WATER: A Multidisciplinary Research Journal

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Fourth Annual Conference on the Physics, Chemistry and Biology of Water

Chair: Gerald H. Pollack

October 22-25, 2009
West Dover, Vermont

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Agenda

Thursday, October 22

Session TH-I: Water: Global Considerations

Chairs: Martin Chaplin and Yolene Thomas

13:45	Gerald Pollack, Thomas Lowell	Welcome
14:00	Eshel Ben Jacob *Tel Aviv University*	Bacteria-guided reflections on water's unusual properties
15:00	Barry Ninham *Australian National University*	Waterless water: The Faustian bargain of physical chemists and biologists
15:35	REFRESHMENTS	

16:00	Gerald Pollack *University of Washington*	Unexpectedly long-range effects of hydrophilic surfaces on the contiguous aqueous phase
17:00	Emilio del Giudice *INFN Milan*	Formation of dissipative structures and emergence of novelties in liquid water
17:35	Fabio Bruni *University of Rome*	Is there a minimum density in confined water?
18:10	Reception (hearty hors d'oeuvres and beverages served)	

Session TH-II: Water-Droplet Behavior

Chairs: Barry Ninham and Michael Mross

19:30	Karl Bohringer *University of Washington*	Droplet transport on microstructured superhydrophobic surfaces
20:05	Kenichi Yoshikawa *Kyoto University*	Self-Running Droplet: An Isothermal Chemical Motor

Friday, October 23

Session F-I: Water and Light

Chairs: Vladimir Voeikov and Marie-Claire Bellisent-Funel

09:00	Shigezo Shimokawa, Tetsuro Yokono *Hokkaido University*	Sunlight-induced structural change in liquid water
09:35	Franco Musumeci *University of Catania*	Aqueous ionic solutions investigated by time-resolved delayed luminescence
10:10	Nikolay Bunkin *Gen. Physics Inst.*, Moscow	Structure of stable nanobubbles of dissolved air in water
10:45	REFRESHMENTS	
11:10	Roumiana Tsenkova *Kobe University*	Aquaphotomics
11:45	Elmar Fuchs *WETSUS*, Holland	The inner structure of a floating water bridge
12:20	LUNCH TOGETHER	

Session F-II: Long-range Interactions

Chairs: Barry Ninham and Michael Mross
Chairs: David Anick and Nigel Dyer

13:20	Yosef Scolnik *Weizmann Institute*, Israel	Deviation from identity of macroscopic properties of enantiomers via water chiral preference - Indication for long range order in water?
13:55	D. James Morré *Purdue University*	Oscillations of the ortho/para ratio of liquid water drive the ultradian regulator of the cell's biological clock
14:30	Rustum Roy *Penn State University*	Structures and thermodynamics in the (paracrystalline) polymorphism of liquid water
15:30	REFRESHMENTS	
16:00	Lior Miller *DO-COOP*, Israel	Nanoparticle-doped water: from particle structure to water properties
16:35	John Dore *University of Kent*	Water and ice in a confined hydrophobic environment
17:10	Vladimir Korenbaum *Pacific Ocean Institute*, Vladivostok	Study of water-based electronic-homeopathic nosodes
17:45	DINNER (on your own)	
19:30-21:30	POSTER SESSION	Beverages and Wine Served

Saturday, October 24

Session Sat-1: Biology and Water

Chairs: Hans Frauenfelder and Ryszard Grygorczyk

09:00	Vladimir Voeikov *Moscow University*	Intrinsic sustained activity of bicarbonate aqueous solutions
09:35	Fumio Hirata *Okazaki National Research Institute*	Biomolecules in water and water in biomolecules
10:10	Jeff Fredberg *Harvard University*	Universal behavior of the osmotically compressed cell and its analogy to the colloidal glass transition
10:45	REFRESHMENTS	
11:15	Abraham Stroock *Cornell University*	What can we learn from plants about water at negative pressures?
11:50	Yuko Yoshikawa *Ritsumeikan University*	Giant DNA in water: Conformational transition and radio-sensitivity
12:25	Lunch together	
13:30	Free Time until 16:00	

Session Sat-II: Proteins and Water

Chairs: Jeff Fredberg and Yolene Thomas

16:00	Hans Frauenfelder *Los Alamos Nat'l Lab*	The role of hydration in protein dynamics
16:35	Marie Claire Bellisent-Funel *CNRS Saclay*, France	Water at Interfaces: Phase transitions and connection to protein dynamics
17:10	Kim, Chae Un *Cornell University*	Phase behavior of water inside protein crystals
18:30	Dinner & Entertainment/ Announcement of Award for Best Poster	

Sunday, October 25

Session Sun-I: Biology and Water – 2

Chairs: Eran Gabbai and Wei-Chun Chin

09:00	James DeMeo *Orgone Bio-Phys. Lab*	Water as a resonant medium for unusual external environmental factors
09:35	Yolene Thomas *CNRS*	Gurvitch experiments revisited (Yolene unable to attend)

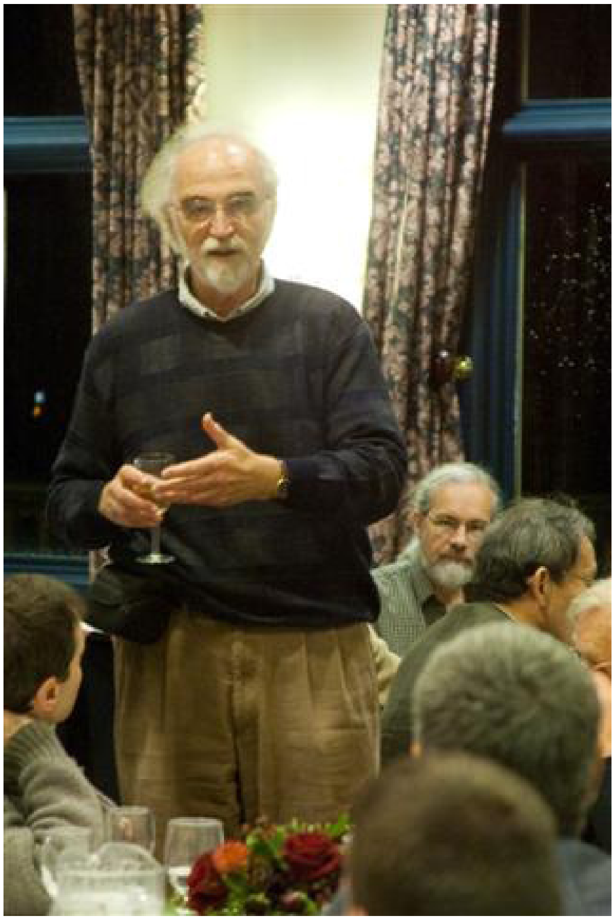
10:10	A. Sommer and D. Zhu *University of Ulm*	Interfacial water and biolubrication / Six ways to probe interfacial water layers non-destructively
10:55	REFRESHMENTS	
11:20	Phil Snyder / Geo Whitesides *Harvard University*	Why is it so hard?
11:55	Round Table Discussion	

A Letter from D. James and Dorothy M. Morré

Being first time attendees at the Annual Conference on the Physics, Chemistry and Biology of water, we were indeed both pleased and honored by our invitation to the fourth convening of scientists interested in varied properties of water.

