (2005).
[30] J. L. F. Abascal and C. Vega, "A general purpose model for the condensed phases of water: TIP4P/2005," J. Chem. Phys. **123**, 234505 (2005).
[31] H. W. Horn, W. C. Swope, J. W. Pitera, J. D. Madura, T. J. Dick, G. L. Hura, and T. Head-Gordon, "Development of an improved four-site water model for biomolecular simulations: TIP4P-Ew," J. Chem. Phys. **120**, 9665 (2004).
[32] J. L. F. Abascal and C. Vega, "The water forcefield: Importance of dipolar and quadrupolar interactions," J. Phys. Chem. C **111**, 15811–15822 (2007).
[33] J. D. Bernal and R. H. Fowler, "A theory of water and ionic solutions, with particular reference to hydrogen and hydroxyl ions," J. Chem. Phys. **1**, 515–548 (1933).
[34] V. Molinero and E. B. Moore, "Water modeled as an intermediate element between carbon and silicon," J. Phys. Chem. B **113**, 4008–4016 (2009).
[35] S. Izadi, R. Anandakrishnan, and A. V. Onufriev, "Building water models: A different approach," J. Phys. Chem. Lett. **5**, 3863–3871 (2014).
[36] L.-P. Wang, T. J. Martinez, and V. S. Pande, "Building force fields: An automatic, systematic, and reproducible approach," J. Phys. Chem. Lett. **5**, 1885–1891 (2014).
[37] R. Fuentes-Azcatl and J. Alejandre, "Non-polarizable force field of water based on the dielectric constant: TIP4P/ε," J. Phys. Chem. B **118**, 1263–1272 (2014).
[38] S. Piana, A. G. Donchev, P. Robustelli, and D. E. Shaw, "Water dispersion interactions strongly influence simulated structural properties of disordered protein states," J. Phys. Chem. B **119**, 5113–5123 (2015).
[39] D. Van Der Spoel, E. Lindahl, B. Hess, G. Groenhof, A. E. Mark, and H. J. C. Berendsen, "GROMACS: Fast, flexible, and free," J. Comput. Chem. **26**, 1701–1718 (2005).
[40] C. Vega, J. L. F. Abascal, and I. Nezbeda, "Vapor-liquid equilibria from the triple point up to the critical point for the new generation of TIP4P-like models: TIP4P/Ew, TIP4P/2005, and TIP4P/ice," J. Chem. Phys. **125**, 034503 (2006).
[41] S. Dufal, T. Lafitte, A. J. Haslam, A. Galindo, G. N. I. Clark, C. Vega, and G. Jackson, "The A in SAFT: Developing the contribution of association to the Helmholtz free energy within a Wertheim TPT1 treatment of generic Mie fluids," Mol. Phys. **113**, 948 (2015).
[42] C. Vega and E. de Miguel, "Surface tension of the most popular models of water by using the test-area simulation method," J. Chem. Phys. **126**, 154707 (2007).
[43] M. A. González and J. L. F. Abascal, "The shear viscosity of rigid water models," J. Chem. Phys. **132**, 096101 (2010).
[44] M. M. Conde, M. A. Gonzalez, J. L. F. Abascal, and C. Vega, "Determining the phase diagram of water from direct coexistence simulations: The phase diagram of the TIP4P/2005 model revisited," J. Chem. Phys. **139**, 154505 (2013).
[45] J. L. Aragones, L. G. MacDowell, and C. Vega, "Dielectric constant of ices and water: A lesson about water interactions," J. Phys. Chem. A **115**, 5745–5758 (2011).
[46] C. Vega, J. L. F. Abascal, M. M. Conde, and J. L. Aragones, "What ice can teach us about water interactions: A critical comparison of the performance of different water models," Faraday Discuss. **141**, 251–276 (2009).
[47] C. Vega and J. L. F. Abascal, "Simulating water with rigid non-polarizable models: A general perspective," Phys. Chem. Chem. Phys. **13**, 19663–19688 (2011).
[48] A. J. C. Ladd and L. V. Woodcock, "Triple-point coexistence properties of the Lennard-Jones system," Chem. Phys. Lett. **51**, 155 (1977).
[49] R. García Fernández, J. L. F. Abascal, and C. Vega, "The melting point of ice I_h for common water models calculated from direct coexistence of the solid-liquid interface," J. Chem. Phys. **124**, 144506 (2006).

