Journal of Molecular Liquids 270 (2018) 1–6

Contents lists available at ScienceDirect

Journal of Molecular Liquids

journal homepage: www.elsevier.com/locate/molliq

Editorial Overview

In memory of Lesser Blum

This issue is devoted to the memory of Lesser Blum, one of the leaders of the modern theory of electrolyte solution. We express our deepest condolences to his family, colleagues, and friends.

Lesser was born in Berlin in 1934. This was not an auspicious time and place for a Jew. Fortunately, he and his family were able flee to Argentina in 1942, just before the 'final solution'. Lesser attended the University of Buenos Aires and obtained his Ph.D. in 1956. Unfortunately, at this time there was little encouragement for research in Argentina so Lesser spent a few years as an industrial chemist. His position was in the docks of Buenos Aires. He related an amusing story about a Scandinavian ship that was docked next to his employer. The ship was painted a gleaming white. Presumably it was painted with a lead based paint. The scrubber of the factory failed and plume of noxious gases was emitted. The ship's paint turned black instantly and the ship's captain came out screaming. Who paid for the repainting is not known to us.

In 1955 Juan Peron was ousted and the atmosphere for research improved and Lesser was able to return to the University of Buenos Aires and engage in research and assist in rebuilding the scientific program of the university. Several scholars visited the university. One was Roger Parsons, who lectured on electrochemistry. This had a lasting influence on Lesser.

Lesser was able to obtain fellowships to work in Ottawa, Canada, and Brussels, Belgium. In Brussels he worked with Prigogine and became skilled in statistical mechanics. Around this time, he met and married Elisa (Lita) Sasson. It was a happy marriage. They had three sons Jorge (George), Steven, and Leonardo (Lennie). He was a devoted husband and father.

The situation in Argentina, with frequent coups, led Lesser and Lita to leave Argentina. First, he worked with Zevi Salsburg at Rice University on chemically reactive fluid systems and kinetic theory [1–5]. Later in 1968 he accepted a position at the University of Puerto Rico (UPR), where he remained for most of his scientific career. At the UPR, Lesser played a significant role in the development of statistical mechanics/condensed matter research areas in the Department of Physics during his 37 year career, and helped seal international recognition for the University for pioneering research in these areas. An important contribution in this regard was his effort to attract important scientists to visit the Department, which had lasting positive influence on the academic environment. It was at the UPR that Lesser began to work of the physics and chemistry of electrolyte solutions and electrochemistry He was also a member of the UPR Academic Senate during the years 1980-1982 representing the Faculty of Natural Sciences. He retired from the UPR in 2005 and moved to New Jersey to be near his children and sister. He held visiting positions at Rutgers and Princeton and was active until his health failed. A photograph of Lesser that was taken during his retirement ceremony is part of this essay. We thank Ronald Selsby of the Department of Physics, UPR, for the photograph and his permission to reproduce it.

The word that comes to mind when thinking about the long academic career of Lesser is ***prolific***. His scholarly productivity throughout his career has been truly ***prolific*** in every sense of the word. Having published his first research paper in 1959 [6], he never looked back, and over the next five decades published around 300 more and established collaborations with scientists in at least five continents. Along the way he was on the organizing committee of many international scientific conferences and was on the editorial boards of many scientific journals. He received several awards. Among them was a Guggenheim Fellowship (1978), fellowship in the American Physical Society (1982), and the Joel Hildebrand Award of the American Chemical Society (2003). He also served as Programme Director of the Theoretical Chemistry Division of the National Science Foundation in 1996-1997, while being an Adjunct Professor of Chemistry at Georgetown University.

https://doi.org/10.1016/j.molliq.2018.10.118
0167-7322/

Most of the scientific works of Lesser are connected with the analytical solutions of the Ornstein-Zernike integral equation for different fluid models in the mean spherical approximation (MSA) introduced by Lebowitz and Percus [7]. For ionic fluids he found [8–10] the solution for an electrolyte model consisting of ions with arbitrary size and charge. Here he introduced the now famous parameter Γ, that is a generalization of the Debye-Hückel screening parameter κ [11]. Lesser showed that this parameter is sufficient for the description of thermodynamic and structural properties of ionic systems. The MSA results for thermodynamics were successfully used for the description of thermodynamical properties of electrolyte solutions [12–15]. Lesser next turned his attention to the case of an electrolyte next to a charged interface, otherwise known as electric double layer phenomenon —— one of the important problems in electrochemistry. The results for pair distribution functions in framework of the Henderson-Abraham-Barker theory [16] were successfully applied for the description of such electrolyte solutions near charged surfaces [17–27]. In collaboration with Henderson and Bhuiyan [28] the analytic solution of the classical Gouy-Chapman-Stern theory for the planar electric double layer was found for electrolytes that are asymmetric in both ion size and charge. Some important exact results were formulated in this field such as the contact theorem for density profile of ions near charged wall [19,20].

In parallel with the MSA treatment of ionic models Lesser considered more realistic models for electrolyte solutions, which include the polar solvent molecules explicitly. Since the pair correlation functions for molecules with electrostatic interactions have orientation dependencies, Lesser developed the general scheme of orientational invariant expansions for pair correlation functions and formulated a general scheme of the MSA solution for the coefficients of these expansions [29–32]. The simplest such ion-molecular model is the ion-dipolar model represented by a three-component mixture of positively and negatively spheres and hard spheres with embedded dipoles with the equal ionic and molecular sizes. The MSA solution for such a simplified ion-dipole model was first obtained by Lesser [33,34] and later this solution was simplified and analyzed by him and coworkers [35–37]. The MSA solution was also generalized for the ion-dipole model with different ionic and molecular sizes [38–43]. The obtained results are more complicated than for ionic model. However it was found in this solution the two scaling parameters, Γ for ions and λ for dipoles [43–45], define the thermodynamic properties of ion-dipole model. The obtained results obtained for the ion-dipole model were successfully applied for the description of the Gibbs' solvation energies of monovalent monoatomic ions in different polar solvents [46,47]. For the description of aqueous solutions Lesser improved the model of dipolar hard sphere by adding the tetrahedral orientational interactions [48–50]. He used the results for the ion-dipole model successfully for the description of electrolyte solutions near charged hard walls [51–54]. Around this time Lesser, along with other co-authors, formulated the exact sum rules for an inhomogeneous charged system connected with the effects of the screening of electrostatic interactions [55–57]. Some other exact asymptotic relations, for thermodynamic properties of charged systems were formulated by L. Blum together with Y. Rosenfeld [58–60].

