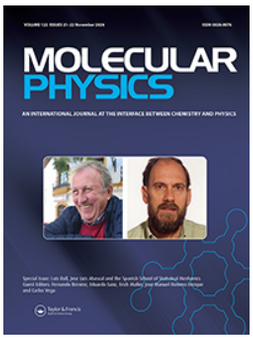

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INTRODUCTION

On the contributions of Luis F. Rull and José Luis F. Abascal to the development of the school of statistical mechanics in Spain

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ABSTRACT
A scientific biography serves as an introduction to a collection of papers honoring the significant contributions to the field of Statistical Mechanics by the late Luis Felipe Rull (1949-2022) and José Luis Fernandez Abascal (1952). Both dedicated their careers to the understanding of condensed matter systems, not only making substantial scientific contributions but also pioneering and expanding computer simulation methods in Spain. They were instrumental figures in the Spanish Statistical Mechanics School, which has flourished due to the efforts of a generation, including Luis and José Luis, who transformed Spanish science since 1975 and laid the foundation for our current achievements.

KEYWORDS
Statistical mechanics; computer simulations; liquid crystals; water; Monte Carlo; molecular dynamics

1. Luis F. Rull 1949–2022

On February 14, 2022 Luis Felipe Rull Fernández (Figure 1) passed away. He was emeritus professor of the department Atomic, Molecular and Nuclear Physics (FAMN) of the University from Seville; member of the Governing Board of the Royal Spanish Society of Physics (RSEF) between 2013 and 2017, and president of the Local Section of the RSEF in Seville between 2017 and 2019.

Born in Almería (Spain), he moved to Seville to attend secondary school. He graduated in Sciences, Physics Section, from the University of Seville in 1971 and he received his doctorate from said University in January 1976, under the direction of Juan de la Rubia Pacheco. During this period he initiated his career in the area of computer simulations applied to the Statistical Mechanics of liquids. He completed a postdoctoral stay between 1981 and 1982 at the University of Copenhagen (Denmark), where he collaborated with Soren Toxvaerd, as well as several short stays in the group of Keith E. Gubbins at Cornell University (USA) between 1986 and 1988. As an Assistant Professor since 1979, in 1983, he became Associate Professor at the University of Seville, and in 1995, he took up the position of Full Professor in the area of Theoretical Physics in the FAMN department of the University of Seville. After his retirement in 2019, he was appointed Professor Emeritus by the University of Seville, a position he held until his death.

Luis was a pioneer in the field of computer simulation in Spain. His extensive research activity, which was reflected in a multitude of publications and collaborations with various national and international groups were developed in this area, mainly in its application to the study of thermodynamic properties, transport, and phase diagrams of simple and complex liquids, especially liquid crystals, within Statistical Physics. In addition, he initiated many researchers in this field (among them José Manuel Romero Enrique and Erich Muller), infecting us with his enthusiasm for science and providing us with all the means at his disposal for our progress in the scientific field. Among his many merits, it is worth highlighting that he was a member of the board of the Liquids Section of the European Physical Society between 1996 and 2000, and he was a member of the editorial team of Molecular Physics and Molecular Simulation journals. He also co-directed the NATO-ASI and Enrico Fermi Summer School 'Observations and Predictions of Phase Transitions in Complex Fluids' in 1994 in Varenna (Italy) and organised the VI Meeting of Statistical Physics FisEs'94 in Seville. Despite being close to his definitive retirement, he enjoyed doing science. In recent times, he became interested in the use of Statistical Physics techniques in other,

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Figure 1. Luis Rull, in his beloved Sevilla, late 2021.

more applied areas. Thus, he participated in a project that investigated the incidence of cardiovascular accidents in stroke patients in Andalusia based on data recorded in the Andalusian Health Service.

