Special issue on soft matter research in Latin America

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Preface

Special issue on soft matter research in Latin America

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1. Introduction

The term soft matter was coined to describe systems in which the effective interaction between the basic components can be modified by small changes in temperature and external fields, or alternatively as a type of matter which, subjected to slight disturbances or because of minute structural modifications, completely changes its properties. In principle this implies that the strengths of the interactions are of the order of few $k_{\mathrm{B}}T$. The expression 'matière molle' was coined by Madeleine Veyssié in the 70s [1] as a joke since the word in French has a double meaning. The detailed explanation of the meaning of soft matter was given by de Gennes in his Nobel prize lecture [2]. The field includes a diversity of systems such as polymers, colloids, micelles, surfactants, lipids, foams etc all of which exhibit by this feature of softness. Indeed soft matter systems are present in our everyday lives in the form of ice cream, milk, blood, paint, glues, and many other common substances [2].

In simple systems, such as mixture of gases as the rare gases or hydrogen or nitrogen, at room temperatures and pressures the interaction between atoms and molecules fully characterizes its macroscopic structure and dynamics. This is not strictly the case in soft matter systems, in which—even though atoms and molecules are relevant—their physical behavior involves many length scales. Due to this inherent complexity, many soft matter systems are also referred to as complex fluids. This term highlights an important feature shared by some soft matter systems: complexity. At the atomistic length scale the system might appear disorganized but at mesoscopic ranges structures appear, displaying in some cases self-organization. Such is the case of liquid crystals, surfactants, micelles, liposomes, and colloidal systems, to name a few.

Soft matter behavior also appears in mixtures of mesoscopic-sized solutes with microscopic-scaled solvents, i.e. in particular water, but also salts, etc when competing length scales are present. In such a scenario the phase behavior brings about new structures not present in the individual systems. Hydrated biological systems are examples of this type of behavior.

Another important feature of some soft matter systems is the presence of non-Newtonian dynamics. While most materials behave as Newtonian fluids with the shear stress proportional to shear rate, this is not the case of quite a few complex fluids: here one finds that viscosity is not constant but depends on the stress.

The unusual dynamic behavior of soft matter does not restrict itself to the viscoelastic stress dependence. The mixing of polymers such as DNA or proteins with water gives rise to a dynamic behavior both in the polymer and in the water which it is non linear with temperature. Another dynamic aspect of soft matter

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worth mentioning is the propensity for a glassy behavior upon cooling and/or compression. This type of dynamics is able to create self-organization as observed in colloidal, polymeric, and electrostatic systems.

In this special issue, a selection of 30 articles from researchers of Latin America is presented with the aim of showing how this scientific community is active in soft matter and to promote future scientific collaborations among them and with other soft matter groups in the world. It is worth to mention that Statistical Mechanics groups have been formed in different Latin American countries since long time ago, and the actual soft matter groups emerged mainly from them. In this issue several countries are participating: Argentina, Brazil, Chile, Colombia, Mexico, and, Uruguay.

In the Brazilian community this area emerges in the 1990 Brazilian Physical Society Condensed Matter Report as complex systems [3], 'sistemas complexos' meaning studies of polymers, colloids, microemulsions and liquid crystals. The word soft matter does not translate well in Portuguese, therefore the field was denominated as complex systems and later, copying the US denomination, complex fluids [4]. Even though, with a focus in studies of liquid crystals, the community also emerges with contributions in charged systems and core-softened interactions bridging between physics, chemistry, biological and material sciences.

The first works on soft matter in Argentina were produced through the study of liquids. Perhaps the first precedent was the arrival to Argentina of Octavio Fabricio Mossotti, who settled in the University of Buenos Aires around 1828, and where, as he describes in his work, began to think about the dielectric properties of liquids [5]. Slightly more than a century later, in 1939, Félix Cernuschi published, along with Henry Eyring, a theory of critical phenomena in liquids based on particles moving in a regular array of sites in a lattice [6]. Some years later, Antonio Rodriguez developed, under Max Born's supervision, a numerical method to obtain the equation of state of simple liquids within the framework of a general kinetic theory [7]. Starting from these initial works, the field expanded towards the study of more complex systems, such as electrolyte solutions and hydration of proteins and macromolecules, resulting in a numerous and active community in the country that has been meeting annually and continuously for the last 20 years at the Regional Congress of Statistical Mechanics and Applications to Condensed Matter (TREFEMAC) and also at the Soft Matter Division of the Argentine Physics Association, making diverse contributions in colloids, lipids and membranes, active matter, foams, glasses, nanoparticles, interfaces, granular matter, etc.