Lesser also considered the MSA solution for fluids with Yukawa type of inter-particle interactions. The results were used to the study bulk and surface properties and for the improvement of the closure relations in the Ornstein-Zernike equation [61–65]. For the MSA solution for fluids with multi-Yukawa interactions it was shown that for such fluids it is also possible to introduce a scaling parameter Γ and the structural and thermodynamic properties can be described in term of this parameter [66–71].

A new promising approach for the investigation of adsorption of fluids on crystalline surfaces was developed by Lesser together with Badiali and Rosinberg in 1986 [72]. In this paper, the interface between solid and fluid is modelled by a flat surface with sticky sites placed on a regular lattice. After averaging over the fluid configuration, the model was mapped into a two-dimensional lattice-gas model with the interaction energies of the particles on the sites related to the potential of mean force in an inhomogeneous fluid. It was shown that the first layer of a fluid at contact with solid can exhibit an order-disorder phase transition which can be interpreted as cooperative adsorption. Later this effect was investigated in more detail by Lesser together with Huckaby [73–75] and it was used by them for interpretation of different phenomena at the interface electrode-electrolyte solutions [76–79].

During the final decade of the last century Lesser was a regular summer visitor at the Universite P. et M. Curie in Paris. Strong collaboration with the laboratory of P. Turq opened the possibility of applying the MSA approach to describe transport properties of electrolyte solutions [80–83]. Around this time Lesser, together with his coworkers, generalized the results of the MSA for ionic fluids for the presence of ionic associations. Towards this aim, within the framework of the Wertheim-Ornstein-Zernike integral equation theory [84,85], the associative mean spherical approximation (AMSA) [86] and the binding mean spherical approximation (BIMSA) [87] were formulated. These approaches are practically identical. The results for ionic fluids that included ionic dimerization [88], were generalized to encompass more complex ionic associations such as the formation of ionic chains [89], networks [90], polyelectrolytes [91], and highly asymmetric ionic fluids [92]. Again it was shown that the AMSA solution for ionic system with different types of associations can be given in the terms of a single screening parameter Γ_B, which plays the same role as the parameter Γ in the MSA theory for simple electrolytes. With his French colleagues Lesser used the MSA and the AMSA results for the description of thermodynamic properties of electrolyte solutions [93–95]. An interpolation scheme as a combination of the MSA and the AMSA was proposed for ionic fluids. It was shown that such scheme reproduces satisfactorily computer simulation data for the critical point in ionic fluids [96,97]. In Paris, Lesser collaborated successfully with the theoretical group of B. Jancovici from Orsay Universite. This collaboration led to some interesting exact results for one and two dimensional coulombic systems [98–100].

Lesser was the one of the leaders of modern liquid matter theory. He collaborated and had joint publications with other leaders such as H.L. Friedman, K. Gubbins, D. Henderson, J.L. Lebowitz, G. Stell, J.M. Prausnitz, M. Wertheim and others. Lesser also developed close connection with experimentalists. For example, he collaborated with such known specialists in neutron scattering as A.H. Narten. They used the MSA for the description of the structure of liquid metals [101]. From neutron diffraction they extracted atom pair distribution functions of liquid water [102]. He also collaborated with a known specialist in electrochemistry, W.R. Fawcett, and many others.

We should note that the analytical solution of MSA for different models that Lesser treated is not so simple. It involves complex and tedious algebra but the final results are usually very clear. But with his insightful imagination Lesser knew the results intuitively from the beginning and the complex mathematics was only a means to that end.

MH knew Lesser from his first papers about the MSA for the ion-dipole model. He reproduced these results and then tried to generalize this for size-asymmetric ion-dipole systems, but with Lesser it was impossible to be in competition and later MH collaborated with Lesser on the AMSA solution for different models of ionic fluids. MH met Lesser personally for the first time at a conference in Asilomar, California, in 1990, and later at other conferences and during their mutual visits to Paris. MH found Lesser to be very attractive and intelligent personality. He was equally fluent in English, French, Spanish and German. He could also speak Italian and Portuguese.

OB was doing his PhD thesis in Paris when he met Lesser during one of his visits to the laboratory of P. Turq. At first OB did not know MSA and HNC theories. Lesser was presenting his work on sticky electrolytes – another curiosity at the time. Lesser's suggestion prompted OB to apply simply the distribution functions given by MSA to the description of transport properties of electrolyte solutions.

Later, this collaboration was continued with the introduction of the MSA approach in the framework of the Wertheim-Ornstein-Zernike integral equations to describe the ionic dimerization and the formation of charged chains. Lesser invited OB to visit him in Puerto Rico which the latter did in 2002. Lesser was a very welcoming host and this visit generated stimulating scientific discussions. We also keep the memory of pleasant scientific meetings with him, especially during CECAM workshops in Lyons, France. The last time we saw Lesser in Paris was in May 2011. He continued his research enthusiastically despite health issues.

