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Aqueous Solutions at the Interface with Phospholipid Bilayers

MAX L. BERKOWITZ*,† AND ROBERT VÁCHA‡

†Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, North Carolina 27599, United States, and ‡Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB21EW, United Kingdom

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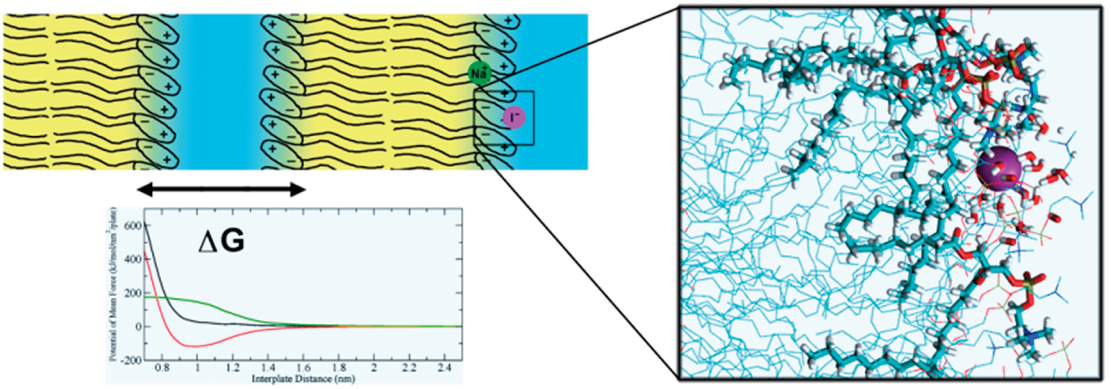

In a sense, life is defined by membranes, because they delineate the barrier between the living cell and its surroundings. Membranes are also essential for regulating the machinery of life throughout many interfaces within the cell's interior. A large number of experimental, computational, and theoretical studies have demonstrated how the properties of water and ionic aqueous solutions change due to the vicinity of membranes and, in turn, how the properties of membranes depend on the presence of aqueous solutions. Consequently, understanding the character of aqueous solutions at their interface with biological membranes is critical to research progress on many fronts.

The importance of incorporating a molecular-level description of water into the study of biomembrane surfaces was demonstrated by an examination of the interaction between phospholipid bilayers that can serve as model biological membranes. The results showed that, in addition to well-known forces, such as van der Waals and screened Coulomb, one has to consider a repulsion force due to the removal of water between surfaces. It was also known that physicochemical properties of biological membranes are strongly influenced by the specific character of the ions in the surrounding aqueous solutions because of the observation that different anions produce different effects on muscle twitch tension.

In this Account, we describe the interaction of pure water, and also of aqueous ionic solutions, with model membranes. We show that a symbiosis of experimental and computational work over the past few years has resulted in substantial progress in the field. We now better understand the origin of the hydration force, the structural properties of water at the interface with phospholipid bilayers, and the influence of phospholipid headgroups on the dynamics of water. We also improved our knowledge of the ion-specific effect, which is observed at the interface of the phospholipid bilayer and aqueous solution, and its connection with the Hofmeister series.

Nevertheless, despite substantial progress, many issues remain unresolved. Thus, for example, we still cannot satisfactorily explain the force of interaction between phospholipid bilayers immersed in aqueous solutions of NaI. Although we try to address many issues here, the scope of the discussion is limited and does not cover such important topics as the influence of ionic solutions on phases of bilayers, the influence of salts on the properties of Langmuir monolayers containing lipid molecules, or the influence of aqueous solutions on bilayers containing mixtures of lipids. We anticipate that the future application of more powerful experimental techniques, in combination with more advanced computational hardware, software, and theory, will produce molecular-level information about these important topics and, more broadly, will further illuminate our understanding of interfaces between aqueous solutions and biological membranes.