21 October 2026 13:04:58

Published under an exclusive license by AIP Publishing

[50]M. M. Conde, C. Vega, and A. Patrykiejew, "The thickness of a liquid layer on the free surface of ice as obtained from computer simulation," J. Chem. Phys. **129**, 014702 (2008).
[51]C. Vega, M. Martin-Conde, and A. Patrykiejew, "Absence of superheating for ice I_h with a free surface: A new method of determining the melting point of different water models," Mol. Phys. **104**, 3583–3592 (2006).
[52]H. L. Pi, J. L. Aragonés, C. Vega, E. G. Noya, J. L. F. Abascal, M. A. González, and C. McBride, "Anomalies in water as obtained from computer simulations of the TIP4P/2005 model: Density maxima, and density, isothermal compressibility and heat capacity minima," Mol. Phys. **107**, 365–374 (2009).
[53]J. L. F. Abascal and C. Vega, "Widom line and the liquid-liquid critical point for the TIP4P/2005 water model," J. Chem. Phys. **133**, 234502 (2010).
[54]P. H. Poole, F. Sciortino, U. Essmann, and H. E. Stanley, "Phase behavior of metastable water," Nature **360**, 324 (1992).
[55]P. G. Debenedetti, F. Sciortino, and G. H. Zerze, "Second critical point in two realistic models of water," Science **369**, 289–292 (2020).
[56]P. Gallo, K. Amann-Winkel, C. A. Angell, M. A. Anisimov, F. Caupin, C. Chakravarty, E. Lascaris, T. Loerting, A. Z. Panagiotopoulos, J. Russo *et al.*, "Water: A tale of two liquids," Chem. Rev. **116**, 7463–7500 (2016).
[57]L. C. Jacobson, W. Hujo, and V. Molinero, "Thermodynamic stability and growth of guest-free clathrate hydrates: A low-density crystal phase of water," J. Phys. Chem. B **113**, 10298 (2009).
[58]M. M. Conde, C. Vega, G. A. Tribello, and B. Slater, "The phase diagram of water at negative pressures: Virtual ices," J. Chem. Phys. **131**, 034510 (2009).
[59]A. Falenty, T. C. Hansen, and W. F. Kuhs, "Formation and properties of ice XVI obtained by emptying a type sII clathrate hydrate," Nature **516**, 231 (2014).
[60]J. L. Aragones, M. M. Conde, E. G. Noya, and C. Vega, "The phase diagram of water at high pressures as obtained by computer simulations of the TIP4P/2005 model: The appearance of a plastic crystal phase," Phys. Chem. Chem. Phys. **11**, 543–555 (2009).
[61]J. L. Aragones and C. Vega, "Plastic crystal phases of simple water models," J. Chem. Phys. **130**, 244504 (2009).
[62]Y. Takii, K. Koga, and H. Tanaka, "A plastic phase of water from computer simulation," J. Chem. Phys. **128**, 204501 (2008).
[63]M. Rescigno, A. Toffano, U. Ranieri, L. Andriambariarijaona, R. Gaal, S. Klotz, M. M. Koza, J. Ollivier, F. Martelli, J. Russo, F. Sciortino, J. Teixeira, and L. E. Bove, "Observation of plastic ice VII by quasi-elastic neutron scattering," Nature **640**, 662 (2025).
[64]M. M. Conde and C. Vega, "Determining the three-phase coexistence line in methane hydrates using computer simulations," J. Chem. Phys. **133**, 064507 (2010).
[65]M. M. Conde and C. Vega, "A simple correlation to locate the three phase coexistence line in methane-hydrate simulations," J. Chem. Phys. **138**, 056101 (2013).
[66]D. Gonzalez-Salgado and C. Vega, "A new intermolecular potential for simulations of methanol: The OPLS/2016 model," J. Chem. Phys. **145**, 034508 (2016).
[67]C. Vega, "Water one molecule, two surfaces, one mistake," Mol. Phys. **113**, 1145 (2015).
[68]A. Z. Panagiotopoulos, "Direct determination of phase coexistence properties of fluids by Monte Carlo simulation in a new ensemble," Mol. Phys. **61**, 813 (1987).
[69]B. Garzón, S. Lago, C. Vega, E. de Miguel, and L. F. Rull, "Computer simulation of vapor-liquid equilibria of linear quadrupolar fluids. Departures from the principle of corresponding states," J. Chem. Phys. **101**, 4166 (1994).