LBB began his career at the UPR as Lesser's post-doc in the early 1980's and was greatly impressed by Lesser's unflinching devotion to science, an infectious enthusiasm for research, his tireless hard-working nature, and phenomenal output. All this, coupled with an amiable, friendly disposition made Lesser a role model at the Department of Physics and the Natural Sciences Faculty.

DH first met Lesser at one of Joel Lebowitz's Statistical Mechanics meeting in 1967 and again at a meeting in Mexico City in 1975. At the Mexico City meeting, Lesser invited DH to visit UPR, which he did in 1976. This was the first of several visits. Lesser was always a stimulating colleague and a hospitable host. Many pleasant weekends were spent at Dorado Beach and other parts of the island.

The last time DH saw Lesser was at a meeting in Puerto Vallarta, Mexico, in 2003. Lesser, Yurko Duda, and DH had lunch together at the end of the meeting. On this occasion, Lesser forecast that he and DH would live about ten years more and die at about the age of 80. Surprisingly, it was Yurko, who was much younger, who died first. However, Lesser was quite accurate about himself. He passed away in New Jersey at the age of 82 on April 24, 2016, surrounded by his family. He is missed, personally and scientifically.

This special issue contains articles by collaborators, former students, and friends of Lesser. The contents can be separated approximately into three parts. The first one is connected with the studies of the bulk properties of liquids and solutions [103–117]. The second part is devoted to investigations of surface properties of liquids and solutions [118–126]. The third part includes some biological aspects [127–131]. Nine papers [103–111] are connected with the development and applications of MSA and AMSA approaches, one of the favorite topics of Lesser. In particular Kalyuzhnui, Reščič, Holovko, and Cummings [103] developed the AMSA theory for several versions of primitive models of room temperature ionic liquids modeled as two-component mixture of hard-sphere anions and linear chain cations represented by tangentially bonded hard spheres with the charge located on one of the terminal bonds. The theory reduces to solving one nonlinear algebraic equation for the screening parameter Γ and was applied to the description of vapour-liquid phase coexistence. Bernard and Simonin [104] have proposed the AMSA approach for polyelectrolytes considering polyelectrolytic chain formation and associations of counterions on the chains. The expressions for the screening parameters the internal and free energy are established. Herrera [105] has discussed the thermodynamics and structural properties of hard-sphere fluids with multi-Yukawa interactions obtained from the MSA approach. Villard, Bernard and Dufrêche [106] have used the MSA solution for the study the problem of specificity in aqueous electrolyte solutions which is taken into account by association term similar to that in the Bjerrum theory. The activity coefficients obtained are used for the description of pure electrolytes and electrolyte mixtures up to molar concentrations. Luksic, Slejko, and Hribar-Lee [107] used a primitive ionic model in mixture with uncharged hard spheres for the modeling of the influence of the poly(ethylene glycol) on the mean activity coefficients of NaCl aqueous solutions. It was shown that MSA theory for such simple model can be successfully used for the interpretation of experimental data. Holovko and Protsykevich [108] have analysed the analytical solution of AMSA for ion-dipole model and discussed the possibility of using this result for electrolyte solutions. Using the MSA solution for dipolar mixture Bandura, Holovko, and Lvov [109] have derived a new analytical expression for the solvation energy of dipolar molecules in polar solvents which generalizes the Kirkwood classical expression obtained in the framework of dielectric continuum model. This result together with corresponding generalization of Born classical expression for solvation energy of ions in polar solvents obtained from MSA solutions for ion-dipole mixture, were applied by Lvov, Hall, Bandura, and Gamwo [110] in the description of standard molar Gibbs energies of ions and ionic pairs in aqueous solutions above and below the critical point of water. Janc, Vlachy, and Luksic [111] present the calorimetric studies of the enthalpy of mixing of bovine serum albumin in water at different pH with several low molecular weight salts. The MSA was used to estimate the Coulomb effects upon mixing.

Different aspects of bulk properties of liquids and solutions are considered also in papers [112–117]. In particular, in the paper of Rouha, Nezbeda, Hruby, and Moucka [112] the second, third and fourth virial coefficients for the non-polarizable TiP4P/2005 model of water and the polarizable BK3 model are presented and compared with available experimental and pseudo-experimental data. Urbic [113] has studied the structural and thermodynamic properties of two-dimensional fluids with one site associating point by the site-site integral equation theory, the Wertheim's thermodynamics perturbation theory and the Wertheim's integral equation theory for associative fluids. The accuracy of the theories were checked by comparing with the corresponding Monte Carlo results. Patsahan (O), Patashan (T), and Holovko [114] have studied the influence of charge and size asymmetry of ions on vapour-liquid phase transition of ionic fluids in disordered porous media by combine the collective variables and scaled particle theories and the replica method. HØye and Lomba [115] return to investigation of critical properties in framework of the hierarchical reference theory and discuss connection with the self-consistent Ornstein-Zernike approximation. Raineri, Wise, and Ben-Amotz [116] have presented a new statistical-mechanical approach for studying the energetics of solvent restructuring in solvation processes where only the interactions between the solute and solvent molecules change. Vericat, Carlevano, Stoico and Renzi [117] have developed a theory for physical clusters bonded in clusters along a finite time, so-called residence time.