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Introduction

Structural and dynamical properties of membranes strongly influence the function of biological cells, and, in their turn, membrane properties strongly depend on the properties of aqueous solutions at the membrane boundary. Therefore, it is important to understand the character of these solutions at the interface with biological membranes. Since biological membranes represent very complex entities composed of a mixture of lipid molecules, proteins, and carbohydrates, it is advantageous to study properties of simple membranes containing one or few phospholipid components. This model has been also extensively used in the study of the membrane/aqueous solution interface. Different experimental techniques, such as, for example, small angle neutron scattering,[1] X-ray scattering,[2] low temperature magic angle NMR,[3] IR spectroscopy,[4] and vibrational sum frequency generation spectroscopy[5] were employed to study the phospholipid membrane/aqueous solution interface. On the theoretical side, given the complex character of a model membrane/water interface, most of the work employed simulation techniques, such as molecular dynamics[6,7] or Monte Carlo.[8] As a result of this effort, a large number of papers are available in the literature. Some of the issues discussed in the papers are described in the reviews by Milhaud[9] and Berkowitz et al.[10] which depict the status of the field prior to and around 2005. Since that time, substantial progress was achieved in the study of the membrane/aqueous solution interface, both in experiments and in simulations, due to the development of more sophisticated spectroscopic methods and better hardware for simulations. Recent work illustrates that a nice symbiosis between simulations and experiment exists in the field: computer simulations prompt experimental investigations, and new experimental data pose new challenges to simulations. In what follows, we describe briefly progress made in the study of the lipid bilayer/aqueous solution interface with the emphasis on the latest developments that took place in the last 5−6 years and that illustrate the symbiosis between experiments and simulations.

Interfaces between Water and Phospholipid Bilayers

Existence of water in the vicinity of the membrane surface with properties that differ from its bulk properties influences the interaction of biomolecules, such as peptides and proteins, with membranes. The questions that experiments and simulations need to answer are related to the issues of how far the influence of the membrane surface propagates into the water and what are the manifestations of such propagation. One of the earlier experimental measurements that clearly displayed the role of interfacial water next to membranes was the measurement of the hydration force.[11] In these initial measurements, it was determined that when membrane surfaces approach each other at distances below 2 nm a repulsive exponentially decaying force acts between membranes. Since the exponent of the decay, although dependent on the type of phospholipid, was mostly in the range of 0.2−0.3 nm, it was suggested that the force was due to the presence of water in the confined space between membranes. As a result, this previously unobserved force was called the hydration force. Later it was shown that the repulsive force acting between membranes has three components, each dominant in a different regime.[12] At larger distances (above ∼0.9 nm), the main contribution to the force comes from undulation of the membranes; at short distances (below ∼0.4 nm), the force is mostly due to steric interactions between headgroups of the membranes. The proper hydration force appears in the range between ∼0.4 and ∼0.9 nm, when two to three layers of interfacial water are squeezed out upon membrane approach. Initial theoretical work on the hydration force had a phenomenological character and later introduced more molecular features into consideration.[13] Given the complexity of the interface on the molecular level, one should expect that simulations, with their ability to take into account molecular details, will play an important role in the understanding of the nature of the hydration force. Initial simulations performed to study the hydration force concentrated on the study of structural properties of water next to phospholipid bilayers in order to infer if these properties were consistent with the phenomenological theories and also, if possible, justify these theories.[14,15] The simulations showed that water next to phospholipid membranes was different from bulk water and that phenomenological theories were too simplistic, but they did not reveal the quantitative connection between water structure and the hydration force. A direct calculation of the force or the free energy change as a function of distance between phospholipid bilayers was performed in recent simulations. Grunze and collaborators, using grand canonical Monte Carlo technique, calculated the dependence of the pressure acting between lipid bilayer on the distance between bilayers.[16−18] They performed their calculations for DLPE and DLPC bilayers to be able to explain why DLPC has a much larger interbilayer separation at a given pressure, compared to bilayers of DLPE. By separating the pressure into components, they concluded from their