Luis's academic production was very fertile and multidisciplinary. However, it is in the area of the study of the phase diagram of bulk and confined liquid crystals where he made a significant mark. Most of his work was devoted to the study of the Gay-Berne model [1]. This model is a anisotropic version of the Lennard-Jones potential which has become a paradigmatic model for the study of thermotropic liquid crystals. Together with his former PhD student Enrique de Miguel (now full professor at the University of Huelva) and Keith Gubbins, he applied computer simulation techniques to characterise the phase diagram of the Gay-Berne fluid [2–5], paying special attention to its dependence on the potential parameters. Together with his former PhD student Mohammed Houssa, he studied how the presence of permanent electric dipoles may affect the liquid crystal phase diagram [6–9]. Luis Rull and Enrique de Miguel were responsible of introducing the Gibbs Ensemble Monte Carlo method (proposed by Thanos Panagiotopoulos [10] in 1987) in Spain. Luis as a member of the panel evaluating Carlos Vega's thesis suggested to implement this method to the Kihara potential model. That was done in the following years [11,12] along with an excursion to the type of decay of the radial distribution function (oscillatory or exponential) at supercritical temperatures [13]. These papers also marked the beginning of a long term collaboration between Luis Rull and Santiago Lago (reinforced after Santiago Lago movement to Seville in 1998). As a consequence of this collaboration the phase diagram of a number of potentials such as hard and soft spherocylinders [14–16], as well as the Kihara and related models [17–19] was explored in a fruitful collaboration between Luis and the group at Pablo Olavide University formed by Santiago Lago, Bruno Martínez Haya and Alejandro Cuetos. He also was interested on the study of the interfacial phenomena of the Gay-Berne model, such as the anchoring, surface nematization and wetting [20–22] (together with Erich Muller and José Manuel Romero Enrique). Beyond computer simulations, he contributed to the theoretical understanding of these phenomena. For example, in collaboration with his former PhD student Elvira Martín del Río (now an associate professor at the University of Huelva), Enrique de Miguel and Margarida Telo da Gama (U. Lisboa), he applied density-functional theory (DFT) to the study of nematic-vapour interfaces [23,24]. Furthermore, anchoring and wetting transitions at solid-nematic interfaces [25–27] were studied within DFT in collaboration with his former student Inmaculada Rodríguez-Ponce, José Manuel Romero Enrique, Enrique Velasco (UAM, Madrid) and Luis Mederos (ICMM, CSIC, Madrid). In his last years, Luis focused his attention to the study by computer simulation of the formation of nematic droplets and capillary bridges, where the interplay between its shape and nematic ordering and the emergence of topological defects plays an essential role [28,29] (cf. Figure 2). In fact, when he sadly passed away he was working on a paper in collaboration with José Manuel Romero Enrique about how the aspect ratio of a nematic bridge between parallel plates can induce a textural order transition. Unfortunately, he could not see this work published [30]. Although editorial rules did not allow to credit him as an author of the paper, this must be seen as his last contribution and final touch of his brilliant career.

In addition to his work in liquid crystals, he also made high-impact contributions to many other areas of the equilibrium Statistical Physics of liquids. His most cited paper [31] involved a collaboration between four different authors (including Erich Muller) and has been cited more than 450 times, laying the groundwork for the study of the effects of confinement on the adsorption of water. It is also worth mentioning the research line on the properties of square-well fluids [32–34], in collaboration with his former PhD student Lourdes Vega (now full professor at Khalifa University in Abu Dabhi, UAE), Fernando del Río (UAM, México) and George Jackson (Imperial College London, UK), in which they studied by computer simulation how the vapour-liquid transition and its critical point depends on the range of the attractive

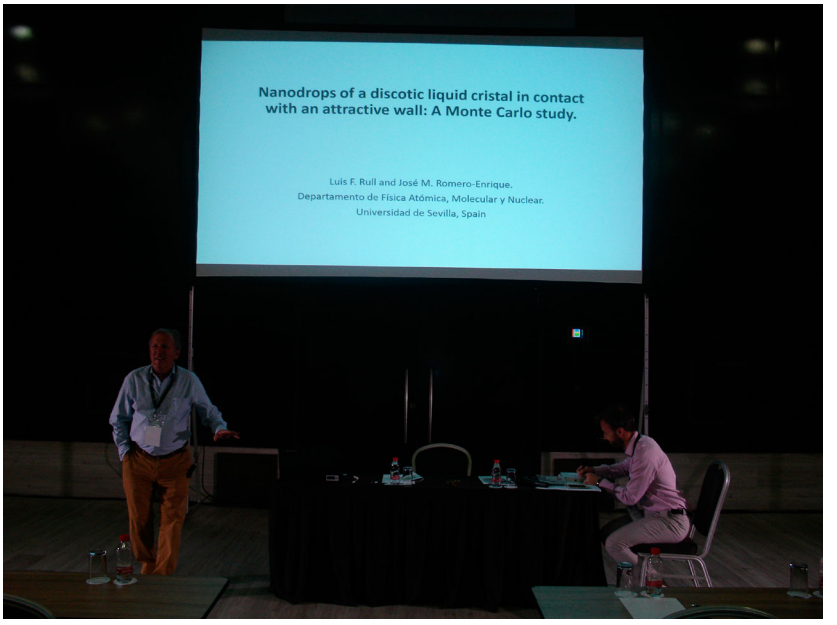

Figure 2. Luis giving a talk in the Thermodynamics'19 conference held in Punta Umbría (Huelva, Spain), June 2019.

part of the potential. In collaboration with G. Jackson, Luis also studied associating fluids and their peculiar phase diagrams, including the appearance of closed loops of immiscibility [35,36]. He also studied this problem from a theoretical point of view [37–41] in collaboration with José Manuel Romero Enrique (as part of his PhD project) and Umberto Marini Bettolo Marconi (U. Camerino, Italy). Last but not least, Luis made relevant contributions in the understanding of the vapour-liquid phase separation of ionic fluids. The role of ion pairing in this phenomenon, akin to associating systems, was not fully understood. Luis, in collaboration with José Manuel Romero Enrique and Athanassios Z. Panagiotopoulos (Princeton Univ.) showed by computer simulation that, in an exact mapping of the ionic fluid as a mixture of associated dipolar pairs and free ions, the absence of free ions enhanced the vapour-liquid phase separation [42]. This was a strong indication that the transition is driven by the associated pair fluids and not the free ions, as many theories proposed at that time. The colloidal counterpart of the restricted primitive model was also studied in collaboration with Antonio Puertas (Univ. Almería) [43]. Subsequent work considered the dependence of the vapour-liquid phase transition of primitive models of imidazolium-like ionic liquids as a function of the aliphatic chain length [44], as well as their glass transition [45].