Seven papers [118–124] from the second part of this issue are connected with different aspects of electrical double layer theory, one of Lesser's enduring research interests spanning over three decades. In particular Ciach [118] presents the simple theory for oscillatory charge profile in ionic liquids near a charged wall in the framework of mesoscopic field theory for ionic systems. By using coarse-grained models and the density theory, Neal, Wesolowski, Henderson, and Wu [119] have investigated the distribution of ions among idealized nanopores in contact with an asymmetric ionic liquid mixture and the effects of the bulk electrolyte composition on the capacitive energy storage. In [120] Patra resorts to density functional theory and Monte Carlo simulations in order to study the effect of multivalent counterions on the spherical electrical double layers with size and charge asymmetric mixed electrolytes. Gonzalez-Tovar, Lozada-Cassou, Bhuiyan, and Outhwaite [121] have studied the zeta potential and structure of a model cylindrical double layer by Poisson-Boltzmann theory, hypernetted chain/mean spherical approximation, the modified Poisson-Boltzmann theory, and the density functional theory. The results are compared with the corresponding Monte Carlo simulations data. In [122] Lee, Ramos(FS), and Ramos(AM) resort to a density functional theory based on the third-order Ornstein-Zernike relation in order to study the adsorption of mixtures of the Yukawa ions near a hard wall. Satisfactory agreements are obtained with corresponded computer simulation results. Spada, Gavryushov and Bohinc [123] have, in framework of a modified Poisson-Boltzmann theory, have investigated the mechanism of attractive interaction between two like-charged surfaces embedded in an electrolyte composed of positively and negatively charged spherical nonoparticles. Bokum, di Caprio, Holovko, and Vikhrenko [124] have studied the influence of vacancies on the charge screening of mobile ions in lattice models. It is shown that the value of

square of inverse Debye-Huckel length is proportional to the product of the concentration of mobile ions and the concentration of vacancies. It is further shown that inclusion of the entropy term connected with vacancies leads to a Fermi-Dirac-like charge distribution at a plain boundary. The influence of the variation of the crystal field near the boundary on the structure and electro-physical characteristics of a double layer are discussed. Borówko, Ryzsko, Sokolowski, and Pizio [125] have considered molecular dynamics and density functional study of the structure of hairy particles at a hard wall. Druchok and Luksic [126] present the molecular dynamics investigation of concept of nanocarries based on carbo-cylated nanotubes with anionic functional groups and tetra-alkyl-ammonium cations acting as corks.

And finally five other papers [127–131] have some biological aspects. Eisenberg [127] has formulated general biological questions to physical systems needed for understanding of fundamental biological problems. Hirata [128] has proposed a theory to analyse the elastic incoherent neutron scattering data of aqueous solutions of protein, based on the generalized Langevin theory combined with the 3D-RISM/RISM equation. In the framework of this theory, the abrupt change of the gradient of the mean square displacement of protein versus the temperature is interpreted as an onset of "solvent-induced elasticity" with increasing temperature. Zhang, Xu, Xiong, Peng, Kumari, ans Wei [129] have presented molecular dynamic simulations showing why calcium ions cause membrane defects and water leakage. Kastelic, Dill, Kalyuzhnyi, and Vlachy [130] have modified Wertheim's theory of associating fluid to model antibody solutions, specifically to study qualitative relations between the structure and interactions of antibodies and the viscosity of solution. Molecular dynamics simulations were used to investigate the dissolution of aspirin nanocrystals in water in the paper of Anand and Patey [131].

We express our gratitude to all of the contributors of this special issue.