Since we are neither physicists nor chemists, we were somewhat apprehensive about coming to a meeting that appeared to be far afield from our area of work. However, it was a pleasure to find just the opposite. It did not take long to realize that nearly every presentation contained knowledge useful to us. The presentations were relevant to water and water is fundamental to life. We had no problem relating to the presentations and garnered much valuable factual and conceptual information. In fact, a number of presenters suggested that a clearer and more exacting definition of “water” be seriously considered.

A hallmark of the meeting was that no idea was dismissed and no concept ignored. Matters relating to the properties of water, however controversial, were discussed openly and seriously with the full expectation that in each might be found vital new information. Presentations were thoroughly discussed often in extended question and answer sessions. The prevailing tone of the meeting was that any and all relevant observations must somehow be accommodated within our understanding of the properties of water. It was both thrilling and refreshing to not only see such an eminent group of established investigators and leading scientists open to different ideas and departures from dogma but also to the participation of young students and in their excellent poster presentations and discussions. We learned much and were pleased to have been included.



Jerry Pollack is a great organizer and interaction stimulator. The Mt. Snow resort is a pleasant, comfortable and accommodating meeting venue providing surroundings conducive to a serious but enjoyable conference. We met many new potential colleagues and opportunities for continuing collaborations.

Regards,

D. James and Dorothy M. Morré, Professors

Emeriti, Purdue University

Towards A Systemic View of Water as the Fabric of Life

Eshel Ben-Jacob

I present a concise summary of the "Fourth Annual Conference on the Physics, Chemistry and Biology of Water", Vermont 2009. The summary is presented from a personal perspective with an attempt to present my own impression of the meeting and explain why I think most of us found it so exciting. In a nutshell, I feel that this meeting might mark the beginning of a paradigm shift in our perception of water; A shift from the current molecular-level based approach (focusing on individual or several molecules) that underpinned our perception of water to a new, systemic view of water. According to the molecular-level based paradigm, water is a passive and homogeneous solvent close to equilibrium. This is in contrast to the new, systemic view of water as an active substance which adaptively responds to external and internal constraints, cues and signals by generation of complex, sustainable organization on all scales. That complex organization, in turn, can have singular effects on substances immersed in water and in particular on the functioning of biological constituents, from molecules to living cells. My take-home message is that we are at the doorstep towards a systemic view of water as an active substance imbued with life-giving properties. And that the notion of water as "life's solvent" should give way to the new realization of water as an active "Fabric of Life"; continuously engaging and interacting with bio-molecules in complex subtle ways.

Three decades ago, in an article entitled "Water Revisited" published in *Science*, Frank H. Stillinger said: "A comprehensive molecular theory for water is needed for two reasons: First, this substance is a major chemical constituent of our planet's surface and as such it may have been indispensable for the genesis of life. Second it exhibits a fascinating array of unusual properties both in pure form and as a solvent. Physical scientists have attempted to respond to this need for nearly a century, but a satisfactory molecular theory has only begun to emerge in the last decade." He referred to the progress made in the 1970s in understanding the water molecule interactions and the "hydrogen bond" concept. The articled focused on the spontaneous creation and annihilation of local patterns (of several water molecules), characterized by strong bonds and nearly tetrahedral angles. The article presented the molecular-level based paradigm saying that "All the properties of water and aqueous solutions ultimately must be explained in terms of intermolecular forces that are present" and a sense of optimism that a general theory of water is at hand.

Two and a half decades have passed, and in a monograph entitled "Water? What's so special about it?", published in the Proceedings of the Royal Society, John L. Finney commented: "Although we pay lip service to the biological importance of water, we do not understand what it is about the molecule that makes it a particularly 'fit' molecule to form the 'matrix of life'". He further proposed that water anomalies should not be perceived as "mysteries" as they can be explained based on the understandings at the molecular level of the water molecules and its interactions. He also claimed that, "Some demystification of water might help us to understand more clearly its role in the molecular-level processes that are important for maintaining life". The focus in this important article was also on the developments in understanding the role of tetrahedral geometry in governing the local order of water and the central role of these understandings in explaining the water anomalies. However, at the same time it was also pointed that the understanding "...may be incidental to the molecular-level biological fitness of water", admitting that the molecular-level based paradigm falls short of providing a comprehensive theory of water's role in the genesis of Life.

Half a decade ago, the consensus was that satisfactory understanding of water has been reached and that once some more details are attained, a sound water theory will be established. While many scientists still hold this notion, it has recently been questioned. Two years ago, in an essay entitled "Water – an enduring mystery" published in *Nature*, Philip Ball abstracted the failure of science to understand water, saying, "It's embarrassing to admit it, but the stuff that covers two-thirds of our planet is still a mystery". And with regard to the prospects of the molecular-level based paradigm ability to change this alarming situation he stated, "Worse, the more we look, the more the problems accumulate: new techniques probing deeper into the molecular architecture of liquid water are throwing up more puzzles".

We all agree that the detailed molecular-level properties of water are very important. Yet, it is becoming evident that they are not sufficient to provide a complete theory of water; we are missing some essential water aspects that cannot be accounted for by the molecular level investigations irrespective of how detailed and sophisticated they will be. The sense during the meeting was that the accumulations of new observations pose new "puzzles" to the extent that a paradigm shift towards a systemic view of water is called for. Generally speaking, the lectures could be sorted into three categories: I. Investigations of the active response of water. II. Development of experimental and theoretical characterizations of water state. Such characterizations are essential for accurate quantifications of the water's active response. III. The effect of water on immersed substances from bio-molecules to living cells.