Along with extensive research, Luis had a vital teaching activity in the Physics and Mathematics degrees at the University of Seville, an activity that he continued to develop until the last moment, as well as management activities. He was Dean of the Faculty of Physics between 1984 and 1989, a member of the University Senate between 1985 and 2000, and on the Social Council of the University of Seville between 1986 and 1989. It is necessary to highlight his commitment to advancing scientific research in Spain. In this sense, in addition to participating in multiple panels of experts and scientific evaluations throughout his long career, he advised groups from across the political spectrum on issues related to the University and Science. He also chaired the Association for the Advancement of Science and Technology in Spain (AACTE) between 2001 and 2003. In all these areas, he always maintained an independent, critical, and consistent stance with his ideas, which he defended passionatelly, although he was always open to constructive debate.

In June 2023 the Faculty of Physics of the University of Seville organised a Symposium in his honour, in which many of his friends, both colleagues and former students, contributed with excellent talks, as well as remembrances of him and his scientific career (cf. Figure 3). Those who knew him agree to highlight his big heart and generosity. Many colleagues with whom he worked felt literally at home when they visited him, revealing to them the charms of his city (cf. Figure 4), which was Seville, even though he was born in Almería. He was a great music lover and an avid reader whose curiosity covered the most varied fields of knowledge. He was fascinated by such abstract topics as the distribution of prime numbers, Gödel's incompleteness theorems, or the origin of human consciousness. In one of his last posts on social networks, he recommended reading the book by Nobel Prize winner in Physics Frank Wilczek, The *World as a*

Figure 3. Picture group of the conference celebrated in Sevilla in June of 2023 devoted to the memory of Luis Rull. First row from left to right George Jackson, Lourdes Vega, Jose Manuel Romero Enrique, Santiago Lago, Juan Antonio Anta, Bruno Martinez Haya. Second row from left to right Carlos Vega, Felipe Blas. Third row Jordi Torné, Álvaro Rodríguez-Rivas, Luis G. MacDowell, Antonio M. Puertas, Pedro Tarazona, Alberto Martín-Molina, Alessandro Patti, his daughter Patricia, Inmaculada Rodríguez-Ponce, Erich Müller, María (Luis's wife), his son Luis and Alejandro Cuetos.

Figure 4. Not everything in life is science. Feria de Sevilla (also denoted as Feria de Abril) and Betis football club were passions of Luis when not doing science. Time to relax. Santiago Lago, George Jackson, María (Luis's wife), Luis Rull and Jose Manuel Romero Enrique, July 1999.

Work of Art. He was a family man and a great friend to his friends, on whom he left an indelible mark. Luis, we will always carry you affectionately in our memories and hearts.

2. José Luis Fernández Abascal

José Luis Fernández Abascal (also known as JL to his friends) was born in a small city in the middle of Spain (Ciudad Real) in the region of 'La Mancha' in 1952. He was the fifth of a family of 11 children. When he was 13, the family moved to Madrid because his parents decided that this move would offer better educational opportunities for their sons and daughters. At high school in Madrid, José Luis got interested in Chemistry and decided to study Chemistry at Universidad Complutense the Madrid (UCM), where he entered in 1970, graduating in 1975 and remaining for more than fifty years until his

retirement December 2020. José Luis was educated in the fundamentals of Chemistry at Complutense University and obtained some training in scientific computation, which soon became one of his passions.

Between 1970 and 1975, Spain remained undemocratic, standing as a unique case in Europe, and dictatorship persisted until Franco died in 1975. The University was a hub of resistance and dissent against Franco, and José Luis actively joined many of his contemporaries in university protests against Franco's rule. These demonstrations frequently ended with the police forcefully entering university buildings. His generation played a crucial role in the anti-Franco movement within universities and intellectual circles leading up to Franco's death in 1975.

After graduating, José Luis found several jobs that were still unrelated to science for a few months, such as a high school chemistry teacher or a chemical industry employee. Both experiences were valuable as he learned about his teaching abilities and capacity to address practical problems. José Luis started a master's thesis under Manuel Lombardero's supervision on the importance of quadrupolar interactions in describing the properties of nitrogen and carbon dioxide. This master thesis was a turning point for José Luis and showed him the path he wanted to follow. He then accepted an offer for a PhD thesis under the guidance of Manuel Lombardero to work on perturbation theories of molecular liquids [46]. This thesis was submitted in 1981.