References

[1] L. Blum, Z.W. Salsburg, Light scattering from a chemically reactive fluid, J. Chem. Phys. 48 (1968) 2292–2309.
[2] L. Blum, On the effect of Breit-Wigner resonances in chemical kinetics, J. Chem. Phys. 49 (1968) 1922–1931.
[3] L. Blum, Z.W. Salsburg, Light scattering from a chemically reactive fluid ii: case with diffusion, J. Chem. Phys. 50 (1969) 1654–1660.
[4] L. Blum, J.L. Lebowitz, Binary collision expansion for kinetic equation, Phys. Rev. 185 (1969) 273–285.
[5] L. Blum, H.L. Frisch, Light scattering from optically active fluids, J. Chem. Phys. 52 (1970) 4379–4384.
[6] L. Blum, N.V. Cohan, Orbital following in tetrahedral molecules, Can. J. Phys. 37 (1959) 1002–1007.
[7] J.L. Lebowitz, J.K. Percus, Mean spherical model for lattice gases with extended hard cores and continuum fluids, Phys. Rev. 144 (1966) 251–258.
[8] L. Blum, Mean spherical model for asymmetric electrolytes. I: Method of solution, Mol. Phys. 30 (1975) 1529–1535.
[9] L. Blum, J.S. Hoye, Mean spherical approximation for asymmetric electrolytes II: Thermodynamic properties and the pair correlation function, J. Phys. Chem. 81 (1977) 1311–1316.
[10] Simple electrolytes in the mean spherical approximation, in: L. Blum, H. Eyring, D.J. Henderson (Eds.), Theoretical Chemistry Advances and Perspectives, Academic Press, N. York, 1980.
[11] P. Debye, E. Huckel, Zur theoretie der elecrtolyte, Z. Phys. 24 (1924) 185–206.
[12] J.R. Grigera, L. Blum, Mean spherical model approximation for the primitive model of sodium chloride, Chem. Phys. Lett. 38 (1976) 486–488.
[13] R. Triolo, J.R. Grigera, L. Blum, Simple electrolytes in the mean spherical approximation, J. Phys. Chem. 80 (1976) 1858–1861.
[14] R. Triolo, L. Blum, M.A. Floriano, Simple electrolytes in the mean spherical approximation III: A workable model for aqueous solutions, J. Chem. Phys. 67 (1978) 5956–5989.
[15] R. Triolo, L. Blum, M.A. Floriano, Simple electrolytes in the mean spherical approximation II: Study of a refined model, J. Phys. Chem. 82 (1978) 1368–1370.
[16] D. Henderson, F.F. Abraham, J.A. Barker, The Ornstein-Zernike equation for a fluid in contact with a surface, Mol. Phys. 31 (1976) 1291–1295.
[17] L. Blum, G. Stell, Solution of the Ornstein-Zernike equation for the wall-particle distribution function, J. Stat. Phys. 16 (1976) 439–449.
[18] L. Blum, Theory of electrified interfaces, J. Phys. Chem. 81 (1977) 136–147.
[19] D. Henderson, L. Blum, Some exact results and the application of the MSA to charged hard spheres near a charged hard wall, J. Chem. Phys. 69 (1978) 5441–5449.
[20] D. Henderson, L. Blum, J.L. Lebowitz, An exact formula for the contact value of the density profile of a system of charged hard spheres near a charged wall, J. Electroanal. Chem. 102 (1979) 315–319.
[21] D.A. McQuarrie, W. Olivares, D. Henderson, L. Blum, On Derjaguin's formula for the force between planar double layers, J. Colloid Interface Sci. 77 (1980) 272–273.
[22] L. Blum, J.L. Lebowitz, D. Henderson, A condition on the derivative of the diffuse layer potential in the primitive model of an electrode double layer, J. Chem. Phys. 72 (1980) 4249–4250.
[23] D. Henderson, L. Blum, Application of the GMSA to the electric double layer, Can. J. Chem. 59 (1981) 1906–1917.
[24] D. Henderson, L. Blum, A simple non-iterative method for calculating the potential of an electric double layer, J. Electroanal. Chem. 111 (1980) 217–222.
[25] D. Henderson, L. Blum, D.A. McQuarrie, W. Olivares, An extended mean spherical approximation calculation for the potential of an electrified interface, Chem. Phys. Lett. 71 (1980) 569–571.
[26] D. Henderson, L. Blum, M. Lozada-Cassou, The statistical mechanics of the electric double layer, J. Electroanal. Chem. 150 (1983) 291–303.
[27] L. Blum, D. Henderson, R. Parsons, The mean spherical capacitance approximation of the double layer for an electrolyte at high concentration, J. Electroanal. Chem. 161 (1984) 389–392.
[28] L.B. Bhuiyan, L. Blum, D. Henderson, The Application of the Modified Gouy Chapman Theory to an Electrical Double Layer Containing Asymmetric Ions, J. Chem. Phys. 78 (1983) 442–445.
[29] L. Blum, A.J. Torruella, Invariant expansion for two body correlations: Thermodynamic functions, scattering and the Ornstein-Zernike equation, J. Chem. Phys. 56 (1972) 303–310.
[30] L. Blum, Invariant expansion II: The Ornstein-Zernike equation for non spherical molecules and an extended solution to the mean spherical model, J. Chem. Phys. 57 (1972) 1862–1869.
[31] L. Blum, Invariant expansion III: The general solution of the mean spherical model for neutral spheres with electrostatic interactions, J. Chem. Phys. 58 (1973) 3295–3303.
[32] L. Blum, A.J. Torruella, Invariant expansion IV: The exponentials of tensorial expressions, J. Chem. Phys. 89 (1988) 4976–4980.
[33] L. Blum, Solution of the mean spherical model for a mixture of charged hard spheres and dipoles, Chem. Phys. Lett. 26 (1974) 200–202.
[34] L. Blum, Solution of a model of solvent electrolyte interaction in the mean spherical approximation, J. Chem. Phys. 61 (1974) 2129–2133.
[35] F. Vericat, L. Blum, Mean spherical model for a mixture of hard ions and dipoles: thermodynamics and correlation functions, J. Stat. Phys. 22 (1980) 593–604.
[36] W. Perez-Hernandez, L. Blum, Explicit solution of the MSA for ions and dipoles, J. Stat. Phys. 24 (1981) 451–454.
[37] L. Blum, F. Vericat, Molecular description of ionic solvation and ion-ion interactions in dipolar solvents, in: R.R. Dogonadze, E. Kalman, A.A. Kornyshev, J. Ulstrup (Eds.), The Chemical Physics of Solvation Part A, Elsevier, North Holland, Amsterdam, 1985.
[38] L. Blum, Solution of the mean spherical approximation for hard ions and dipoles of arbitrary size, J. Stat. Phys. 18 (1978) 451–474.
[39] L. Blum, D.Q. Wei, Analytical solution of the mean spherical approximation for an arbitrary mixture of ions and dipolar solvent, J. Chem. Phys. 87 (1987) 555–565.
[40] D.Q. Wei, L. Blum, Internal energy in the mean spherical approximation (MSA) as compared to Debye-Huckel theory, J. Phys. Chem. 91 (1987) 4342–4343.
[41] D.Q. Wei, L. Blum, Analytical solution of the mean spherical approximation for an arbitrary mixture of ions and dipolar solvent: Approximate solution pair correlations and thermodynamics, J. Chem. Phys. 87 (1987) 2999–3007.
[42] D.Q. Wei, L. Blum, Non-primitive model of electrolytes: Analytical solution of the mean spherical approximation an arbitrary mixture of sticky ions and dipoles, J. Chem. Phys. 89 (1988) 1091–1100.
[43] L. Blum, F. Vericat, W.R. Fawcett, On the mean spherical approximation for hard ions and dipoles, J. Chem. Phys. 96 (1992) 3039–3044.
[44] L. Blum, Scaling in charged fluids: Beyond simple ions, Condens. Matter Phys. 4 (2001) 611–620.
[45] L. Blum, Scaling for a mixture of hard ions and dipoles, J. Chem. Phys. 117 (2002) 756–765.
[46] L. Blum, W.R. Fawcett, Application of the mean spherical approximation to describe the Gibbs' solvation energies of monovalent monoatomic ions in non-aqueous solvents, J. Phys. Chem. 96 (1992) 408–414.
[47] W.R. Fawcett, L. Blum, A simple model for ion solvation with non additive cores, Condens. Matter Phys. 2 (1993) 76–84.
[48] D. Bratko, L. Blum, A. Luzar, A simple model for the intermolecular potential of water, J. Chem. Phys. 83 (1985) 6367–6370.
[49] L. Blum, F. Vericat, J.N. Herrera, On the analytical solution of the Ornstein-Zernike equation with Yukawa closure, J. Stat. Phys. 66 (1992) 249–262.
[50] C.M. Carlevaro, L. Blum, F. Vericat, Generalized Mean Spherical Approximation for a model of water with dipole, quadrupole and short range potential of tetrahedral symmetry, J. Chem. Phys. 119 (2003) 5198–5215.
[51] L. Blum, D. Henderson, Mixtures of hard ions and dipoles against a charged hard wall: Ornstein-Zernike equation, some exact results and the mean spherical approximation, J. Chem. Phys. 74 (1981) 1902–1910.
[52] D. Henderson, L. Blum, A simple theory of the electric double layer including solvent effects, J. Electroanal. Chem. 132 (1982) 1–13.
[53] F. Vericat, D. Henderson, L. Blum, Generalized mean spherical approximation of hard ions and dipoles against a charged hard wall, J. Chem. Phys. 77 (1982) 5808–5815.
[54] F. Vericat, L. Blum, D. Henderson, Non-primitive electrolyte near a charged hard wall: generalized mean spherical approximation, J. Electroanal. Chem. 150 (1983) 315–324.