Within category I we learned about water's active response to: 1. External signals including electromagnetic (EM) fields from very strong ones (e.g. that generate water bridges) to extremely weak ones (e.g. generated due to tides in the ionosphere), acoustic signals and EM radiations at a wide frequency range. 2. External geometrical constraints, forcing the water within confined geometry. 3. Internal geometrical-chemical constraints such as interaction with hydrophobic surfaces and immersed nano-particles. 4. Internal interactions with immersed biological substances from bio-molecules to tissues, organs and living cells. In all cases, the water response included generation of complex organization on all scales, and in some cases with the correlation length (water order) extending over tens of microns and being sustained over long times (hours). In several lectures it was proposed that the strong response of water to weak signals might be mediated via the formation of network of nanobubbles.

From these lectures it became evident that the standard picture of liquid water is too simplistic and even wrong in many cases. This standard picture is rooted in the propositions that: 1. at room temperature water can be assumed to be close to equilibrium; 2. water is in a homogeneous state with no long-range correlations, dissolved substances are homogeneously distributed, and molecules dissolved in water are subject to non-correlated noise. In contrast, we were exposed to a systemic view which posits that: 1. water at room temperature under ordinary conditions (open to the atmosphere) is a non equilibrium open system that exchanges heat and gases with the environment and absorbs electromagnetic (EM) radiation and acoustic signals. 2. Consequently, water is usually in a dynamic state (continuous self-organization) manifested by the formation of complex organization on all scales. 3. The formation of gas nanobubbles in water or immersed nanoparticles or the existence of hydrophobic surfaces change the organization of water from nano scale of local arrangements of tens of molecules up to a scale of tens of microns. 4. The complex water organization can induce spatio-temporal hydrophobic/hydrophilic large scale order and orientation variations which can lead to corresponding variations in pH, chemical affinity, etc.

The category II lectures presented new approaches and technologies (e.g. aquaphotomics) appropriate for real-time and non-invasive monitoring of the water states on all levels, which thus provide new tools to quantify the active response of water. Other lectures presented theoretical characterizations of the active response of water. Both are crucial steps towards the development of a systemic view of water.

New percepts about the state of water were mentioned during some lectures and during discussions among the participants; for example, a new “string theory” of water according to which part of the water molecules form long strings. Much discussion was also devoted to the possibility that water is composed of low-density and high-density water regimes and to the role of nanobubbles in the formation and stability of “water order”. These topics are currently under “hot” debate. Others presented molecular dynamic simulations that support the existence of water clusters (assembly of tens of water molecules in a crystalline structure). There was an agreement that, due to the special interaction of water with a mixture of hydrophobic and hydrophilic substances, intracellular water should be regarded as partially ordered water.

From the category III lectures we learned that water actively engages and interacts with biomolecules in complex, subtle, and essential ways. There is now good reason to regard the “active volume” of molecules such as proteins as extending beyond their formal boundary by virtue of the way they shape and manipulate the shell of water that surrounds them. Moreover, the structure and dynamics of this hydration shell seems to feed back onto those aspects of the proteins themselves so that biological function depends on a delicate interplay between what is currently regarded as distinct entities: the molecule and its environment. Many proteins make use of bound water molecules as functional units, like snap-on tools, to mediate interactions with other proteins or with substrate molecules or to transport protons rapidly to locations deep inside the protein.

Hence, the prevailing notion of water as a passive solvent, that does little more than temper or moderate the basic physicochemical interactions responsible for molecular biology, is a too simplistic and even misleading view of water’s role in the chemistry of life. The role of water structure is perhaps most apparent in the attractive force that operates between two hydrophobic entities (nanobubbles, proteins, and other hydrophobic molecules and particles) in water. Hydrophobic attraction drives the correct folding of protein chains, the binding of some proteins to substrates (or cell membranes), and the aggregation of proteins into functional units. These processes are essential to the understanding of life, implying the need for intensive studies of the interactions of hydrophobic substances with water.

To conclude, the conflict between the systemic view of water that emerged during the meeting, and the molecular-level based view brings to mind the seminal article “More is different”, published in *Physics Today* back in 1972. In this opinion article, Phil Anderson promoted the notion of “constructivism”. He argued that new fundamental principles are needed to explain the higher level (system) properties. More specifically, he proposed that even if we accept that the rules that govern the dynamics at a higher level *in principle* emerge (according to reductionism) from the lower level rules, since *in practice* they are not derivable, we should treat them as fundamental as the rules at the lower level. Three decades later, in a *Nobel Symposium* on “Self-organization: the quest for the origin and evolution of structures”, I proposed the extended “More is different on all levels” principle to account for the changes in biological constituents during self-organization into a new functional system. The observations presented in the Vermont meeting, about the ways water adaptively responds to external and internal constraints, cues and signals by generation of complex organization on all scales are very reminiscent of the adaptive response of living systems. Could it be, then, that “More is different on all levels” fits the systemic view of water as the fabric of life?

Speaker Abstracts

(alphabetical by author)

Water at Interfaces: Phase Transitions and Connection to Protein Dynamics

Bellissent-Funel, MC[1]

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Water is a unique liquid, many of its properties being critical for the continued support of life. In living systems, essential water-related phenomena occur in restricted geometries in cells and at active sites of proteins and membranes or at their surface. The effects of hydration on the equilibrium protein structure and dynamics are fundamental to the relationship between structure and biological function. In particular, the assessment of the perturbation of the structure and dynamics of liquid water by hydrophilic and hydrophobic molecular surfaces is fundamental to the understanding of the stability and enzymatic activity of globular proteins and functions of membranes [1].

Water plays a major role in the stability and catalytic function of proteins. Both the effect of hydration water on the dynamics of proteins [2,3] and the effect of proteins on the dynamics of water [4] have been studied using inelastic neutron scattering, the most direct probe of protein /water dynamics on the picosecond-nanosecond timescale. The peculiar structural and dynamic properties of interfacial water, in particular the phase transitions that interfacial water experiences at low temperature, will be presented. We will discuss: i) the connection between the interfacial water phase transitions and the dynamics of protein, ii) how the protein-hydration water interaction can drive the protein function [5].

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Bacteria Guided Reflections on Water Order and Water Memory

Ben-Jacob, E[1]

[1] Tel Aviv University

Although much effort has gone into trying to understand the ways in which water is involved in life-sustaining processes, current science does not provide clear and convincing answers to what it is about water that makes it a particularly 'fit' substance to form the 'matrix of life'. This state of affairs, which severely limits our ability to understand life, is rooted in the simplistic and misleading assumption of water's role in the chemistry of life as a passive, structureless solvent that is close to thermodynamic equilibrium (under the normal conditions that permit life).