calculations that in case of the DLPE bilayers the short-range repulsion mainly originates from the direct electrostatic lipid/lipid interactions of the headgroups from the opposing leaflets, while in case of the DPPC bilayers the short-range repulsion is mainly due to the lipid/water interaction.[18] Large scale molecular dynamics simulations were employed in the work of Gentilcore et al.[19] to examine the origin of the hydration force between lipid bilayers. They calculated the free energy change as a function of distance between bilayers and observed that the change, in agreement with the experiment, was positive as the bilayers approached each other. Estimates of enthalpic and entropic contributions into the free energy change were performed, and according to these estimates the entropy got reduced as the bilayer separation became smaller, while the enthalpy increased. Therefore, it was concluded that the entropy change was responsible for the repulsion character of the total free energy. Note that the simulations were performed in a canonical ensemble and therefore the amount of water was not determined from the conditions of equal chemical potential for water in the space between bilayers and bulk water. In this respect, Monte Carlo simulations using grand canonical ensemble have an advantage. Inspired by the computational scheme used for the calculation of free energy change when two graphene plates moved toward each other,[20] Eun and Berkowitz[21,22] added to the graphene plates phosphatidylcholine headgroups (creating so-called PC plates) and used these plates as models of the bilayers. The PC plates were immersed in a water bath, and the distance dependent free energy was calculated as the plates were moving toward each other. (See Figure 1 for the illustration of the model, as the figure shows the system setup imitated the conditions of the grand canonical ensemble.) It was observed that the free energy increased as the PC plates approached each other, and that the free energy curve could be fitted by three exponents, each corresponding to a different range of interbilayer space, indicating existence of different regimes for PC plate repulsion. The small distance interplate regime corresponded to steric repulsion between the headgroups. The large distance regime corresponded to the removal of bulk-like water, although bulk-like was still different from the true bulk water.[22] The mid-distance regime, in the interval between ~0.7 and ~0.1 nm, was determined to be the hydration force regime due to the removal of interfacial layers of water. In this regime, the exponent of the free energy decay was ~0.3 nm, in the same range as observed in experiment. The separation into entropic and enthalpic components showed that the repulsive

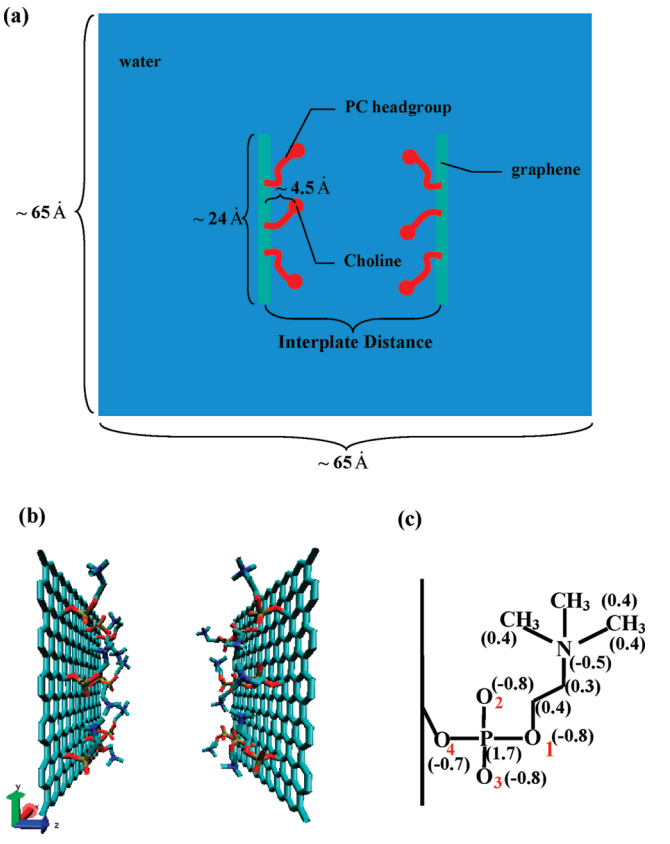

FIGURE 1. (a) Schematic diagram of our model system with associated length scales. (b) Snapshot of the PC headgroup plates. (c) Detailed structure of the PC headgroup. Numbers in parentheses represent themagnitudes of partial charges (in units of the elementary charge, *e*). Reprinted with permission from ref 22. Copyright 2010 American Chemical Society.