[55] L. Blum, J.L. Lebowitz, D. Henderson, C. Gruber, P.A. Martin, A sum rule for an inhomogeneous electrolyte, J. Chem. Phys. 75 (1981) 5974–5975.
[56] L. Blum, C. Gruber, J.L. Lebowitz, P.A. Martin, On perfect screening for charged systems, Phys. Rev. Lett. 48 (1982) 1769–1772.
[57] L. Blum, C. Gruber, D. Henderson, J.L. Lebowitz, P.A. Martin, On the properties of inhomogeneous charged systems, J. Chem. Phys. 78 (1983) 3195–3203.
[58] Y. Rosenfeld, L. Blum, Statistical thermodynamics of charged objects, J. Phys. Chem. 89 (1985) 5149–5151.
[59] Y. Rosenfeld, L. Blum, Statistical mehanics of charged objects: General method and application to simple systems, J. Chem. Phys. 85 (1986) 1556–1566.
[60] L. Blum, Y. Rosenfeld, Relation between the free energy and the direct correlation function in the mean spherical approximation, J. Stat. Phys. 63 (1991) 1177–1190.
[61] L. Blum, J.S. HØye, Solution of the Yukawa closure of the Ornstein-Zernike equation, J. Stat. Phys. 16 (1977) 399–413.
[62] L. Blum, J.S. HØye, Solution of the Ornstein-Zernike equation with Yukawa closure for a mixture, J. Stat. Phys. 19 (1978) 317–324.
[63] D. Henderson, E. Waisman, J.L. Lebowitz, L. Blum, Equation of state of a hard core fluid with a Yukawa tail, Mol. Phys. 35 (1978) 241–255.
[64] D. Henderson, J.L. Lebowitz, L. Blum, E. Waisman, The mean spherical approximation for a Yukawa fluid interacting with a hard planar wall with a Yukawa tail, Mol. Phys. 39 (1980) 47–50.
[65] L. Blum, Solution of the Ornstein-Zernike equation for a mixture of of hard ions and Yukawa closure, J. Stat. Phys. 22 (1980) 661–672.
[66] J.N. Herrera, L. Blum, P.T. Cummings, Equation of state for a Yukawa fluid in the mean spherical approximation, Mol. Phys. 93 (1998) 73–78.
[67] L. Blum, J.N. Herrera, Analytical solution of the Yukawa closure of the Ornstein-Zernike equation II: The full solution, Mol. Phys. 95 (1998) 425–429.
[68] L. Blum, J.N. Herrera, Analytical solution of the Yukawa closure of the Ornstein-Zernike equation III: The 1 component case, Mol. Phys. 96 (1999) 821–826.
[69] O. Vazquer, J.N. Herrera, L. Blum, Thermodynamic properties and static structure factors of a binary mixtures of a Yukawa fluids, Phys. A 325 (2003) 319–332.
[70] L. Blum, J.A. Hernando, Yukawa Fluids: A new solution of the one component case, Condens. Matter Phys. 6 (2003) 447–458.
[71] L. Blum, M. Arias, Structure of Multi-component/Multi-Yukawa mixtures, J. Phys. Condens. Matter 18 (2006) S 2437–S 2450.
[72] J.P. Badiali, L. Blum, M.L. Rosinberg, The discrete site sticky wall model, Chem. Phys. Lett. 129 (1986) 149–154.
[73] D.A. Huckaby, L. Blum, Exact results for the adsorption of a dense fluid onto a triangular lattice of sticky sites, J. Chem. Phys. 92 (1990) 2646–2649.
[74] D.A. Huckaby, L. Blum, A model for sequential first order phase transitions occurring in the underpotential deposition of metals, J. Electroanal. Chem. 315 (1991) 255–261.
[75] L. Blum, D.A. Huckaby, Underpotential deposition of Cu on Au(111): Implications of the hb model, J. Electroanal. Chem. 375 (1994) 69–77.
[76] D.A. Huckaby, L. Blum, Rigorous analysis of low temperature phases in a model for the underpotential deposition copper on the (111) surface of gold in the presence of bisulfate, Langmuir 11 (1995) 4583–4587.
[77] L. Blum, D.A. Huckaby, M. Legault, Phase transitions at electrode interfaces, Electrochim. Acta 41 (1996) 2207–2227.
[78] A. Belkasri, D. Huckaby, L. Blum, Guanidinium nitrate phases, Langmuir 13 (1997) 4887.
[79] D.A. Huckaby, R. Pitis, A.K. Belkasri, M. Shinmi, L. Blum, Molecular mirror images, dense ice phases, organic salts at interfaces and electrochemical deposition: Exotic applications of the Pirogov-Sinai theory, Phys. A 285 (2000) 211–219.
[80] O. Bernard, W. Kunz, P. Turq, L. Blum, Self diffusion in electrolyte solutions: a MSA approach, J. Phys. Chem. 96 (1992) 398–403.
[81] O. Bernard, W. Kunz, P. Turq, L. Blum, Conductance in electrolyte solutions using the mean spherical approximation, J. Phys. Chem. 96 (1992) 3833–3840.
[82] S. Durand-Vidal, P. Turq, O. Bernard, C. Treiner, L. Blum, New perspectives in transport phenomena in electrolyte solutions, Phys. A 231 (1996) 123–143.
[83] O. Bernard, T. Cartailler, P. Turq, L. Blum, Mutual diffusion coefficients in electrolyte solutions, J. Mol. Liq. 73-74 (1997) 403–411.
[84] M.S. Wertheim, Fluids with highly directional attractive forces, J. Stat. Phys 35 (1984) (I Statistical thermodynamics p.19-34. II. Thermodynamic perturbation theory and integral equations. p.35-47).
[85] M.S. Wertheim, Fluids with highly directional attractive forces, J. Stat. Phys 42 (1986) (III. Multiple attraction sites. p. 459-476 IV. Equilibrium polymerization. p. 477-492).
[86] M. Holovko, Yu.V. Kalyuzhnyi, On the effects of association in the statistical theory of ionic systems. analytical solution of the PY-MSA version of the Wertheim theory, Mol. Phys. 73 (1991) 1145–1157.
[87] L. Blum, O. Bernard, The general solution of the associating mean spherical approximation for dimerizing ions, J. Stat. Phys. 79 (1995) 569–583.
[88] O. Bernard, L. Blum, Binding mean spherical approximation for pairing ions: The BIMSA-EXP approximation and thermodynamics, J. Chem. Phys. 104 (1996) 4746–4754.
[89] I.A. Protsykevytch, M.F. Holovko, Yu.V. Kalyuzhnyi, L. Blum, General solution of the polymer MSA for the totally flexible two point electrolyte model, J. Mol. Liq. **73-74** (1997) 1–26.
[90] L. Blum, M.F. Holovko, I.A. Protsykevych, A solution of the multiple binding mean spherical approximation for ionic mixtures, J. Stat. Phys. 84 (1996) 191–204.
[91] O. Bernard, L. Blum, Thermodynamics of a model for flexible polyelectrolytes in the binding mean spherical approximation, J. Chem. Phys. 112 (2000) 7227–7237.
[92] Yu.V. Kalyuzhnyi, L. Blum, M.F. Holovko, I.A. Protsykevytch, Primitive model for highly asymmetric electrolytes: Associative mean spherical approximation, Phys. A 236 (1997) 85–96.