I will present my view of water as an active solvent of complex organization with long-range order (microns) and long-time memory (minutes to hours), actively interacting with biomolecules and engaging in inter- and intra-cellular processes in complex, subtle, and essential ways. This view emerged following over twenty years of theoretical and experimental investigations of self-organization in nonliving systems (snowflake formation and electrochemical deposition) [1], and close to ten years of studying self-organization during bacteria colony development [2,3].

Guided by bacteria response to treated water, I will further reflect on the possibility that water can store biological relevant information, presumably in its complex structural organization (long range water). For that I will present the results of a novel approach of using bacteria, the most fundamental organisms that have the most "intimate relations" with Nature, to sense the effect of rf (radio frequency) treatment and nano particle doping of water. Using the bacteria as biosensors, I could infer that water treatments by rf radiation and nano particle doping induce long-range order, which I will reason occurs through the formation (self-organization) of a network of gas nano-bubbles with non arbitrary complex organization in which information might be stored. This paradigm will be further supported by experimental results of electrochemical deposition in treated water, and the effects of the water treatments on Z-potential. Put together, the physical, chemical and biological results provide important support to the notion of waterformatics – the possibility to induce endured long range order in water [4]. Consequently I will reflect on the possibility that phenomena like "water order", "water memory" and "water information" are real and not artifacts or mysticism as they are still perceived by the scientific community at large. And if so, the existence of water order and memory calls for rethinking of water and the development of a new theoretical framework for the understanding of water.

References

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Droplet Transport on Microstructured Superhydrophobic Surfaces

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Systematic design of microscopic surface roughness can be employed to propel water droplets on flat, inclined, and even upside-down surfaces. Droplets are transported, split, and merged on these engineered surfaces by externally applied mechanical vibration. The conversion of vibration into directed droplet motion is achieved in two ways: (1) by creating surface energy gradients, or (2) by utilizing surface ratchets. In both cases, rough surfaces are designed with microscopic features that trap air between microfabricated pillars, resulting in a superhydrophobic surface where the liquid-solid contact area is confined to the pillar tops ("Fakir state"). For (1), the liquid-solid contact area varies along a track with decreasing apparent contact angle, leading to a hydrophobicity gradient that causes the droplet to move towards regions with lower contact angle; the length of this track is limited by practical geometric constraints. For (2), repetitive surface features produce an anisotropic force bias along the contact line of a vibrating droplet; the resulting tracks have no length limitation and can include loops. This work provides the basis for novel microfluidic systems that process small amounts of liquids on a simple, low-cost, portable platform.

Is there a Minimum Density in Confined Water?

Bruni, F[1]

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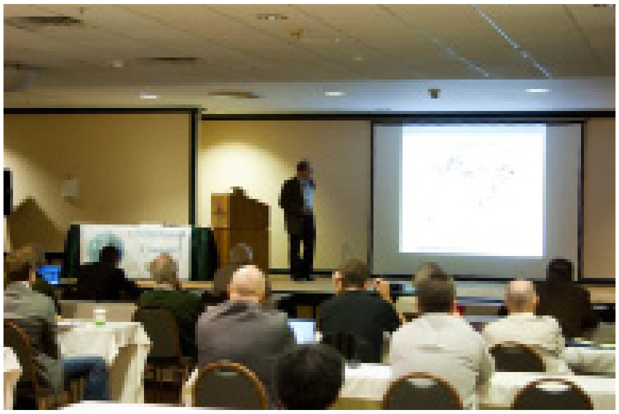
To what extent is it possible to compare the microscopic structure of water confined in nanopores with that of bulk water? Here we use neutron diffraction experiments with isotopic substitution, coupled to coarse graining calculations and atomistic simulations, to investigate water confined in a silica matrix (MCM41-S-15). This comparison is made at 300 K and at 210 K, addressing, in particular, the issue related to the existence of a minimum of density at 210 K, as recently claimed.

The presence of hydrophilic pore surface causes a non homogeneous distribution of water molecules across the pore. As a consequence, we find a clear water density profile, with a layer of higher density near the pore surface and a region of lower density in the pore center. This non uniform pore occupancy is accompanied by sensible changes of the microscopic structure of water compared to bulk, here evidenced by a layer analysis of the site-site radial distribution functions.



Structure of the Stable Nanobubbles of Dissolved Air in Water as Studied by Measurements of Light Scattering Matrix

Bunkin, NF[1]; Suyazov, NV[1]; Shkirin, AV[1]; Prokhorov, AM[1]; Kozlov, VA[2]

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In experiment combining both laser modulation-interference microscopy and scattering matrix measurements (the results of this study have been recently published in [1]) it was established that in the water samples saturated with dissolved air and containing an ionic component, there exist stable (long-living) gas particles at the micron scale having a negative electrical charge. Moreover, it was proved that these micron-sized particles are not monolithic ones but are composed of separate stable nanobubbles containing dissolved air. The solution of inverse scattering problem based on numeric simulation of the angular dependences of the scattering matrix elements has allowed us to estimate the gyration radii of the nanobubble clusters and their fractal dimension. The calibration scatterometry experiments, performed with aqueous monodisperse suspensions of latex particles with various known concentrations have made it possible to define the concentration of the nanobubble clusters. The additives of various salts in the water samples give rise to an increase in the concentration of the nanobubble clusters, while their fractal dimension deceases, and the clusters become “more friable”. It is shown that certain peculiarities in the behavior of aqueous solutions of different salts (here we mean the dependences of the mass density and the dielectric permittivity as functions of the salt concentration) can be explained within the framework of model of electrically charged clusters of the nanobubbles, whose parameters critically depend on the salt concentration as well. The nanobubble clusters as charged particles naturally should distort the hydrogen-bond network in aqueous media and also can affect chemical, in particular, auto-catalityc and biochemical reactions. Additionally, the model of the nanobubble clusters can be applied for an explanation of the mechanism for breath of oceanic animals (for example, fishes). And finally, according to our experimental results, these particles are the centers of natural heterogeneity in liquids being the nuclei for the acoustic and optical (laser) cavitation, as well as for boiling. The proposed model allows us to interpret at a qualitatively new level our earlier experimental results [2] on inducing the hypersonic cavitation in a field of broadband optical pump.