interaction between the PC model bilayers was due to the enthalpic effect, coming from the presence of electrostatic charge/charge interactions between water and zwitterionic headgroups. As a matter of fact, removing these interactions produced attractive force between plates. The model that Eun and Berkowitz considered is simple, and probably suffers from some edge effects due to relatively small size of the PC plates. Nevertheless, it was able to catch all the prominent features of the "hydration" force, when structured interface water is removed from the space between membranes, including the range of the force, its decay exponent and its magnitude.

Grand canonical Monte Carlo simulations do not suffer from edge effects, but the accuracy of pressure measurements is limited due to the precision of water chemical potential control. As a result, reliable comparison between simulations and experiments can be done only for the range of small interbilayer distances. Very recently, Netz and collaborators developed a thermodynamic extrapolation (TE) method that allows, using molecular dynamics simulations,

determination of hydration pressure as a function of distance between infinite surfaces, thus avoiding edge effects. In addition, the TE method does not suffer from problems related to the control of water chemical potential. Netz and collaborators performed a study of a hydration force acting between smooth surfaces and also between lipid bilayers. Good agreement with experiments was observed. It was also observed that in the region where the proper hydration force is dominant, the force shows a universal character.[23]

Computer simulation studies of water density at the water/membrane interface showed that when the features of the water density are properly resolved, it displays existence of oscillations and therefore layering of water.[7,24] From such simulations, it was concluded that there exists a layer of intrinsic water that penetrates the headgroup region, the layer of interface water, and following that layer the water density displayed much smoother character with water properties approaching bulk properties. Layering of water next to phospholipid bilayers was recently observed in the experiments. Fukuma et al.,[25] using the frequency-modulated atomic force microscope technique, were able to obtain the force profile next to supported gel phase DPPC bilayer in phosphate buffer. They concluded that up to two intrinsic hydration layers are present next to the phospholipid bilayer surface.

It is well-known that bulk liquid water's peculiar properties are determined by its hydrogen bonded network.[26] Water molecules at the interface with phospholipid bilayers have some of their water–water hydrogen bonds replaced with water–headgroup hydrogen bonds, specifically with carbonyl oxygen–water hydrogen bonds and phosphate oxygen–water hydrogen bonds.[27] This change should influence both structural and dynamical properties of interfacial water. Computer simulations indicated that the strength of hydrogen bonds follows the order: water–phosphate O > water–carbonyl O > water–water.[24] They also indicated that for waters close to bilayers the number of hydrogen bonds is reduced from a bulk value of ~3.7 on average to the value of ~3.2, but the reduction in bond number is compensated by energetically stronger bonds.[24] Infrared spectroscopy measurements confirm these conclusions.[4] Based on the infrared spectroscopy data, Binder also concluded[4] that water next to membranes is in some way reminiscent of supercooled water at −25 °C. Binder used arguments from a mixture model of water (for a nice review of mixture models of water, see the recent book by Ben-Naim[28]). According to this model, water consists of dynamically transforming domains of two different types: (i) lower density domains where water molecules are part of a more highly ordered hydrogen bonding network and (ii) higher density domains where water is in a less ordered network. The peculiar temperature dependent effects observed for water in bulk are explained by changes in the fraction of water belonging to different domains. Binder argues that IR spectroscopic measurements show that the fraction of ordered water domains is increased at the lipid surface, as it would when we supercool water. As of today, no evidence of such a mechanism at work is obtained from computer simulations, although they do show some decrease in water density next to bilayers, but this can be attributed to the "dilution" of water by the headgroups.