[93] J.P. Simonin, L. Blum, P. Turq, Thermodynamics of real ionic solutions in the mean spherical approximation: Simple salts in the primitive model, J. Phys. Chem. 100 (1996) 7704–7709.
[94] J.P. Simonin, O. Bernard, L. Blum, Real ionic solutions in the mean spherical approximation 3: Osmotic and activity coefficients for pure associating electrolytes in the primitive model, J. Phys. Chem. **B** 102 (1998) 4411–4417.
[95] J.P. Simonin, O. Bernard, L. Blum, Ionic solutions in the binding mean spherical, approximation: Thermodynamic properties of mixtures of associating electrolytes, J. Phys. Chem. **B** 103 (1999) 699–704.
[96] J.W. Jiang, L. Blum, O. Bernard, J.M. Prausnitz, S.I. Sandler, Binding mean-spherical approximation for charged hard dumbbells, J. Chem. Phys. 116 (2002) 7977–7982.
[97] J.W. Jiang, L. Blum, O. Bernard, J.M. Prausnitz, Thermodynamics and phase equilibria of charged hard-sphere chain model for polyelectrolyte solution, Mol. Phys. 99 (2001) 1121–1128.
[98] L. Blum, B. Jancovici, An exactly solvable model for the interaction of two parallel charged plates in a ionic media, J. Phys. Chem. 88 (1984) 2294–2297.
[99] A. Alastuey, B. Jancovici, L. Blum, P.J. Forrester, M.L. Rosinberg, Comment to the ideally polarizable interface: A solvable model and general sum rules, J. Chem. Phys. 83 (1985) 2366–2367.
[100] F. Cornu, B. Jancovici, L. Blum, The two dimensional one component plasma in a doubly periodic background: Exact results, J. Stat. Phys. 50 (1988) 1221–1243.
[101] L. Blum, A.H. Narten, The mean spherical model for the structure of liquid metals, J. Chem. Phys. 56 (1972) 5197–5198.
[102] A.H. Narten, W.E. Thiessen, L. Blum, Atom pair distribution functions of liquid water at 25^0C from neutron diffraction, Science 217 (1982) 1033–1034.
[103] Y.V. Kalyuzhnyi, J. Reščič, M. Holovko, P.T. Cummings, Primitive models of the room temperature ionic liquids. Liquid-gas phase coexistence, J. Mol. Liq. 270 (2018) 7–13.
[104] O. Bernard, J.-P. Simonin, Association of counterions on polyelectrolytes: Thermodynamic properties in the binding mean spherical approximation, J. Mol. Liq. 270 (2018) 14–24.
[105] J.N. Herrera, Thermodynamic and structural properties of fluids with a hard-sphere plus multi-Yukawa interaction potential, J. Mol. Liq. 270 (2018) 25–29.
[106] A. Villard, O. Bernard, J.-F. Dufrêche, Non additivity of ionic radii in electrolyte solutions: Hofmeister effect on mixtures modelled by an Associated MSA model, J. Mol. Liq. 270 (2018) 30–39.
[107] M. Luksic, E. Slejko, B. Hribar-Lee, The influence of the poly (ethylene glycol) on the mean activity coefficients of NaCl aqueous solutions. The application of the MSA and HNC method, J. Mol. Liq. 270 (2018) 40–45.
[108] M. Holovko, I. Protsykevich, On the application of the associative mean spherical approximation to the ion-dipole model for electrolyte solutions, J. Mol. Liq. 270 (2018) 46–51.
[109] A.V. Bandura, M.F. Holovko, S.N. Lvov, The chemical potential of a dipole in dipolar solvent at infinite dilution: Mean spherical approximation and Monte Carlo simulations, J. Mol. Liq. 270 (2018) 52–61.
[110] S.N. Lvov, D.M. Hall, A.V. Bandura, I.K. Gamwo, A semi-empirical molecular statistical thermodynamic model for calculating standard molar Gibbs energies of aqueous species above and below the critical point of water, J. Mol. Liq. 270 (2018) 62–73.
[111] T. Janc, V. Vlachy, M. Luksic, Calorimetric studies of interactions between low molecular weight salts and bovine serum albumin in water at pH values below and above the isoionic points, J. Mol. Liq. 270 (2018) 74–80.
[112] M. Rouha, I. Nezbeda, J. Hruby, F. Moucka, Higher virial coefficients of water, J. Mol. Liq. 270 (2018) 81–86.
[113] T. Urbic, Two dimensional fluid with one site-site associating point. Monte Carlo, integral equation and thermodynamic perturbation theory study, J. Mol. Liq. 270 (2018) 87–96.
[114] O. Patsahan, T. Patsahan, M. Holovko, Vapour-liquid critical parameters of a 2:1 primitive model on ionic fluids confined in disordered porous media, J. Mol. Liq. 270 (2018) 97–105.
[115] J.S. HØye, E. Lomba, Critical properties of the hierarchical reference theory: Further investigations, J. Mol. Liq. 270 (2018) 106–113.
[116] F.O. Raineri, P. Wise, D. Ben-Amotz, Solvent scaling scheme for studying solvent restructuring thermodynamics in solvation processes, J. Mol. Liq. 270 (2018) 114–127.
[117] F. Vericat, C.M. Carlevaro, C.O. Stoico, D.G. Renzi, Clustering and percolation theory for continuum systems: clusters with non specific bonds and a residence time in their definition, J. Mol. Liq. 270 (2018) 128–137.
[118] A. Ciach, Simple theory for oscillatory charge profile in ionic liquids near a charged wall, J. Mol. Liq. 270 (2018) 138–144.
[119] J.N. Neal, D.J. Wesolowski, D. Henderson, J. Wu, Electric double layer capacitance for ionic liquids in nanoporous electrodes: Effects of pore size and ion composition, J. Mol. Liq. 270 (2018) 145–150.
[120] C.N. Patra, Effects of multivalent counterions on the spherical electric double layers with asymmetric mixed electrolytes: A systematic study by Monte Carlo simulations and density functional theory, J. Mol. Liq. 270 (2018) 151–156.
[121] E. Gonzalez-Tovar, M. Lozada-Cassou, L.B. Bhuiyan, C.W. Outhwaite, Comparison of zeta potentials and structure for statistical mechanical theories of a model cylindrical double layer, J. Mol. Liq. 270 (2018) 157–167.
[122] L.L. Lee, F.S. Ramos, A.M. Ramos, Adsorption of mixture of the Yukawa-ions near a hard wall: A density functional study based on the third-order Ornstein-Zernike relation, J. Mol. Liq. 270 (2018) 168–177.
[123] S. Spada, S. Gavryushow, K. Bohinc, Uniformly charged nanoparticles between like-charged walls, J. Mol. Liq. 270 (2018) 178–182.