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Formation of Dissipative Structures in Liquid Water

Del Giudice, E[1]

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Self-organisation is the dominant feature of the dynamics of living organisms. According to the findings of the thermodynamics of irreversible processes (Prigogine) the possibility of self-organisation is connected with the formation of dissipative structures , namely open subsystems able to decrease their own entropy as a consequence of their dynamics.

In this presentation it is shown that such features appear in liquid water at interfaces with hydrophilic surfaces , provided that molecular impurities (for instance, atmospheric gases and bicarbonates) are present. This result emerges from Quantum ElectroDynamics (QED) . QED prescribes that water molecules in the liquid state may oscillate in unison within extended Coherent Domains (CD) between two configurations: the first configuration is one where all electrons are tightly bound to their molecule , in the second configuration one electron per molecule is almost free. In this way a CD includes a reservoir of quasi-free electrons that can be further excited giving rise to vortices. Since the vortex motion is coherent, is also frictionless , so that the life time of the vortices could be extremely long (weeks, months). Consequently CDs become machines able to store a large amount of energy , transforming it from high entropy to low entropy energy. This stored energy can be released to non aqueous molecules when the frequency of oscillation of these ones matches the frequency of oscillation of the CD. In this way selected molecules get activated and an intelligent biochemistry could emerge. Furthermore , since the output energy of the chemical reaction is taken by the CD , changing its frequency of oscillation and hence the nature of the resonating species, the possibility of an evolutive biochemistry emerges.

Water as a Resonant Medium for Unusual External Environmental Factors

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One of the significant proofs for a new scientific finding is the independent discovery and/or verification of it by other researchers. During the last Century, there were multiple lines of converging evidence, suggesting the existence of a dynamic plasmatic energy existing within living organisms and water, existing as a background medium filling the atmosphere, and found within the deep vacuum of space itself. The biologist Frank Brown, investigating the external biological clock mechanism, observed an unshieldable cosmic *solar-lunar* phenomena capable of affecting the behavior and metabolism of many living creatures. "Tidal" forces could be transmitted through laboratory walls into controlled aquaria, for one example, where isolated creatures followed the rhythms of the lunar tide, which they could not react to via known measures. Physicians such as Harold Burr and Bjorn Nordenstrom argued for a specific *electro-dynamic* energy in the body, which they measured independently via bioelectricity and other measures, showing its similarities to the *acupuncture energy* of Chinese medicine. Such experiments typically utilized water as a *carrier* for the charge of this previously unknown energy phenomenon. Intuitive naturalist Viktor Schauberger argued for a specific quality of alive or *living water*, and made practical applications of this in forestry. Biologist Jacque Benveniste investigated and proved the *memory of water* effect, as employed by homeopathic medicine. Wilhelm Reich's experiments indicated a specific life-energy, the *orgone*, which was reflectable by metals and more active at higher altitudes, able to charge up water, and possessed of cosmic, biological and meteorological functions. Biochemist Giorgio Piccardi also discovered a similar *bio-cosmic, physico-chemical fluctuating phenomenon* at work in physical chemistry, reflectable by metal plate, more active at higher altitudes, and possessing significant solar-terrestrial, biological and meteorological components. His findings showed fluctuations in the freezing of super-cooled water, tied to sunspot variations. Much of this same work integrates with diverse astrophysical theory which today argues for an *interstellar medium*, variously termed *cosmic plasma*, *dark matter*, or even *cosmic ether*. Physicist Dayton Miller confirmed a dynamic cosmic ether, moving faster at higher altitudes, and slowed or reflected by dense materials such as metals or stone. His work has been confirmed "down to the details" by radiophysicist Yuri Galaev, and others. All of these natural scientists undertook decades of careful experimental work, indicating the presence of a very similar water-affecting cosmic medium. They mostly did not know of each other's existence. All were maligned and assaulted by the dogmatic orthodoxy of science. I have been privileged to replicate some of these experiments, notably using the highly unorthodox orgone accumulator of Reich to affect an approximate 40% increase in sprouting seeds as compared to controls. Another of Reich's apparatus was evaluated for its ability to influence clouds from a distance, with basic confirmation. The effect appears water-moderated in most cases. Taken together these studies are suggestive of a major scientific breakthrough, ignored or dismissed prematurely during the 20th Century.

Studies of Water in Hydrophobic Confinement

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The last decade has seen a great interest in the study of water in confined geometry. Most of the experimental work has been undertaken with a range of mesoporous silicas in which the surface interaction is essentially hydrophilic. The behaviour of the water [and ice] in these systems shows a strong dependence on a number of factors, such as pore size, pore morphology and fractional filling-factors. Furthermore the nucleation to produce ice is complex, producing a mixture of hexagonal [I_h], cubic [I_c] and disordered states that are temperature-dependent and may also exhibit hysteresis effects; the solid phase has been likened to that occurring in rotationally-disordered crystals and has been referred to as 'plastic ice.'

Consequently, it is of interest to study the behaviour of water in a hydrophobic mesopore environment although this poses a number of technical problems. Two approaches have been adopted that will be reported in this presentation. The first method uses a surface modification technique that introduces a layer structure on to the internal substrate to make the basic interaction hydrophobic. Neutron and NMR techniques have been used to investigate the difference in water/ice characteristics for the modified and non-modified samples; the latest results will be presented. Another approach is to use a different substrate. It is well-known that water is readily adsorbed into carbon nanotubes, despite the fact that the water-graphene interaction is primarily hydrophobic. Experimental measurements have been made for water/ice in carbon nanohorns with a mean pore diameter of 30 Å. In this case, the water features are quite unusual with a lower temperature-dependence, evidence of enhanced connectivity in the H-bond network and a much reduced density. Some recent DINS measurements suggest that there is possibly evidence for de-localisation effects in the H-bond, which will require more detailed investigation.

The Role of Water in Protein Dynamics

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Without proteins and water, life as we know it would not be possible. Texts and most publications show proteins naked, without a hydration shell and without bulk solvent. Experiments show, however, that the bulk solvent and the hydration shell are essential for proteins to function. What is their role? In particular, how is water involved? Recent experiments have shed some light on these problems using and extending concepts borrowed from the physics of glasses and supercooled liquids (PNAS 106, 5129, 2009). Proteins are dynamic systems; they must fluctuate in order to work. Glasses show two main types of fluctuations, α and β. Proteins and their environment also experience similar fluctuations. The α fluctuations originate in the bulk surrounding and influence the shape of proteins. The β fluctuations originate in the hydration shell, two layers of water around proteins, and control the internal breathing. The role of water and of fluctuations is becoming clearer and the path to further directed experiments is now open.