After his PhD defense in 1982, Jose Luis visited Jack G. Powles' lab at the University of Kent (UK), where he used for the first time simulation methods, in particular, the technique of Molecular Dynamics that he applied to study the impact of nuclear quantum effects on the properties of Neon [47]. Manuel Lombardero educated José Luis in Statistical Mechanics, while visiting Powles changed his career, as he instantly fell in love with computer simulations. At that time the experience with simulations at Complutense was small and reduced to the code developed by Alberto Bañon and Jesus Santamaria (another former PhD student of Manuel Lombardero). Notice that at this time one had to write Fortran codes to run simulations. Public codes for simulations as Gromacs or DLPOLY were developed later in the 90s. At the beginning of 1984, José Luis obtained a permanent position at UCM.

Soon after this period, he began to tackle increasingly complex computer simulation challenges. He employed Monte Carlo methods to examine the structures of quadrupolar and dipolar fluids and compared these findings with theoretical predictions derived from integral equations. He became increasingly interested in simulating systems composed of charged particles and implemented state-of-the-art methods to deal with the long-range nature of the interactions. During the 1985–1986 academic year, he took a sabbatical in Paris under the guidance of Pierre Turq at the Université Pierre et Marie Curie – Paris VI, where he worked on Brownian dynamics applied to electrolytes [48]. He developed computational strategies for cluster analysis and structural studies using Voronoi tessellations. A few years later, he successfully published a paper on the application of Voronoi polyhedra in structural studies [49]. His stay in Paris was enjoyable, as he could travel with his wife, Mercedes, and their first son, Javier. José Luis and Mercedes have been married for nearly five decades and have two children, Javier and Mercedes.

When returning to Spain, José Luis decided to continue with electrolytes but now moving to polyelectrolytes. For this reason, he started to work on the structure of ions around rigid polyelectrolytes as DNA. Thus, he started a research line about the influence of ions on the B-Z ADN structural transition using a simple but physically inspired coarse-grained model of DNA. That work was reflected in several essential papers about how a coarse-grained model could capture the physics of this transition. Motivated by this interest, he visited the labs of John Prausnitz (1992) [50] and J. Andrew McCammon (1997). At that time, water was not explicitly introduced in the description, so these simulations were with implicit solvent.

Electrolytes are found not only in solution but also as molten salts. A simple model of a molten salt consists of a model of hard spheres, having half positive and half negative charges. This is usually denoted as the Restricted Primitive Model. In a first approach to the problem, José Luis and his group performed computer simulations of this system (using Ewald sums) and compared the structural predictions from integral equations with those obtained from the simulation. He got interested in studying the liquid-solid equilibria of the RPM, along with Fernando Bresme (a PhD student at that time) and Carlos Vega. José Luis and Carlos have known each other since long ago, as they used to have lunch together along with Eduardo Enciso, Santiago Lago and other departmental colleagues. They used to have lunch around 14:00 and coffee afterwards around 15:00. Who paid for the coffee? The group played 'Chinos', and the loser paid for the coffee. In the 'Chinos' game, each player had a maximum of three coins and could choose between 0 and 3. Then, each one, in turn, would have to guess the total number of coins hidden in all the players' hands. The game was Statistical, but not Mechanics. The group played this game for about 12 years, and all the statistics, winners, and losers were recorded on a web page, maintained by, who else?

Figure 5. Relaxing in Snowdonia National Park in the early 90s.Left: Fernando Bresme and José Luis. Right: Eduardo Enciso, José Luis, and Juan Carlos Gil Montoro.

The problem of determining the phase diagram of RPM was exciting and José Luis F. Abascal, Fernando Bresme, Carl McBride, and Carlos Vega decided to work together on this project, leading to several exciting publications [51,52], including the discovery of a new phase at low temperatures where the ions ordered on an fcc lattice [53]. This was the first of a long list of collaborations between José Luis F. Abascal and Carlos Vega that lasted almost three decades (1996–2025). According to José Luis, the time he shared with his two PhD students (second half of the 90s), namely, Juan Carlos Gil Montoro working [54] on DNA and Fernando Bresme working on water, electrolytes, integral equations, and RPM was one of his most productive and happiest times [54,55] (see Figure 5 for a picture of this time). That period witnessed the setup of the 'Decpacho' with the incorporation of the first Dec workstation used initially to compute virial coefficients with Monte Carlo simulations, as well as the development by the group of the code Poly, which incorporated pre-processing capabilities and performed Monte Carlo, Molecular Dynamics or Brownian Dynamic simulations, depending on the user needs.