The first evidence of a formation of a soft matter network in Mexico occurred around 1986, in an event supported by the National Science Foundation and organized by Roberto Alexander, from Universidad Autónoma Metropolitana (UAM) and a group of USA researchers that were interested in polymers and colloids. In parallel, a theoretical group interested in the dynamics of colloidal dispersions developed in the Physics Department of the Centro de Investigación y Estudios Avanzados from the Instituto Politécnico Nacional (CINVESTAV). This group started a productive partnership with the group of Complex Fluids of Rudolf Klein from the University of Konstanz, whose 1988 visit to Mexico triggered the occurrence of a joint UAM-CINVESTAV short summer school, whose success led to the organization in 1989 of the Second 'Encuentro de Ciencia y Tecnología de Coloides y Fluidos Complejos'. One year later, Magdaleno Medina Noyola moved to Universidad Autónoma de San Luis Potosí (UASLP), where the third edition of this meeting took place. Afterwards, a multi-institutional and national coordination allowed this event to be hosted yearly by UASLP over more than two decades. The only interruption occurred early in 2003, when this meeting was substituted by the First Mexican-American

Symposium on Complex Fluids, co-organized by Fyl Pincus, who was an active and enthusiastic supporter of the development of our national soft matter community and of its articulation with its international counterparts. At present, the Meeting on Complex Fluids is still alive and has promoted the relations among multidisciplinary researchers and opened the scope of the meeting to other topics, like biomaterials. Along this process, in the first decade of this century, a young but vigorous national academic community of soft condensed matter could be identified in different universities all over the country. This community was sponsored by the federal Ministry of Education to constitute the first version of a national network in this field, led by José Luis Arauz Lara from UASLP. In 2009, the National Council of Science and Technology (CONACyT) promoted the formation of research networks to attend to national complex problems. Rolando Castillo, from Universidad Nacional Autónoma de México (UNAM), officially structured the Mexican soft matter community, to become the present Soft Condensed Matter Network, which in 2020 had 300 participants from 28 Mexican states. The members of this network are very active and keep collaborating with researchers from different countries.

In this special issue, a number of some of the essential soft matter features mentioned above, as specified in the list of the contributions below.

1.1. Phase behavior and structure of soft matter systems

Soft matter systems can exhibit a number of phases, including glass phases (and related transitions) which can be difficult to be described. Hernandes and collaborators [8] analyze a system of particles interacting through a continuous shouldered well potential. Systems which interact through core-softened two length scales potentials exhibit a number of phases, some of which are difficult to be identified. The authors use neural networks combined with rotational and translational order parameters to identify the phases and to define the order of the transitions.

Another type of soft matter systems that has been considered in this section are the liquid crystals. In such systems the shape of the molecules is responsible for the type of phases present. Salgado-Blanco and co-authors [9] explore by Monte Carlo simulations the phase space of discotic liquid crystals and the phase behavior of this system changes under confinement.

Critical behavior of fatty acids is relevant for the cost reduction in biodiesel production. The liquid–vapor phase diagram of the fatty acids is a complex problem which requires a modeling which takes into account bond distances and angles. Gonzalez *et al* [10] represent this complexity by using a united atom transferable potential designed for phase equilibrium calculations, obtaining not only the liquid–gas coexistence but also the critical point of the fatty acid systems.

Liposomes exhibit a transition from a gel (liquid) to a liquid (gel). At this transition the structure and the size of the liposomes is changed. Velez-Saboya *et al* [11] attempt to shade some light into this particular transition by performing experiments. They show that the phase transition of the liposomes can equally well be described by differential scanning calorimetry or dynamic light scattering methods.

Also from the experimental point of view Wouk *et al* [12] analyze the morphology and energy transfer between conjugated polymers thin films.