Universal Behavior of the Osmotically Compressed Cell and its Analogy to the Colloidal Glass Transition

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Mechanical robustness of the cell under different modes of stress and deformation is essential to its survival and function. Under tension, mechanical rigidity is provided by the cytoskeletal network; with increasing stress, this network stiffens, providing increased resistance to deformation. However, a cell must also resist compression, which will inevitably occur whenever cell volume is decreased during such biologically important processes as anhydrobiosis and apoptosis. Under compression, individual filaments can buckle, thereby reducing the stiffness and weakening the cytoskeletal network. However, the intracellular space is crowded with macromolecules and organelles which can resist compression. A simple picture describing their behavior is that of colloidal particles; colloids exhibit a sharp increase in viscosity with increasing volume fraction, ultimately undergoing a glass transition and becoming a solid. We investigate the consequences of these two competing effects and show that as a cell is compressed by hyperosmotic stress it becomes progressively more rigid. Although this stiffening behavior is dependent somewhat upon cell type, starting conditions, molecular motors, and cytoskeletal contributions, its dependence upon solid volume fraction is exponential in every instance. This universal behavior suggests that compression-induced weakening of the network is overwhelmed by crowding-induced stiffening of the cytoplasm. We also show that compression dramatically slows intracellular relaxation processes. The increase in stiffness, combined with the slowing of relaxation processes, is reminiscent of a glass transition of colloidal suspensions, but only when comprised of deformable particles. Our work provides a means to probe the cytoplasm under compression, and leads to results that are universal across cell type.

The Inner Structure of a Floating Water Bridge

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When high voltage is applied to distilled water filled into two beakers close to each other, a water connection forms spontaneously, giving the impression of a floating water bridge (Fuchs et al. 2007 *J. Phys. D*: *Appl. Phys.* 40: 6112-4, 2008 *J. Phys. D*: *Appl. Phys.* 41: 185502, Woisetschläger et al. 2009 Exp. Fluids (submitted)). This phenomenon is of special interest, since it comprises a number of phenomena currently tackled in modern water science. The first data on neutron scattering of a floating heavy water bridge and the preliminary results of inelastic UV scattering seem to support the 'bubble hypothesis' suggested earlier (Fuchs et al. 2009, J. Phys. D: Appl. Phys 42 2009 065502). These measurements can be interpreted in accordance with the presence of electrically induced cavitation nano bubbles. The quantum field theory prediction of coherent domains (Del Giudice, Vitiello, personal communication 2008) cannot be excluded either, since such domains would reveal similar neutron scattering characteristics. However, since both nano bubbles and coherent domains are said to carry charge, an electrostatic mesoscopic network formed by either of them can be held directly responsible for the stability of the bridge and may thus explain one key feature of the phenomenon.

Biomolecules in Water and Water in Biomolecules

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It is a common understanding that the molecular recognition is an essential elementary process for protein to function. The molecular recognition is a thermodynamic process which is characterized by the free energy difference between two states of a host-guest system, bound and unbound. On the other hand, the time to reach the thermodynamic equilibrium depends on the free energy barrier mainly associated with the conformational fluctuation of protein. Therefore, the molecular recognition is a thermodynamic process conjugated with the conformational fluctuation of protein.

We have been developing a new theory for the molecular recognition by protein based on the statistical mechanics of liquids, or the 3D-RISM/RISM theory. The theory has demonstrated its amazing capability of "predicting" the process from the frist principle. [1] However, what we have investigated so far is an entirely equilibrium process both in protein conformation and solvation.

Recently, we have started to incorporate the conformational fluctuation of protein into the molecular recognition process in two ways. The first of those is a "static" one in which we just shake the protein conformation to find the local minimum of the free energy surface by the combined 3D-RISM/RISM with conformational sampling algorithms, and to see if one can find the distribution of a guest molecule in the recognition site. One example of such studies will be presented in the talk. [2] The other method is to take the "dynamic" fluctuation of protein conformation into account. The process can be described by hybridized 3D-RISM/RISM with the generalized Langevin dynamics theories. The methodology is currently under construction, and some prospective view of the theory will be presented in the lecture.

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Phase Behavior of Water Inside Protein Crystals

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Protein crystals typically consist of 40 - 60 % water. The internal water forms solvent channels (2 - 4 nm in diameter) inside the crystals. We have studied the phase behavior of water inside protein crystals using a novel crystal freezing method: high-pressure cryocooling. Using X-ray diffraction, we demonstrated that the high-density amorphous (HDA) ice induced inside the high-pressure cryocooled protein crystal undergoes a phase transition to low-density amorphous (LDA) ice as the crystal is warmed from 80 to 170 K. We found that the intermediate states in the temperature range from 80 to 170 K can be reconstructed as a linear combination of HDA and LDA ice, suggesting a first-order transition. We also found evidence for a liquid state of water during the ice transition by monitoring the protein crystallographic data, suggesting a glass transition of HDA ice. These results provide new insights into the anomalous behavior of supercooled water and open a host of unanswered questions.

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Study of Water-Based Electronic Homeopathic Nosodes

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Apart from traditional homoeopathic copies prepared by the dilution/potentiation of parent substances, the electronic-homeopathic nosodes – preparations made by electronic-homeopathic copying the parent substance onto water with the help of M. Rae's or other (J. Benveniste) devices - have received a certain acceptance in some fields of complimentary medicine such as Electropunctural diagnostics, Applied Kinesiology in spite of a significant deficit of scientific data on their nature. The objective of the study is double blind estimation of biophysical differences between water-based electronic homeopathic nosodes (EHN) and blank water carrier. Two investigations were carried out.

The first one was connected to verification of biomedical effect of EHN with a biological model. 4 double blinded randomized trials for the estimation of influence of water-based EHN of organic fertilizer biohumus and placebo on growth and weight of tomato seedlings were handled. The electronic-homeopathic copying was carried out with "Simulator" (Metabolics Ltd, GB) apparatus. The tomato seeds were soaked in preparations then planted out in plastic boxes by 40-49 pieces. In the first experiment one box was separated in equal sections, in other experiments separate boxes were used. Equal exposition of plants to external conditions was achieved. The groups of plants were fed by preparations (200-300 ml) once a week. Duration of each experiment was 38 day. Nonparametric Mann-Whitney U-test and Wald-Wolfovitz runs test were used for statistical analysis. Significant distinctions in mass or/and growth of green part of plants fed by EHN and placebo were found in the last 3 experiments.