At the end of the 90s, José Luis decided to incorporate water into his ADN coarse-grained model so that simulations of ADN would be performed in explicit water. However, the closure of the computer centre at UCM ended this line of research. When a door is closed, another door opens, so that this closure was responsible for the 'water adventure'. Carlos Vega, had a PhD student at that time, Eduardo Sanz, pursuing a thesis proposal devoted to the solubility of aminoacids in water. It was soon evident that to describe aminoacids in water, an appropriate potential model should be used, and there were reasons to believe that a model with an accurate melting point would be a good option. After a lunch conversation with José Luis, it was suggested that SPC/E [56] was the best option. Somewhat surprisingly, the melting point of many water models was unknown. Since Carlos had experience with free energy calculations of solids using the Frenkel-Ladd method [57] (acquired during his post-doc in 1992 with Peter Monson [58]) Eduardo started to determine the melting point of SPC/E using free energy calculations that were already incorporated in a Monte Carlo code that Carlos developed along the years (with parts added by Luis G. MacDowell and parts added by Eduardo Sanz). Ewald sums were incorporated using José Luis background on electrolytes. Eduardo Sanz determined the melting point of SPC/E and other water models. It was shown that the melting point of SPC/E and TIP4P water models was quite low. It was decided at this time to join the computer resources of José Luis and Carlos for an ambitious goal: the first determination of the phase diagram of a water model (SPC/E) by using computer simulations. Eduardo's thesis was taking a different route than initially conceived (not aminoacids at all but just water) and Luis G. MacDowell joined the research team. By combining free energy calculations, thermodynamic integration and Gibbs Duhem integration method [59], the phase diagram of SPC/E was obtained. After one year of hard work, the results were somewhat frustrating: the agreement with the experiment was not very good. After a meeting where frustration was undoubtedly present, it was decided to spend four additional months determining the phase diagram for another model, TIP4P [60]. This decision changed everything. The phase diagram of TIP4P was in better agreement with the experiment. At that time, it was not unusual for José Luis and Carlos to work late at night modifying the input files (sometimes simultaneously) to launch new simulations. Difficult to forget the enthusiasm of this time. The paper with the first diagram of water obtained from simulations was published [61] in Physical Review Letters in 2004. Although the phase diagram of TIP4P was reasonable, the melting point was low [62] (230 K); thus, it was decided to develop a new TIP4P model with the correct melting point, and that was the birth of TIP4P/Ice [63]. After realizing that at room pressure reproducing simultaneously the melting point and the temperature of the maximum in density (TMD) was not possible within the TIP4P geometry [64] another model was developed to describe the temperature of the maximum density of water at room temperature [65]: TIP4P/2005. No doubt, 2005 was a good year! The two water models TIP4P/ICE and TIP4P/2005 are highly regarded in the community of simulations of water and are used worldwide nowadays.

Eduardo Sanz left the group by the end of 2005 for a post-doc position. The solubility of amino acids in water was the initial scope of his thesis but was never performed since life happens, and the water research was exciting (although at least the solubility of NaCl in water was determined by computer simulations within his thesis). In 2006, with the help of Ramón García Fernández, Gromacs was installed in several computers of the group. Until this moment, all the runs had been done with the Monte Carlo code that the group developed over the years. According to José Luis, this code was not elegant and should be rewritten from scratch, but this code rewriting never happened. The first MD simulations arrived at the group. They were devoted to testing if the melting point of ice Ih for water models obtained from free energy calculations would be consistent with those obtained from direct coexistence methods. That was indeed the case [66], and this work contributed to the increasing popularity of direct coexistence methods to get phase equilibria. The following years were devoted to determining some additional properties of TIP4P/2005 and TIP4P/ICE, namely the viscosity [67], vapour-liquid equilibria [68], surface tension [69] and nuclear quantum effects [70] (in collaboration with Eva G. Noya, Luis Sesé and Rafael Ramírez). The TIP4P/2005, in particular, performed extraordinarily well (better even than anticipated), and it was decided in 2009 and 2011 to evaluate the performance of water models more quantitatively (starting with a more qualitative test done in collaboration with Maria M. Conde and Juan Luis Aragones [71]), and continuing with a more elaborate proposal that is now denoted as the Vega-Abascal test [72]. A pedagogical paper describing how to determine phase diagrams by computer simulations appeared [73] in 2008 with the help of Eva G. Noya (a postdoct in the group at that time). A picture of the group around 2010 is shown in Figure 6. Since TIP4P/2005 was a good model, it was decided to analyse its performance at low temperatures to analyse if its behaviour was consistent with the existence of a second critical point. This was indeed the case [74–76] and confirmed a few years later in 2020 by Gul H. Zerze, Francesco Sciortino and Pablo G. Debenedetti [77] (see Figure 7 with a picture of the visit of Pablo G. Debenedetti to Complutense)

In the last 10 years, water research has continued, taking different routes. On the one hand, after the return of Eduardo Sanz and the incorporation of Chantal Valeriani into the group, they led our effort to understand the nucleation of ice. The seeding technique, developed within the PhD thesis of Jorge R. Espinosa, was proposed and first implemented to estimate the nucleation rate of ice using TIP4P/2005 and TIP4P/ICE water models

Figure 6. Group at UCM by 2010. From left to right, Luis G. MacDowell, Carlos Vega, José Luis F. Abascal, Miguel Angel Gonzalez, Carl McBride, Eva G. Noya, María M. Conde, Juan Luis Aragonés and Briesta S.González.

Figure 7. From left to right Pablo Debenedetti during his visit to Madrid in March 2024, Carlos Vega, Eduardo Sanz and Jose Luis Fernandez Abascal. The picture is taken at the corridor of the Physical Chemistry department of Complutense University where the water models TIP4P/ICE and TIP4P/2005 were developed.