1.2. Interaction potentials in soft matter

The collection of papers presented in this section shows the possibility to model the complex behavior of soft matter systems by using effective interaction potentials that have as a key component simple interaction potentials models as for example, hard spheres, square-well, square-shoulder interactions or a

combination of them. These discrete potentials have been successfully applied in liquid state theories. Their main advantage is that they have simple mathematical expressions that simplify their treatment with Statistical Mechanics methods and in some cases analytical expressions for some of their thermodynamic and structural properties can be obtained. The combination of these simple discrete potentials are able to produce a great variety of phase diagrams that make them suitable to model the behavior of complex fluids.

The first contribution of this section is written by de Santiago *et al* [13] and shows that the extended law of corresponding states of Noro and Frenkel, originally developed for pair potentials of variable range, can also be applied to short-range pair potentials with both attractive and repulsive anisotropic interactions. As an illustrative example the authors considered oblate hard ellipsoids with varying short-range square-well interactions using perturbation theory and simulations.

Although discontinuous potentials have a simple mathematical expression problems occur when one wants to use a simulation method that requires the evaluation of forces, since the related forces diverge at the discontinuities of the discrete potentials. This type of problem appears for molecular dynamics or Brownian simulations. To avoid this problem there have been some works reported in the literature that provide a continuous version of some discontinuous potentials that are able to accurately describe the properties of the equivalent original discontinuous potential. With this goal in mind, the second contribution by Munguía-Valadez *et al* [14] presents a generalized continuous multiple step interaction potential that provides a continuous representation of the square-well, square-shoulder potentials and for some combinations of them for their implementation in simulations.

Another effort in this direction is presented in the third paper of this section written by Sandoval-Puentes *et al* [15] who present an alternative solution to provide a continuous version of two discontinuous potentials: square-well and square-shoulder. The criterion to build this soft version of the potential is an extension of the one proposed for hard-spheres [16] that suggests to match the second virial coefficients of both potentials.

The last contribution to this section was written by Perdomo-Pérez *et al* [17] and is devoted to study the impact of competing interactions. The authors study a system of particles interacting through a potential that is a combination of a short-ranged square-well, an intermediate-ranged square-shoulder, and, a long-ranged square-well interactions. This potential is interesting because it exhibits a very rich phase diagram and because it allows to easily analyze the impact of each of the components on the phase behavior, the emerging microstructure, the morphology of the resulting aggregates and the transport phenomena of these fluids.

1.3. Soft matter mixtures

The papers collected in this section address structural and dynamic properties of complex soft matter mixtures, both in equilibrium and non-equilibrium states.

As opening contribution, Tavera-Vázquez *et al* [18], review the experimental approaches to measure the mesoscopic scales of complex fluids embedded in giant cylindrical micelles. Using mean squared displacements determined from quasi-elastic light scattering (diffusive wave spectroscopy) and the inverse adding double method to recover optical parameters, the authors show how it is possible to access properties such as contour, persistence and entanglement lengths, i.e. key quantities in the description of complex fluids such as polymer melts, colloids or biomolecular aggregates.

In the subsequent contribution, Torres-Carbajal and Ramírez-González [19], revisit the process of formation of dynamically arrested states during gelification. The authors illustrate the difference between equilibrium and non-equilibrium gels resorting to a comparison between systems with short range attractive-long range repulsive interactions (SALR) and systems with short range attractive interactions undergoing a quenching process. While the former system first aggregates and then gets trapped into a gel-like phase due to cluster agglomeration (being the liquid vapor transition preempted by the repulsive component of the interaction), in the latter, the vapor–liquid transition itself is interrupted by the quenching process. This contribution illustrates the different dynamics between equilibrium (SALR) system and non-equilibrium gels, despite notorious similarities in their structural properties.

The presence of charges is known to introduce substantial complications in the behavior of physico-chemical systems, and their role is essential in biological soft matter. In their contribution, Bertolotto and Umazano [20] review and extend Manning's counterion condensation theory for the cases of finite saline and polymeric concentrations. The theory they present allows for a satisfactory comparison with experimental data for DNA osmotic coefficients.

A more abstract problem connected with charged systems is analyzed by Salazar *et al* [21], who in their contribution compare an analytical electrostatic description of a gaped surface electrode, modeled in terms of a two-component Coulomb gas, with the corresponding Monte Carlo simulations, evidencing significant differences in the strong coupling regime.