If water next to lipid surfaces is different from bulk water, should not we see some substantial changes in its dynamic properties? Because the water–lipid headgroup hydrogen bonding is stronger, should this result in the slow-down of the translational diffusion of water? Indeed, computer simulations showed that the lateral diffusion coefficient for water at the water/lipid bilayer interface is reduced.[24,29,30] Recent molecular dynamics results confirmed that translational dynamics of water at the interface with (DPPC) lipid membrane is slowed down.[31] Moreover, these simulations also show that the motion is not simply diffusive; it displays a ballistic character at short time scales (within 40 fs). At longer time scales, within 5 ps, interfacial water displays subdiffusive character (i.e., in the relationship connecting mean square displacement and time, $\langle r^2 \rangle \sim Dt^{\alpha}$, α is less than 1). Computer simulations also predicted the slowing down of the orientational motion of water at the water/lipid bilayer interface as measured by the decay of the dipole–dipole correlation function. Bhide and Berkowitz found that some of the waters that get trapped in the interior pockets created by the headgroups contribute a long-time component into this decay, extending the reorientional relaxation time of water by a factor of ~100 compared to bulk water.[32] When the simulations were done for water next to frozen lipid groups, the relaxation slowed down by a factor of around 30–40 due to a coupling between the motions of water and slow motion of the headgroups. It needs to be emphasized that these prolonged relaxation times are due to the presence of water molecules that spend a long time deep inside the interface. Most of the water molecules move quickly between different interface regions, and therefore, although display a slowing down of their rotational motion, the slowing-down is not that substantial (with the orientational relaxation time just a few times larger than that in bulk).[32] Simulations showed that the reason for slower dynamics

displayed by the interface water is due to the presence of the strong hydrogen bonds between water and the headgroups. It is proper to mention here that the nature of orientational dynamics of water, even in bulk, was understood only recently. Previously, it was assumed that water orientational relaxation occurs through rotational diffusion, but studies performed by Laage and Hynes showed that relaxation occurs through the molecular jump mechanism (MJM) when water molecules switch hydrogen bonding partners through jumps.[33,34] Simulations showed that the MJM is also applicable in the case of orientational motion of water at the interface with lipids.[35] They also showed that the decay time of the orientational correlation function increases as the degree of lipid hydration decreases, as was observed in the nonlinear ultrafast spectroscopic experiment performed by Zhao et al.[36] This decrease was assigned to the reduction in the number of partners for the jump motion, since the number of water−water hydrogen bonds decreases as the hydration level decreases. Often, the time dependence of the orientational correlation function is fitted by a sum of two or three exponents and physical meaning is assigned to these exponents. It was inferred from simulations that the values of the exponents depend on the length of time for which the correlation data are available[35] and, therefore, one has to be careful when dealing with fits to correlation functions.

In our opinion, we are still lacking clear understanding of water properties at the surfaces of biomembranes and at the surfaces of biomolecules such as proteins and DNA. Recent experimental work that uses more advanced spectroscopic techniques, such as ultrafast vibrational pump−probe spectroscopy,[36] two-dimensional infrared spectroscopy,[37] and other surface-specific spectroscopy techniques,[5,38] illustrated the power of these methods to supply detailed, time-resolved information on water structure and dynamics. Combining such information with the data from simulations and theoretical ideas will provide us with the complete understanding of how "biological" water behaves.