The second investigation was connected to determination of differences in EHN and hidden control (placebo) by means of absorption spectroscopy. During double blind randomized procedure 7 names of EHN and blank placebo were copied on ampoules with saline solution by means of «Simulator» (Metabolics Ltd, GB). There were 63 ampoules of nosodes (9 of each name) and 27 ampoules of the placebo. The absorption spectra were determined by UV – 2101 PC (Shimadzu, Japan) double-beam spectrometer in the band of 800 – 600 nm (increment of 0.5 nm). Nonparametric Mann-Whitney U-test was used for statistical analysis for each wavelength. Absorption spectra of five EHN names had narrowband regions marked by statistically-efficient ($p<0.05$ for at least two adjacent wavelengths) differences from placebo, in the band of 800 – 700 nm. Spectral differences of all EHN were represented by increase of absorption in the band of 702 – 743 nm, and decrease of absorption in the band of 779.5 – 790 nm re placebo.

Revealed distinctions between EHN and placebo points to the reality of the electronic-homeopathic copying phenomenon. This leaves no alternative than to suppose, agreeing with J. Benveniste, that water is able to "memorize" non-contact electronic actions. It does not seem anymore much incredible in the context of physics either (S. Lo, 1996; O. Ponomarev, 2000; S. Pershin, 2009). But how are the non-contact actions produced by M. Rae's apparatus capable of influence on water? Assuming that these actions are due to weak electromagnetic fields, the human body is a source of wide-band electromagnetic disturbances associated with the vital activity of cells and organs. Moreover, all this takes place against the background of magnetotelluric field, along with a field of permanent magnet set in M. Rae's apparatus placed beside the operator's body. Conceivably, the copied preparation interpreted as a certain passive resonator (Yu. Shaub, 1998) might modify the field of electromagnetic emission of the operator's organism or the interaction between this field and the aforesaid magnetic fields. In its turn this modified field is superimposed onto water. Thus EHN seems "commits to memory" not the self-field of preparation copied but an operator's response to the preparation. Hence there is well known operator's personality dependence of the prepared EHN effectiveness or experimenter effect of J. Benveniste's electronic preparations (J. Ives, 2006).

The Influence of Water on Physical States of Soft Condensed Matter (foods) as Observed by the "State" Diagram

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When water interacts with a dissolved solute or with amorphous or crystalline materials, the thermodynamics of the system changes such that the free energy of the water is decreased. This is manifested by a decreased vapor pressure in the gas phase reduced water activity or a_w, a reduced freezing point curve as a function of amount of interacting material as well an increased boiling point and melting point of any solutes. These three curves represent the thermodynamic equilibrium conditions. One can superimpose the glass transition curve (T_g as a function of moisture content) of an appropriate solid component onto the equilibrium diagram to show the transition between the two solid amorphous non-equilibrium states of matter, ie. a glass to/from rubber transition. This state diagram can be used to illustrate the non-equilibrium physical state changes as a function of moisture content during water removal and effects of moisture change during storage. The processing of foods with sugars such as cotton candy and sugar coatings for cereal will be used to illustrate the influence of position (rubber vs glass) on the state diagram. An increase in %RH and temperature will cause the amorphous glassy state to transform into a rubber followed by collapse, caking and recrystallization of the sugar (measured by X-ray diffraction). Controlling this in coating a cereal will allow for a glaze or a frosted state. The third example will show that the same recrystallization phenomenon occurs in soft cookies which undergo hardening after baking. In the last example the hardness of a sugar snap cookie will be used to relate the baking end point position (T_{-m}) on the state diagram with respect to the brittle ductile transition curve. This is similar to loss of crispness for fried snacks like chips. These applications show that combining thermodynamics with T_g can more easily illustrate state changes in processing and storage.

Nanoparticle Doped Water: From Particle Structure to Water Properties

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Water is the second-most common molecule in the universe and the most studied material on earth. It covers 71% of the earth's surface, and the human body contains 60-70% water. Surprisingly though, many of the water functions and properties are poorly understood.

In this talk, I will describe water that is doped with insoluble nanoparticles. The doping process, which is owned by Do-Coop Technologies Ltd., takes advantage of water anomalies, and results in water with different properties. This doped water contains 10-100 times more CO_2 than deionized water, it can dissolve and disperse organic compounds in a different manner than deionized water, increases heat stability and activity of protein and the wetting behavior is different from deionized.

From the particle point of view, there is a significant change in the shape and the crystallographic symmetry of the nanoparticles *following the doping process*. While the source powder contains agglomerates of rectangular particles with a cubic symmetry, following the doping process the particles are separated, are spherical and have different symmetry. In addition, they are surrounded by a water layer that is stable even under extreme physical conditions.

Oscillations of the Ortho/Para Ratio of Liquid Water Drive the Ultradian Regulator of the Cell's 24 h Biological Clock

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Our laboratory has investigated extensively a homodimeric, growth-related and time-keeping hydroquinone oxidase (ENOX1) of the eukaryotic cell surface capable of oxidizing externally supplied NAD(P)H. The protein has a binuclear copper center and exhibits characteristics of an ultradian driver of the biological 24 h circadian clock including a recurring complex 2 + 3 set of oscillations with a period length of 24 min. The period length is temperature independent and entrained by light, melatonin and low frequency EMF. Mutant proteins with period lengths of 22, 36 or 42 min transfected into mammalian COS cells yield circadian periods of 22, 26 or 42 h. The oscillations require bound copper and are recapitulated in solution by copper salts. Period lengths of both the ENOX1 proteins and of the copper II oscillations are increased from 24 min to 30 min by solvation in D_2O in keeping with the characteristic 30 h circadian day of organisms grown in D2O. Our hypothesis supported by experiment is that the oscillations are inherent in the protein associated copper II hexahydrate and derive from periodic variations in the ratios of ortho and para nuclear spins of the paired hydrogen or deuterium atoms of the elongated octahedral structure of the protein-bound copper hexahydrate. This is the only microscopic periodic process that occurs on a similar time scale. Interconversion of the ortho and para isomers in liquid water requires from several min to several h to reach a 3:1 ortho to para equilibrium ratio in ortho or para-enriched samples depending on the ionic composition of the medium. Tikhonov and Volkov enriched a sample to a 10:1 ortho-para ratio, and 18.6 min period was present in the decay of ortho water. This time scale corresponds with the independently measured period length in water's absorption of x-rays at a copper k-edge of 8.9. Data analysis indicated that the bond angles between the equatorial and axial oxygen atoms of the copper (II) hexaaqua ion changed with the same characteristic five-peak pattern as redox potential and NADH oxidation. These results suggest that a ca. 18 min period to ortho-para conversions is inherent in water itself. In the presence of copper salts, the period length is increased to 24 min. Extremely low frequency (ELF) magnetic fields result in phasing the ultradian time keeping mechanism. The target of ELF magnetic fields again appears to be water. Why the ortho-para isomer compositions should exhibit a regular pattern of oscillations from their equilibrium ratio of 3:1 remains unexplained. However, such variation would provide a physical rather than chemical basis for the oscillatory behavior of the redox potential and catalytic activity of aqueous solutions to explain our time keeping model and, at the same time, account for the temperature independence of the circadian period length.