[78]. That was further expanded to nucleation studies on cavitation of water under tension [79,80] in collaboration with Frederic Caupin and Cristoph Dellago. The behaviour of water at very low temperatures was further expanded by José Luis and Chantal Valeriani with the help of Miguel Angel González (their PhD student at that time, see Figure 8) and in collaborations with Frederic Caupin, Mikhail A. Anisimov and Pablo G. Debenedetti [81–83]. Finally from 2015 to 2022, the interest in electrolytes in water returned, and it was decided to develop a force field for electrolytes in water, with the help of

our Mexican friends, Ana Laura Benavides and Iván M. Zeron and that of Samuel Blazquez (a PhD student at that time). That was the beginning of the Madrid force field [84–86]. In addition José Luis was convinced of the importance of modelling seawater as a problem of high interest for our future on Earth [87] and on the importance of determining electrical conductivies properly in computer simulations in collaboration with the group at Delft of Othonas Moultos and Thijs Vlugt [88].

In 2020 Covid came, and in December 2020 José Luis retired as some lung health issues turned the nice duty of teaching into a high-risk activity (see Figure 9 for a photo group just after his retirement). A few years before retirement, José Luis had published 100 papers, garnering in December 2024 over 14000 citations in Google Scholar. He was PhD advisor of six PhD students: Claudio Martin (coadvisor Manuel Lombardero), Enrique Lomba (coadvisor Manuel Lombardero), Fernando Bresme (coadvisor Enrique Lomba), Juan Carlos Gil Montoro, Sonia Jorge (coadvisor Enrique Lomba) and Miguel Angel González (coadvisor Chantal Valeriani). Enrique Lomba and Fernando Bresme founded independent groups in the National Research Council of Spain (CSIC) and Imperial College, respectively, and developed successful careers. Also Miguel Angel Gonzalez his last PhD student, has just started an Assistant Professor position at U.Rey Juan Carlos in Madrid. Enrique, Fernando and Miguel Angel can be regarded as José Luis' academic sons.

Throughout his career, José Luis had a profound passion for computers. His expertise extended to Linux, numerical methods, hardware maintenance (such as disassembling computers and swapping components), initiating the faculty of Chemistry's first internet connections, and developing and executing his computational codes and simulations. Beyond mere execution, he also meticulously analysed the outcomes and crafted his software programs. From the onset of his career, he has personally managed program execution and results analysis. José Luis was a hands-on scientist, frequently leaving the lab at 9:00 PM when his Linux terminal would remind him, 'Es muy tarde'. Despite his significant scientific contributions, José Luis remained humble, forming strong bonds with younger colleagues and was always eager to assist. He approached his work with unwavering rigour, unconcerned about rushing to publish or amassing a high publication count, but intensely focused

Figure 8. José Luis with Chantal Valeriani, PhD advisors of the last PhD student of José Luis, Miguel Angel González, Christmas 2021.

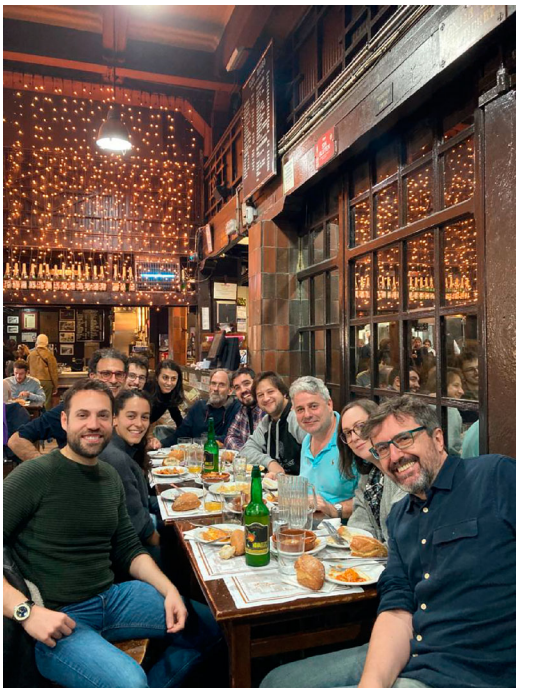

Figure 9. Group picture just after José Luis retirement, Christmas 2022, from left to right Jorge R. Espinosa, Cintia Pulido, Eduardo Sanz, Javier Oller, Eva G. Noya, José Luis F. Abascal, Miguel Camarillo, Samuel Blázquez, Carlos Vega, María M. Conde and Jorge Ramírez.

Figure 10. José Luis in Tomellosa, the place on Earth he likes the most, with gris grand son, Darío, summer 2023.

on ensuring the reliability and accuracy of published findings. While somewhat absent-minded in everyday life, he was exceptionally precise in his professional endeavours. He was among the first to recognise that immediate email responses were unnecessary (eschewing mobiles or WhatsApp) and that distractions detracted from what truly mattered: personal time and focus. He believed that managing one's time should be a personal choice, not dictated by others. The students admired him for his informal and unique approach. In his final years before retirement, he laid the groundwork for the practical training component of Molecular Modelling at the Faculty of Chemistry, which encompasses hands-on experience with Quantum Calculations and Molecular Dynamics. Beyond this, he is an outstanding ping-pong player, having defeated all the research group members over the years. These matches typically took place after lunch at his house in Tomellosa, a quaint village in Guadalajara, and one of his most beloved places (see Figure 10).