[70]E. de Miguel and C. Vega, "The global phase diagram of the Gay-Berne model," J. Chem. Phys. **117**, 6313 (2002).
[71]E. G. Noya, C. Vega, and E. de Miguel, "Determination of the melting point of hard spheres from direct coexistence simulation methods," J. Chem. Phys. **128**, 154507 (2008).
[72]G. J. Gloor, G. Jackson, F. J. Blas, and E. de Miguel, "Test-area simulation method for the direct determination of the interfacial tension of systems with continuous or discontinuous potentials," J. Chem. Phys. **123**, 134703 (2005).
[73]A. P. Thompson, H. M. Aktulga, R. Berger, D. S. Bolintineanu, W. M. Brown, P. S. Crozier, P. J. in 't Veld, A. Kohlmeyer, S. G. Moore, T. D. Nguyen, R. Shan, M. J. Stevens, J. Tranchida, C. Trott, and S. J. Plimpton, "LAMMPS—A flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales," Comput. Phys. Commun. **271**, 108171 (2022).
[74]C. Vega, F. J. Blas, and A. Galindo, "Extending Wertheim's perturbation theory to the solid phase of Lennard-Jones chains: Determination of the global phase diagram," J. Chem. Phys. **116**, 7645 (2002).
[75]J. M. Míguez, M. M. Conde, J.-P. Torré, F. J. Blas, M. M. Piñeiro, and C. Vega, "Molecular dynamics simulation of CO_2 hydrates: Prediction of three phase coexistence line," J. Chem. Phys. **142**, 124505 (2015).
[76]E. G. Noya, C. Vega, J. P. K. Doye, and A. A. Louis, "Phase diagram of model anisotropic particles with octahedral symmetry," J. Chem. Phys. **127**, 054501 (2007).
[77]E. G. Noya, C. Vega, J. P. K. Doye, and A. A. Louis, "The stability of a crystal with diamond structure for patchy particles with tetrahedral symmetry," J. Chem. Phys. **132**, 234511 (2010).
[78]C. McBride, E. G. Noya, and C. Vega, "A computer program to evaluate the NVM propagator for rigid asymmetric tops for use in path integral simulations of rigid bodies," Comput. Phys. Commun. **184**, 885 (2013).
[79]C. McBride, C. Vega, E. G. Noya, R. Ramírez, and L. M. Sesé, "Quantum contributions in the ice phases: The path to a new empirical model for water: TIP4PQ/2005," J. Chem. Phys. **131**, 024506 (2009).
[80]C. Vega, M. M. Conde, C. McBride, J. L. F. Abascal, E. G. Noya, R. Ramirez, and L. M. Sesé, "Heat capacity of water: A signature of nuclear quantum effects," J. Chem. Phys. **132**, 046101 (2010).
[81]C. McBride, E. G. Noya, J. L. Aragones, M. M. Conde, and C. Vega, "The phase diagram of water from quantum simulations," Phys. Chem. Chem. Phys. **14**, 10140 (2012).
[82]C. Valeriani, E. Sanz, and D. Frenkel, "Rate of homogeneous crystal nucleation in molten NaCl," J. Chem. Phys. **122**, 194501 (2005).
[83]A. Reinhardt, J. P. K. Doye, E. G. Noya, and C. Vega, "Local order parameters for use in driving homogeneous ice nucleation with all-atom models of water," J. Chem. Phys. **137**, 194504 (2012).
[84]E. Sanz, C. Vega, J. R. Espinosa, R. Caballero-Bernal, J. L. F. Abascal, and C. Valeriani, "Homogeneous ice nucleation at moderate supercooling from molecular simulation," J. Am. Chem. Soc. **135**, 15008–15017 (2013).
[85]J. R. Espinosa, E. Sanz, C. Valeriani, and C. Vega, "Homogeneous ice nucleation evaluated for several water models," J. Chem. Phys. **141**, 18C529 (2014).
[86]J. R. Espinosa, C. Vega, C. Valeriani, and E. Sanz, "Seeding approach to crystal nucleation," J. Chem. Phys. **144**, 034501 (2016).
[87]J. R. Espinosa, C. Vega, and E. Sanz, "The mold integration method for the calculation of the crystal-fluid interfacial free energy from simulations," J. Chem. Phys. **141**, 134709 (2014).