Finally, Pastorino *et al* [22], address a problem in which the effects of inhomogeneity meet with those of nano-confinement under non-equilibrium conditions. Specifically these authors study the effects of surface modification on the heat flow through a liquid–vapor interface in a nano-channel. To that aim a non-equilibrium molecular dynamics simulations is set up thermostating the walls of the nano-channel (slit) at different temperatures, which in in turn are subjected to surface modification by grafting polymer chains using a coarse-grained model. Thermodynamic conditions are set as to induce a vapor-liquid transition inside the nano-channel. The results illustrate how the heat flow can be enhanced by the presence of grafted polymers.

1.4. Biological soft matter systems

This section comprises a series of papers in which soft matter methodologies are applied to a wide range of biological systems.

The first contribution is due to Casafuz *et al* [23], who investigate the morphological changes and spatio-temporal fluctuations of mitochondria in live *Xenopus laevis* melanophores. The authors used an automatic method based on confocal microscopy images to characterize the shape of the mitochondria. Their findings offer insight into the connection between mechanical forces and the shape of mitochondria, and the impact this has on their biological function.

In the second article, Paulo Netz investigates the dynamic behavior and structural properties of water molecules that solvate DNA using classical molecular dynamics simulations [24]. He utilizes various TIP4P family models at a wide range of temperatures. Netz's findings indicate that the TIP4P/2005 and TIP4P-Ew water models exhibit the highest degree of consistency with experimental diffusion coefficient values. These conditions significantly affect the behavior of biological molecules over the whole temperature range.

Next, Olivera *et al* [25] conduct a comprehensive analysis of the structure, composition, and morphology of nanostructured ordered mesoporous silica. This material has a promising potential as antigen carrier in the development of oral vaccines. The team employs a range of experimental techniques, including small angle x-ray scattering, nitrogen adsorption isotherm, and light scattering,

complemented by scanning and transmission electron microscopy, as well as neutron and x-ray tomography.

Yan Barreto and Adriano Alencar have conducted a study on the transport of sugar molecules across biological membranes [26]. Their focus was on the dynamics of glucose uptake by the sodium-glucose transporter of type 2, which they approached using a seven-state model with stochastic steps. Furthermore, they introduced an additional state into the model so as to incorporate an inhibition mechanism. Their study successfully reproduced the experimental dependence of glucose intake on the inhibitor concentration, indicating that the eight-state model effectively captures the underlying physics of this process.

Quercetin is a widely consumed flavonoid and is abundant in the human diet. Mario Campo and Griselda Corral have studied with the help of molecular dynamics simulation quercetin solutions at three different concentrations [27]. The authors have identified the hydrophobic and hydrophilic regions of the quercetin molecule and have observed its effect on the water structure. Through their research, Campo and Corral have found that the hydration behavior of quercetin leads to the formation of aggregates in a π-stacking configuration with increasing concentration.

In one of the many examples of Argentine-Brazilian collaboration, Cathcarth *et al* [28] developed a molecular thermodynamic theory to investigate the adsorption of proteins (cytochrome c, green fluorescent protein, lysozyme, and myoglobin) onto a charge-regulating silica-like surface. Their study encompasses a wide range of experimental conditions, including pH, salt, and protein concentrations. Among several interesting findings, they discover that properly accounting for protonation equilibrium is critical to accurately describing the interactions of proteins with these surfaces.

Closing this section, de la Guerra and Poiré offer a plausible explanation for the prevalence of coughing among healthy individuals [29]. Their study involved a theoretical examination of the dynamics of a fluid mixture consisting of a low viscosity Newtonian fluid and a viscoelastic fluid, propelled by a pulsatile pressure gradient. Through application of their analytical findings to the flow of air and mucus in the trachea, the researchers have identified the frequency that maximizes the dynamic permeability of mucus, which corresponds to the empirically observed frequency of coughing.

1.5. Dynamic and relaxation in soft matter systems

If the presence of many length scales makes the thermodynamics of soft matter systems complex, the dynamics brings along new phenomena. Many of these materials are out of equilibrium with a relaxation dynamics being similar to the slowing down in glasses, other systems present a far from equilibrium with a dynamics which becomes dependent of the two length scales.