Interfaces between Aqueous Solutions and Phospholipid Bilayers

In biological systems, ions are always present in aqueous solutions, and this presence plays a very important role. As a matter of fact, complicated mechanisms exist to regulate the amount of ions in the extracellular and intracellular environment for the cells' proper functioning. The ion membrane interaction not only regulates the number of ions; it also regulates the physical properties of the cell membranes. For example, recent experiments showed that monovalent cations influence bending rigidity of the lipid membranes.[39] It was also observed that the force needed to puncture the membrane increased with salt concentration.[40]

A large variety of ions is usually present in biological systems; the ions can be either complicated biomolecules or simple atoms, such as halides and alkali metals. In this Account, we will concentrate on systems containing model lipid membranes solvated in aqueous solutions of alkali halide salts dissolved in water. Our choice is dictated by the fact that a largest amount of experimental, simulation, and also theoretical work was done for these systems. The Poisson−Boltzmann equation, based on the mean-field approach to ions and continuum description of water, can be used as a first approximation to a description of complex phenomena involving solvated ion/biomembrane interaction. More detailed treatments are necessary to explain observed ion specific effects, since this equation does not distinguish between cations, such as Na^+ or K^+, or anions, such as Cl^- or Br^-.

Ion specific effects in biological systems were first studied by Hofmeister,[41] who ordered salts based on their ability to precipitate egg-white proteins from the aqueous solution. Later experiments on a large variety of different salt−biomolecular systems demonstrated more general validity of this sequence, and ions were arranged in two series, called Hofmeister or lyotropic series. One series is for cations, and one for anions. For halide anions, the strength to destabilize proteins follows the sequence $I^- > Br^- > Cl^- > F^-$, that is, from large sized "soft" ions to smaller sized "hard" ions. For alkali metal cations, the sequence is opposite: from small "hard" ions to large "soft" ions,; that is, the sequence is $Li^+ > Na^+ > K^+$. Although Hofmeister series were discovered long time ago, the explanation of their nature is still not satisfactory.

Earlier studies on the subject of ion influence on model lipid membrane properties concentrated on the effect of cations, especially Ca^{2+} and Mg^{2+}, in view of biological importance of these ions.[42,43] More recently, systematic studies on the influence of halide anions on lipid membranes were performed.[44−47] Again, as in the case of pure water, a large variety of experimental techniques was employed to study lipid/aqueous solution interface. In addition to the spectroscopic methods that were already mentioned when we described the study of the pure water/membrane interface, such methods as zeta potential measurements[48,49] fluorescence measurements[50] and calorimetric methods were also used.[49] The general consensus reached from the experiments is that the strength of interactions between

lipid membranes and halide anions or alkali metal cations follow Hofmeister series in the order written above (i.e., for anions, the strength of interaction decreases from I^- to F^-, and for cations from Li^+ to K^+).

The interactions between membranes and ions depend strongly on the fine details characterizing ion location and their distribution. This information is very difficult to obtain directly from the experiments, especially the ones that provide microscopically averaged information; however, it can be obtained from computer simulations. A number of different simulations were performed recently that focused on the behavior of ions next to the phospholipid bilayer, especially of halide anions and alkali metal cations.[10,50−60] The simulations used different force fields and also different ensembles, but most of the simulations reached similar conclusions with respect to cation behavior: binding of ions to the bilayer followed the order $Li^+ > Na^+ > K^+$, the same order as in the Hofmeister series. It was also observed that Na^+ ions bind inside the bilayer at the location of carbonyl or phosphate oxygens. In the case of anions, earlier simulations[58] performed over a short time period showed that a large sized anion binds more deeply in the bilayer than Na^+ or Cl^-. Later simulations, performed over longer time periods, but using a different force field, had not observed such a deep penetration.[50] Nevertheless, they showed that I^-, in agreement with the Hofmeister series rule, penetrated deeper than Cl^- into the membrane headgroup region. In Figure 2, we display ion density profiles obtained from simulations of four systems; each system contained a DOPC bilayer immersed into a 1 M aqueous solution of either NaCl, NaI, KCl, or KI salt.[50] As we can see, when salt contains Na^+ cation, there is a substantial separation between the cation and anion distributions and ions create a double layer. While Na^+ penetrates the headgroup region and has a preferred location somewhere around phosphate oxygens or around carbonyl oxygens (depending on the force field used), the peak of anion distribution is small and is located at the interface between membrane and aqueous solution where choline groups are located. Such creation of an ionic double layer is not present when the cation is K^+. It is very important at this point to emphasize that the results of simulations on systems containing ions at the water interface with other substances crucially depend on the force field used in the simulation. It is possible that more refined force fields will change the detailed results, especially details about the degree of ion adsorption into the bilayer (we learned that recent simulations, which used a different force field for K^+ ion, predict its stronger adsorption into the