[88]J. R. Espinosa, C. Vega, and E. Sanz, "Ice-water interfacial free energy for the TIP4P, TIP4P/2005, TIP4P/ICE and mW models as obtained from the mold integration technique," J. Phys. Chem. C **120**, 8068–8075 (2016).
[89]J. R. Espinosa, P. Sampedro, C. Valeriani, C. Vega, and E. Sanz, "Lattice mold technique for the calculation of crystal nucleation rates," Faraday Discuss. **195**, 569 (2016).
[90]I. Sanchez-Burgos, A. R. Tejedor, C. Vega, M. M. Conde, E. Sanz, J. Ramirez, and J. R. Espinosa, "Homogeneous ice nucleation rates for mW and TIP4P/ICE models through Lattice Mold calculations," J. Chem. Phys. **157**, 094503 (2022).
[91]Z. Mester and A. Z. Panagiotopoulos, "Temperature-dependent solubilities and mean ionic activity coefficients of alkali halides in water from molecular dynamics simulations," J. Chem. Phys. **143**, 044505 (2015).
[92]F. Moučka, I. Nezbeda, and W. R. Smith, "Molecular force fields for aqueous electrolytes: SPC/E-compatible charged LJ sphere models and their limitations," J. Chem. Phys. **138**, 154102 (2013).
[93]J. L. Aragones, E. Sanz, and C. Vega, "Solubility of NaCl in water by molecular simulation revisited," J. Chem. Phys. **136**, 244508 (2012).
[94]E. Sanz and C. Vega, "Solubility of KF and NaCl in water by molecular simulation," J. Chem. Phys. **126**, 014507 (2007).
[95]A. L. Benavides, J. L. Aragones, and C. Vega, "Consensus on the solubility of NaCl in water from computer simulations using the chemical potential route," J. Chem. Phys. **144**, 124504 (2016).
[96]I. S. Joung and T. E. Cheatham, "Determination of alkali and halide monovalent ion parameters for use in explicitly solvated biomolecular simulations," J. Phys. Chem. B **112**, 9020–9041 (2008).

21 October 2026 13:04:58

Published under an exclusive license by AIP Publishing

[97]J. R. Espinosa, J. M. Young, H. Jiang, D. Gupta, C. Vega, E. Sanz, P. G. Debenedetti, and A. Z. Panagiotopoulos, "On the calculation of solubilities via direct coexistence simulations: Investigation of NaCl aqueous solutions and Lennard-Jones binary mixtures," J. Chem. Phys. **145**, 154111 (2016).
[98]A. L. Benavides, M. A. Portillo, V. C. Chamorro, J. R. Espinosa, J. L. F. Abascal, and C. Vega, "A potential model for sodium chloride solutions based on the TIP4P/2005 water model," J. Chem. Phys. **147**, 104501 (2017).
[99]I. Leontyev and A. Stuchebrukhov, "Accounting for electronic polarization in non-polarizable force fields," Phys. Chem. Chem. Phys. **13**, 2613–2626 (2011).
[100]B. J. Kirby and P. Jungwirth, "Charge scaling manifesto: A way of reconciling the inherently macroscopic and microscopic natures of molecular simulations," J. Phys. Chem. Lett. **10**, 7531–7536 (2019).
[101]L. F. Sedano, S. Blazquez, and C. Vega, "Accuracy limit of non-polarizable four-point water models: TIP4P/2005 vs OPC. Should water models reproduce the experimental dielectric constant?," J. Chem. Phys. **161**, 044505 (2024).
[102]P. Montero de Hijes, J. R. Espinosa, E. Sanz, and C. Vega, "Interfacial free energy of a liquid-solid interface: Its change with curvature," J. Chem. Phys. **151**, 144501 (2019).
[103]B. J. Block, S. K. Das, M. Oettel, P. Virnau, and K. Binder, "Curvature dependence of surface free energy of liquid drops and bubbles: A simulation study," J. Chem. Phys. **133**, 154702 (2010).
[104]P. Montero de Hijes, J. R. Espinosa, V. Bianco, E. Sanz, and C. Vega, "Interfacial free energy and Tolman length of curved solid-liquid interfaces from equilibrium studies," J. Phys. Chem. C **124**, 8795 (2020).