It's fair to assert that José Luis was, and remains, a remarkably talented individual, an extraordinary person, and primarily a dedicated scientist with an immense curiosity that persists. He believed that science wasn't merely about securing large funding or forming massive teams, but about maintaining rigour, executing serious work, and having fun while pursuing discoveries, with the hope that one or two of your contributions might eventually make a significant impact on the community. We consider him an enduring example worth emulating.

3. Statistical mechanics in Spain

To understand the state of science in Spain between 1976 and 1982, it's crucial to note the impact of the post-civil war era. After the civil war ended in 1939, more than half of the country's professors emigrated, leading to Spain's isolation and a significant decline in scientific advancement for forty years. As an illustration, it wasn't until the 1970s that a paper from Spain was published in the Journal of Chemical Physics, despite the journal being established in 1933. In the late 70s and early 80s, several groups focusing on statistical mechanics emerged. Due to the existence of numerous groups, we will only highlight a few, which probably only reflects our familiarity with them and apologise for maybe missing some other important groups.

In Madrid, two groups emerged. One was located at Universidad Autónoma de Madrid, with Guillermo Navascués as the founder and Pedro Tarazona as one of the most representative members, along with many others, such as Enrique Velasco, Luis Mederos, Rafael Delgado-Buscalioni and Enrique Chacón (CSIC), among others. In Complutense University, Manuel Lombardero's figure should be mentioned. Although belonging to CSIC he worked during his entire life at the Physical Chemistry Department of UCM. Manuel Lombardero was the PhD advisor of José Luis F. Abascal and also of Santiago Lago, Eduardo Enciso and Enrique Lomba. The figure of Lombardero played a key role not only in the life of José Luis, but also in several generations that followed. Enrique Lomba led the statistical mechanics research in CSIC by funding a group at the Rocasolano Institute (now Blas Cabrera Institute) with Noe García Almarza (deceased prematurely) and Eva G. Noya and Juan Antonio Anta, who moved to Seville. The statistical thermodynamics group at Complutense continued having new members, some remaining at UCM and some spreading in the country. A few names are Carlos Vega and Sofia Calero (Santiago Lago being their PhD advisor), Eduardo Sanz, Luis G. MacDowell, Jorge. R. Espinosa, María M. Conde (now at UPM), Juan Luis Aragonés (now at UAM). Carlos F. Tejero (who recently passed away) also founded another group at the Faculty of Physics of UCM, and the statistical mechanics activity continues there with Victor Martín Mayor, Juan Manuel R. Parrondo, Ricardo Brito, Juan José Mazo and Chantal Valeriani. At the University Carlos III a multidisciplinary group on complex systems based on Statistical Physics was founded, with Anxo Sánchez, José Antonio Cuesta, Rodolfo Cuerno, Carlos Rascón and Yuri Martínez Ratón as some of its members. Susanna Manrubia in CSIC also works on Complex systems. At the Universidad Politécnica de Madrid there is another strong group on Statistical Physics applied to complex systems led by Rosa Benito. Other groups in Madrid worked on nuclear quantum effects as the group of Luis Sesé (UNED), or that of Carlos Herrero and Rafael Ramirez (CSIC). Also in Madrid the group led by Pep Español at UNED was involved with the development of dissipative particle dynamics.

In Barcelona, Miguel Rubí's group has contributed significantly to equilibrium and non-equilibrium statistical Mechanics, and on the simulation side, Joan Angel Padró and Antoni Giró. The tradition in Barcelona continues with many others as Elvira Guardia, Jordi Martí, Ignacio Pagonabarraga, David Reguera, Giancarlo Franzese, Alberto Fernandez Nieves among others. In Tarragona a group working in Statistical Mechanics is located at the Faculty of Chemical Engineering, with Allan Mackie, Josep Bonet Avalos, and Felix Llovell (a scientific grand son of Luis Rull). Starting in Barcelona but moving to Baleares islands emerges the figure of Maxi San Miguel that created a strong group in Palma de Mallorca with persons such as Pere Colet or Raul Toral.