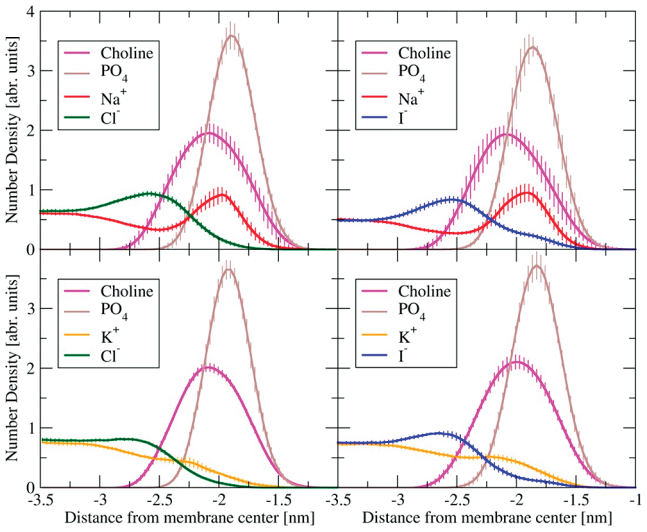

FIGURE 2. Ion density profiles in four different 1 M salt solutions (NaCl, KCl, NaI, and KI) next to DOPC membrane. Density profiles of choline and phosphate groups of the lipids are also included. Reprinted with permission from ref 50. Copyright 2010 American Chemical Society.

bilayer, which is in agreement with the recent isothermal titration calorimetry measurements;[49] Knecht, private communication). In addition, as it was learned from the previous simulation studies of aqueous clusters[61] containing ions and systems containing an aqueous solution/vapor interface,[62] it is important to include the electronic polarizability effect into simulations, especially when systems contain anions. Inclusion of polarizability enhanced hydrophobic tendencies of anions. How important is the inclusion of polarizability into simulations containing lipid bilayer/aqueous solution interfaces? Vacha et al. performed simulations on DOPC bilayers in the KI aqueous solutions using a force field that included polarizability.[50] These simulations showed that inclusion of polarizability results in a larger penetration of I^- ions into the headgroup region, which is presumably more hydrophobic compared to water. Consideration of hydrophobicity may provide some clue toward understanding of ion behavior next to a lipid bilayer; an additional clue can be obtained from considering the ion pairing concept of "matching water affinities" proposed by Collins.[63] According to this concept, the tendency for ion pairing in aqueous bulk solutions is highest for ions (charged groups) of opposite charge and matching free energy of hydration (i.e., small cations prefer small anions, while large ions pair more with large ones). If we extend the application of this principle to the interface between membrane and water, we can conclude that cations such as Na^+ would prefer to pair with oxygens of the headgroups, while anions such as I^- would prefer to pair with the bulkier "softer"

choline group. The Coulomb interaction between salt anions and cations also plays a role. A stronger Coulomb attraction to membrane adsorbed Na^+ ions explains why Cl^- ions are located closer to headgroups for the NaCl case, compared to the KCl case.