[105]P. Montero de Hijes, K. Shi, E. G. Noya, E. E. Santiso, K. E. Gubbins, E. Sanz, and C. Vega, "The Young-Laplace equation for a solid-liquid interface," J. Chem. Phys. **153**, 191102 (2020).
[106]J. W. Gibbs, "On the equilibrium of heterogeneous substances," Transactions of the Connecticut Academy of Arts and Sciences **3**, 108–248 (1876).
[107]J. W. Gibbs, "On the equilibrium of heterogeneous substances," Transactions of the Connecticut Academy of Arts and Sciences **3**, 343–524 (1878).
[108]M. de Jager, C. Vega, P. M. de Hijes, F. Smallenburg, and L. Filion, "Statistical mechanics of crystal nuclei of hard spheres," J. Chem. Phys. **161**, 184501 (2024).
[109]P. Rosales-Pelaez, I. Sanchez-Burgos, C. Valeriani, C. Vega, and E. Sanz, "Seeding approach to nucleation in the NVT ensemble: The case of bubble cavitation in overstretched Lennard-Jones fluids," Phys. Rev. E **101**, 022611 (2020).
[110]W. Gispen, J. R. Espinosa, E. Sanz, C. Vega, and M. Dijkstra, "Variational umbrella seeding for calculating nucleation barriers," J. Chem. Phys. **160**, 174501 (2024).
[111]J. R. Espinosa, C. Vega, C. Valeriani, D. Frenkel, and E. Sanz, "Heterogeneous versus homogeneous crystal nucleation of hard spheres," Soft Matter **15**, 9625 (2019).
[112]J. R. Espinosa, A. Garaizar, C. Vega, D. Frenkel, and R. Collepardo-Guevara, "Breakdown of the law of rectilinear diameter and related surprises in the liquid-vapor coexistence in systems of patchy particles," J. Chem. Phys. **150**, 224510 (2019).
[113]N. D. Pasquale, J. Algaba, P. M. de Hijes, I. Sanchez-Burgos, A. R. Tejedor, S. R. Yeandel, F. J. Blas, R. L. Davidchack, J. R. Espinosa, C. L. Freeman, J. H. Harding, B. B. Laird, E. Sanz, C. Vega, and L. Rovigatti, "Solid-liquid interfacial free energy from computer simulations: Challenges and recent advances," Chem. Rev. **125**, 5003 (2025).
[114]V. Bianco, P. M. de Hijes, C. P. Lamas, E. Sanz, and C. Vega, "Anomalous behavior in the nucleation of ice at negative pressures," Phys. Rev. Lett. **126**, 015704 (2021).
[115]P. Montero de Hijes, J. R. Espinosa, C. Vega, and C. Dellago, "Minimum in the pressure dependence of the interfacial free energy between ice I_h and water," J. Chem. Phys. **158**, 124503 (2023).
[116]I. M. Zeron, J. L. F. Abascal, and C. Vega, "A force field of Li^+, Na^+, K^+, Mg^{2+}, Ca^{2+}, Cl^- and SO_4^{2-} in aqueous solution based on the TIP4P/2005 water model and scaled charges for the ions," J. Chem. Phys. **151**, 134504 (2019).
[117]I. M. Zeron, M. A. Gonzalez, E. Errani, C. Vega, and J. L. F. Abascal, "In silico seawater," J. Chem. Theory Comput. **17**, 1715–1725 (2021).
[118]S. Blazquez, M. M. Conde, J. L. F. Abascal, and C. Vega, "The Madrid-2019 force field for electrolytes in water using TIP4P/2005 and scaled charges: Extension to the ions F^-, Br^-, I^-, Rb^+, and Cs^+," J. Chem. Phys. **156**, 044505 (2022).
[119]S. Blazquez, L. F. Sedano, and C. Vega, "On the compatibility of the Madrid-2019 force field for electrolytes with the TIP4P/Ice water model," J. Chem. Phys. **161**, 224502 (2024).
[120]S. Blazquez, M. M. Conde, and C. Vega, "Scaled charges for ions: And improvement but not the final word for modeling electrolytes in water," J. Chem. Phys. **158**, 054505 (2023).
[121]V. M. Trejos, M. de Lucas, C. Vega, S. Blazquez, and F. Gámez, "Further extension of the Madrid-2019 force field: Parametrization of nitrate (NO_3^-) and ammonium (NH_4^+) ions," J. Chem. Phys. **159**, 224501 (2023).