In Andalucia several groups should be mentioned. In Seville, the figure of Luis F. Rull emerged after founding a strong group at the U.Sevilla. Also in Sevilla there was another strong group led by José Javier Brey, and including María José Ruíz Montero (who sadly passed away a few years ago), Álvaro Domínguez, Pablo Maynar and Maribel García de Soria. More recently, new groups emerged in Seville, as the one led by Antonio Prados. José Manuel Romero Enrique continued the tradition that Luis F. Rull started there, and many other scientists educated by Luis moved to other Universities, such as Lourdes Vega (that moved to Abu Dabhi), and Enrique de Miguel and Elvira Martín del Río (that moved to Huelva), and Felipe J. Blas, who moved to Tarragona first and to Huelva later on to continue the Statistical Mechanics group in Huelva. Also, Santiago Lago moved to Seville in the late 90s and founded a group with Sofía Calero, Juan Antonio Anta, Bruno Martínez-Haya, Alejandro Cuetos and Carmen Gordillo. At the University of Sevilla (Physical Chemistry Department) we find the group of Enrique Sánchez Marcos and Rafael Pappalardo. In Granada, there are two groups created by Joaquín Marro and Roque Hidalgo, respectively, which very active in the Statistical Physics area, with Pedro Garrido, Miguel Angel Muñoz and Pablo Hurtado, on one hand, and Arturo Moncho Jorda, Alberto Martín-Molina and Alessandro Patti on the other hand, as representative members. More research groups can be found in other universities, such as the group of Antonio Puertas in Almeria, Manuel Quesada in Jaén and Juan José Pereda in Malaga.

Other groups also emerged in other parts of Spain as Extremadura (with a good connection with Seville), such as Andrés Santos, Santos Bravo Yuste, Angel Mulero, Vicente Garzó y Francisco Cuadros and in Cantabria, José Ramón Solana and Julio Largo, having all these groups a strong tradition in studies (both simulation and theory) of hard bodies. In Valladolid David González y Luis Enrique González studied in detail liquid metals via computer simulations with collaborations with Moisés Silbert (that passed away a few years ago). In Canary Islands we have the group of Javier Hernández Rojas with a strong background in the study of the statistical thermodynamics of clusters. In Valencia we have the group of Germán Sastre focused on zeolites. In Zaragoza we found the groups of Yamir Moreno, Jesus Gómez Gardeñes working on complex systems and Alfonso Tarancón, that worked on spin glasses.

In Galicia we have several groups, that nucleated around U.Santiago, as the group of Luis Javier Gallego that studied liquid metals and more recently ionic liquids, a tradition now continued by Luis Miguel Varela. The experimental thermodynamic group of Inmaculada (Ada) Andrade (who passed away recently) in Santiago was responsible of many younger researchers that moved to statistical mechanics and simulations in several

Figure 11. Luis and José Luis legacy. Picture of the Spanish simulation group, June 2017. On the second row (right hand side) Luis Rull and José L.F. Abascal along with the younger generations.

Universities of Galicia as Claudio Cerdeiriña, Diego González Salgado, Jacobo Troncoso in the group led by Luis Romaní in Ourense, Manuel Piñeiro (U.Vigo) and Angel Piñeiro (U. Santiago).

Some Spanish groups have worked on the Statistical Mechanics of flexible molecules, and it is worth mentioning the group of José García de la Torre (Murcia), Juan Freire (UNED), Antonio Rey (UCM), Jorge Ramírez and Manuel Laso (UPM).

Nowadays, the Statistical Physics in Spain is internationally recognised as an active, worldwide high-impact research area. The Statistical Physics and Non-linear Physics specialised group of the Spanish Royal Society of Physics (GEFENOL) has more than 300 members and organises regularly meetings on Statistical Physics every year and a half (FisEs conferences), among other activities. On the other hand, the Thermodynamics specialised group of both the Spanish Royal Societies of Physics and Chemistry, led by Manuel Piñeiro and Felipe J. Blas or, more recently, the Soft Matter section of the Condensed Matter Physics specialised group of the Spanish Royal Society of Physics, led by Alberto Fernández-Nieves and Ignacio Pagonabarraga, have also strong ties with the Statistical Physics and promote synergies with other related research areas. Finally, it is worth mentioning the Spanish Network on Simulation, first organised by Felipe J. Blas and currently led by Eva G. Noya, that gathers most of the researchers in the area of computer simulation applied to Equilibrium Statistical Physics. The vitality of this community (see Figure 11) is, beyond doubt, the most important legacy of both Luis and José Luis.

4. Epilogue

We are delighted to introduce this special issue dedicated to Luis F. Rull and José Luis F. Abascal. It features over forty top-tier papers, illustrating their extensive impact in Spain and internationally. Luis and José Luis exemplify the pioneers of Spain's Statistical Mechanics School, which includes many notable figures. Following a period from 1939 to 1975 when Spain played a minor role in science, the arrival of democracy in 1975 heralded a wave of talented individuals who undertook post-doctoral experiences abroad, undertaking the challenging task of rebuilding from the ground up. Luis and José Luis exemplify this transformative generation, significantly impacting Spain's scientific landscape. Luis placed Sevilla on the global Statistical Mechanics map, while José Luis did the same for Madrid. It is gratifying to acknowledge that Spain's scientific standing has improved dramatically over the past 50 years, with exceptional researchers across most fields. We owe much to individuals like Luis and José Luis, who contributed significant groundwork (see Figure 11 for a picture of Luis and José Luis with the young members of the simulation community of Spain). Our sincerest gratitude goes to both of you. You have helped forge the path to our current achievements.

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Disclosure statement

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