The study of Varela *et al* [30] analyzes the temperature dependence of the relaxation time of two charged colloids separated by a distance L interacting in the medium of their N counterions. The authors show that the counterions relaxation time, τ, in one dimension depends basically on N. For odd values of N, τ decreases with increasing temperature while for even N values, τ increases with increasing temperature. The authors attribute this unusual behavior of odd number of counterions to the misfit of one couterion at the double layer.

Peredo-Ortiz *et al* [31] also analyzed the dynamics of systems with charges. In their case the group has studied a suspension of dipolar colloidal systems. The authors applied either an isochoric temperature quench or a sudden isothermal compression. After quenching or compressing the system was carried to one of two non-ergodic conditions: either in a finite time to a new equilibrium state or aging forever to a glassy state. The analysis of these two pathways allow the understanding of the dynamics of colloidal systems.

The description of the dynamics of growing film in the submonolayer regime presents challenges due to the different time scales involved. The traditional way to analyze the kinetics is a one-step growth, where the basic growth units or monomers present a kinetic at constant rate. This process creates the layer formation. In an effort to avoid the interplay of the different time scales, Camargo and González[32] employed a two-step deposition protocol. Using molecular dynamics simulations the authors have studied colloidal particles confined to micro-grooved channels and suggest that their results can be compared with future experiments.

The mobility of polymers at high concentrations depends on a number of factors, including the size of the polymer, the interaction between the monomers and the particular concentration. Guerrero-García *et al* [33] proposed that the activation energy and other dynamic quantities of a spherical tracer immersed into a wormlike micellar network can be described by a Brownian dynamics simulations of a single particle interacting with an effective potential. The method applies for systems in which caging effects are present.

Obtaining the experimental mechanical properties of viscoelastic fluids is also challenging. One of the possible techniques to tackle this problem is the rotational microrheology which is able to measure mechanical properties of optically anisotropic spherical probes. Arauz-Lara *et al* [34] have analyzed the rotation and translation of dumbbell-shaped particles. The authors obtained the complex shear modulus by applying a microrheological approach. Their experimental results indicate that the translational and the rotational mobility of dumbbell shaped particles give similar mechanical properties of the confined viscoelastic media.

1.6. Kinetics of soft matter systems

The papers included in this final section focus on studying various aspects related to the kinetics of soft matter systems.

Olivares *et al* [35] studied the problem of aerosol particle resuspensions, extending a previous model developed in their group, similar to the treatment of heterogeneous surface desorption. Using a Monte Carlo method, the authors have incorporated new mechanisms involving in the resuspension process (rolling, sliding, and taking-off) into the model. The results agree with experimental measurements, showing that the shearing stress required to initiate resuspension decreases as the particle size increases.

Next, Renzo Guido and collaborators addressed, experimentally and through computational simulations, the development and decay of viscoelastic fluid vortices between two coaxial cylinders [36]. They find that—unlike the Newtonian case—the azimuthal velocities of the vortices are non-monotonic, characterized by the presence of maxima or minima followed by a decay to a steady state when the inner cylinder is suddenly put in motion or is abruptly stopped.

In his paper [37], Jason Gallas reports the discovery of non-quantum chirality in the frequency versus amplitude control parameter plane of a Brusselator, by recording how the number of spikes of periodic oscillations evolve when changing the parameters of classical rate equations of motion. Chirality emerges in specific regions of the control parameter space as a macroscopic collective property, due to a large number of distinct trajectories. This is an example of how isospike diagrams can be used to analyze models represented by sets of ordinary differential equations.

The agricultural food industry and manufacturers of rubber-like materials have a keen interest in the development of portable, low-cost devices for measuring the shear elasticity of solids. Nicolás Benech and his colleagues are working in this direction by proposing a simplified Green's function for soft solid elastic plates,

which can retrieve the shear elasticity from near-field measurements [38]. To test the effectiveness of their method, the authors have conducted experiments on agar-gelatin phantoms and mozzarella cheese, and the results showed a good agreement between the theoretical predictions and the experimental observations.

The closing paper of this issue presents a theoretical study conducted by Leticia Rubio Puzzo and her collaborators [39]. Their research shows—similar to equilibrium systems—that the short-time dynamics (STD) technique can be utilized to investigate the order–disorder transition in the Vicsec model with vector noise. This suggests that STD can be an effective tool for analyzing active systems without requiring the system to reach a stationary state, and has the potential to inspire further research in complex systems.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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