[122]M. Cruz-Sánchez, F. Gámez, C. Vega, and V. M. Trejos, "The role of charge distribution in the modeling of polyatomic ions: The nitrate anion case," J. Chem. Phys. **164**, 214503 (2026).
[123]S. Blazquez, J. Troncoso, P. L. Francesca, P. Gallo, M. M. Conde, and C. Vega, "Extending the Madrid-2019 force field to the perchlorate anion: Role of charge distribution and validation with experiments on Mars-relevant aqueous solutions," J. Mol. Liq. **435**, 128035 (2025).
[124]P. Habibi, A. Rahbari, S. Blazquez, C. Vega, P. Dey, T. J. H. Vlugt, and O. A. Moultos, "A new force field for OH^- for computing thermodynamic and transport properties of H_2 and O_2 in aqueous NaOH and KOH solutions," J. Phys. Chem. B **126**, 9376–9387 (2022).
[125]M. de Lucas, S. Blazquez, J. Troncoso, C. Vega, and F. Gámez, "Dressing a non-polarizable force field for OH^- in TIP4P/2005 aqueous solutions with corrected Hirshfeld charges," J. Phys. Chem. Lett. **15**, 9411–9418 (2024).
[126]S. Blazquez, J. L. F. Abascal, J. Lagerweij, P. Habibi, P. Dey, T. J. H. Vlugt, O. A. Moultos, and C. Vega, "Computation of electrical conductivities of aqueous electrolyte solutions: Two surfaces, one property," J. Chem. Theory Comput. **19**, 5380–5393 (2023).
[127]L. F. Sedano, S. Blazquez, E. G. Noya, C. Vega, and J. Troncoso, "Maximum in density of electrolyte solutions: Learning about ion–water interactions and testing the Madrid-2019 force field," J. Chem. Phys. **156**, 154502 (2022).
[128]C. P. Lamas, C. Vega, and E. G. Noya, "Freezing point depression of salt aqueous solutions using the Madrid-2019 model," J. Chem. Phys. **156**, 134503 (2022).
[129]L. F. Sedano, L. C. Pardo, G. Madrigal, E. G. Noya, and C. Vega, "Structure making and breaking in electrolyte solutions explained by water energetics," Proc. Natl. Acad. Sci. U. S. A. **123**, e2531352123 (2026).
[130]J. Grabowska, S. Blazquez, E. Sanz, I. M. Zerón, J. Algaba, J. M. Míguez, F. J. Blas, and C. Vega, "Solubility of methane in water: Some useful results for hydrate nucleation," J. Phys. Chem. B **126**, 8553–8570 (2022).
[131]J. Algaba, I. M. Zerón, J. M. Míguez, J. Grabowska, S. Blazquez, E. Sanz, C. Vega, and F. J. Blas, "Solubility of carbon dioxide in water: Some useful results for hydrate nucleation," J. Chem. Phys. **158**, 184703 (2023).
[132]J. Grabowska, S. Blazquez, E. Sanz, E. G. Noya, I. M. Zerón, J. Algaba, J. M. Míguez, F. J. Blas, and C. Vega, "Homogeneous nucleation rate of methane hydrate formation under experimental conditions from seeding simulations," J. Chem. Phys. **158**, 114505 (2023).
[133]J. Grabowska, S. Blazquez, C. Vega, and E. Sanz, "Bulk versus interface nucleation of CO_2 hydrates from computer simulations," J. Phys. Chem. B **130**, 3717 (2026).
[134]S. Blazquez, J. Algaba, J. M. Míguez, C. Vega, F. J. Blas, and M. M. Conde, "Three-phase equilibria of hydrates from computer simulation. I. Finite-size effects in the methane hydrate," J. Chem. Phys. **160**, 164721 (2024).
[135]S. You, M. Ladd-Parada, K. Nam, A. Karina, S. Lee, M. Shin, C. Yang, Y. Han, S. Jeong, K. Park, K. Kim, M. Ki, R. Tyburski, I. Andronis, K. Ralf, J. H. Lee, I. Eom, M. Kim, R. Ma, D. Jang, F. Perakis, P. H. Poole, K. Amann-Winkel, K. H. Kim, and A. Nilsson, "Experimental evidence of a liquid-liquid critical point in supercooled water," Science **391**, 1387 (2026).

21 October 2026 13:04:58

Published under an exclusive license by AIP Publishing