[124] G. Bokun, D. di Caprio, M. Holovko, V. Vikhrenko, The system of mobile ions in lattice models: Screening effects, thermodynamic and electrophysical properties, J. Mol. Liq. 270 (2018) 183–190.
[125] M. Borówko, W. Rzysko, S. Sokolowski, O. Pizio, Molecular Dynamics and density functional study of the structure of hairy particles at a hard wall, J. Mol. Liq. 270 (2018) 191–202.
[126] M. Druchok, M. Luksic, Carboxylated carbon nanotubes corked with tetraalkylammonium cations: A concept of nanocarriers in aqueous solution, J. Mol. Liq. 270 (2018) 203–211.
[127] B. Eisenberg, Asking biological questions of physical systems: the device approach to emergent properties, J. Mol. Liq. 270 (2018) 212–217.
[128] F. Hirata, On the interpretation of the temperature dependence of the mean square displacement (MSD) of protein; obtained from the inelastic neutron scattering, J. Mol. Liq. 270 (2018) 218–226.
[129] H.-Y. Zhang, Q. Xu, Y. Xiong, S.-L. Peng, K.M. Kumari, D.-Q. Wei, Membrane defect and water leakage caused by passive calcium permeation, J. Mol. Liq. 270 (2018) 227–233.
[130] M. Kastelic, K.A. Dill, Y.V. Kalyuzhnyi, V. Vlachy, Controlling the viscosities of antibody solutions through control of their binding sites, J. Mol. Liq. 270 (2018) 234–242.
[131] A. Anand, G.N. Patey, Molecular dynamics simulations of aspirin dissociation, J. Mol. Liq. 270 (2018) 243–250.

Douglas Henderson
Lutful Bari Bhuiyan
Olivier Bernard
Myroslav Holovko