We already mentioned that the study of interaction between membrane surfaces immersed in pure water provides us with information about properties of water between such surfaces. What can a similar study tell us about the properties of aqueous solutions enclosed between membranes? Can it provide us with information about the location of cations and anions in the solution? The answers to these questions have a large practical value, since they will help us in understanding such phenomena as cell/cell and cell/vesicle interactions. To get the answers, Petrache and co-workers[64,65] and later Leontidis and co-workers[45,46] performed studies of interactions between neutral lipid bilayers immersed in aqueous solutions. Petrache and co-workers studied the interactions between DLPC bilayers immersed in solutions of salt with different KBr or KCl concentration. They were able to fit the observed pressure–distance curve by adding an electrostatic force to the three forces that are also active in pure water: hydration, undulation, and van der Waals. The electrostatic force acting between neutral bilayers is due to adsorption of ions to the bilayer. The partition of ions between the bilayer and solution was taken into account using a binding (charge regulation) mechanism.[66] It was also assumed that salt changes the Hamaker parameter for the van der Waals interaction; the fit showed that the Hamaker parameter was reduced up to 70% at large salt concentration (1 M). The fit also displayed that Br^- was more adsorbed than Cl^-, although still relatively weakly binding to the bilayer, with a binding constant of 0.22 M^{-1}. Leontidis and co-workers studied interaction between DPPC bilayers immersed in salt solutions of NaCl, NaI, $NaNO_3$, and NaSCN. In addition to measuring pressure–distance dependence, they also measured headgroup area–pressure dependence for their systems. Remarkably, they were not able to achieve a good fit to their data by using the same level of theory as used by Petrache and co-workers in cases of high salt concentration (0.5 M) solutions containing anions such as I^- or SCN^-. According to Leontidis and co-workers, our state of understanding the lipid/water interface remains unsatisfactory.

Our brief Account describing research on properties of aqueous/lipid membrane interfaces shows that a nice advancement in this field was achieved due to a fruitful cooperation among experiment, theory, and computer simulations. Nevertheless, we are still missing a full understanding of the membrane/aqueous solution interface. Hopefully, further progress in experimental techniques that allows for more detailed measurements, advances in hardware and software for simulations, and development of new theoretical ideas will result in deep understanding of this important subject.

BIOGRAPHICAL INFORMATION

Max L. Berkowitz received his M.Sc. in Physics from the Novosibirsk State University, Russia and his Ph.D. in Physical Chemistry from the Weizmann Institute of Science in Israel. After his postdoctoral studies, he joined the Department of Chemistry at the University of North Carolina at Chapel Hill in 1983, where he rose in the ranks from Assistant Professor to Professor. During the years of his work in Chapel Hill, he studied, using molecular dynamics simulation technique, properties of water and aqueous solutions in bulk, in clusters, and at the interfaces. He also performed some theoretical work on the qualitative aspects of quantum density functional theory. The study of properties of hydration force acting between phospholipid bilayers brought him to study properties of biomolecular membranes. Presently, he is involved in the studies of peptide–biomembrane interactions and studies of interactions between nanoparticles immersed in aqueous solutions.

Robert Vácha received his M.Sc. in physics from the Charles University in Prague in 2005 and his Ph.D. in chemistry from the Charles University and the Institute of Organic Chemistry and Biochemistry of the Academy of Sciences. He was also enrolled in the International Max Planck Research School for "Dynamical Processes in Atoms, Molecules and Solids" in Dresden in 2007–2009. Since 2009, he works as a Postdoctoral Research Associate in the Department of Chemistry, University of Cambridge, and in 2010 he became a Junior Research Fellow of Churchill College, Cambridge. As a student, he initially performed research in the field of atmospheric chemistry, focusing on adsorption and behavior of atmospherically relevant molecules and ions at the air/water interface. After that he studied more complex interfaces, such as salt solutions in contact with proteins and phospholipid bilayers. Presently, he studies, on a coarse-grained level, the interaction of proteins with lipid membranes.

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FOOTNOTES

*To whom correspondence should be addressed. E-mail: maxb@unc.edu.

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