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Aqueous Ionic Solutions Investigated by Time Resolved Delayed Luminescence

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Many authors have suggested that liquid water could exists in two states, low-density (LDW) and high-density (HDW), a theory that was firstly used to explain the behaviour of water density in the range between -30° C, the supercooled region, up to 70 C°. According to this view liquid water consists of rapidly inter-converting LDW clusters and HDW clusters and, while the molecular movements in liquid water require constant breaking and reorganization of individual hydrogen bonds on a picosecond time scale, at any instant the degree of hydrogen bonding is very high, more than 95%. This view has been further expanded and consolidated by the Chaplin's two states model of highly ordered icosahedral network that interconverts between a fully expanded low density form and a collapsed high density form.

Chaplin's model succeeded to explain many astonishing properties of water including the existence of a massive exclusion zone (EZ) whose existence has been recently demonstrated and which appears to involve millions of water layers and to be stable for days . In this frame recent spectroscopic measurements have been performed in order to compare the behaviour of the EZ adjacent to Nafion (hydrophilic) surface to that of saturated solution of inorganic salts in which water ordering is expected.

In fact the presence of ions stabilize localized water clusters in the bulk of the solution as they reduce the hydrogen bonding exchanges of the affected water molecules. According to the two-states model of water, there are two classes of solutes, that partition into HDW and LDW, respectively.

In the last few years several studies have demonstrated that the Delayed Luminescence (DL), the photo-induced ultra-weak emission of light which lasts from microseconds up to seconds after the switching off of the illumination source, is able to give structural information on several systems. DL, in facts, is connected to the formation and decay of collective electron states such as excitons or solitons and is then related to the structure of the whole system. For this reason DL should be potentially able to provide useful information on possible structures present in water.

In order to check this possibility the time resolved DL from diluted salt aqueous solutions has been measured. The DL signal from salt solutions is significantly relevant when a prevalence of LDW domains is foreseen. The decay time probability distribution function is characterized by a broad maximum in the microsecond range This suggests the existence of structures characterized by lifetimes in the same time scale. These results, never reported in Literature, appear important.

The Faustian Bargain of Physical Chemists and Biologists

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Waterless Water: A gallimaufry of phenomena in biology and physical chemistry depend on specific ion or Hofmeister effects, inexplicable by classical theories or by simulation. These involve "waterless," water, and ignore all important effects of dissolved gas responsible for long range hydrophobic interactions.

In the classical theories of electrolytes ion specificity occurs only in "hidden variables," fitting parameters like ion size. In simulation the model water is unreal as it ignores solutes. The theories are fundamentally flawed. This is so for concepts like pH, buffers , pKas, interactions of ions with surfaces, membrane and zeta potentials, colloidal interactions and ion pumps. Biochemists and biologists use the techniques and the intuition of the physical chemistry.The interpretation of standard measurements depends on the classical theory. So if the theory is incorrect or flawed so is the meaning of the measurement, e.g., of a pH, pKa, or a membrane potential.

We have a muddle, a mishmash of unexplained phenomena associated with specific ion effects, water structure and hydration glossed over in a kind of Faustian bargain.

The result is a proliferation of parameters that lack predictability in a Ptolemaic system. Except that the Ptolemaic system worked! Add to the situation the fact that dissolved atmospheric gas strongly affects everything else, like hydrophobic interactions in a way that is itself ion specific; and is ignored in simulation. Then the known knowns, known unknowns and unknown unknowns of Rumsfeld all become unknowns.

Despite this depressing scenario, when recent developments of our understanding of specific ion effects are brought to bear, many of the observations do begin to fall into place.

Unexpectedly Long-Range Effects of Hydrophilic Surfaces on the Contiguous Aqueous Phase

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The impact of surfaces on the contiguous aqueous phase is generally thought to extend no more than a few water-molecule layers. We find, however, that colloidal and molecular solutes are profoundly excluded from the vicinity of hydrophilic surfaces, to distances typically several *hundred* micrometers. Such large exclusion zones have been observed next to many different hydrophilic surfaces, and many diverse solutes are excluded. Hence, the exclusion phenomenon appears to be quite general. Others have confirmed its existence.

To test whether the physical properties of the exclusion zone differ from those of bulk water, a variety of different spectroscopic, physical, and imaging methods have been applied. The results, now including IR-absorption spectra, collectively reveal that the solute-free zone is a physically distinct, ordered phase of water that can co-exist essentially indefinitely with the contiguous solute-containing phase. This unexpectedly extensive zone may be a candidate for the long-postulated "fourth phase" of water earlier postulated by others.

The energy responsible for building this charged, low entropy zone comes from light. We found that incident radiant energy including all visible and near-infrared wavelengths induce exclusion-zone growth in a spectrally sensitive manner. IR is particularly effective. Five-minute exposure to weak LED radiation at 3.1 μm (corresponding to OH stretch) causes exclusion-zone-width increase up to three times. Apparently, incident photons cause some change in bulk water that predisposes constituent molecules to reorganize and build the charged, ordered exclusion zone.

Photons from sunlight, then, may have a powerful effect on water that goes beyond mere heating. Solar energy apparently builds order and separates charge between the exclusion zone and the bulk water beyond — the separation effectively creating a battery. Such a light-driven separation of charge bears resemblance to the process of photosynthesis. Indeed, this light-induced energy production would seem relevant not only for photosynthesis-like actions, but also for many realms of nature and engineering involving water and interfaces. The implications are amply discussed in a public lecture http://uwtv.org/programs/displayevent.aspx?rID=22222 and will be presented at the meeting.

Cell Size and Shape by Quantum Models of Water Coherent Domains Dynamics

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characteristics of cells (with a few exceptions, of typically 1-100 μm diameter) which place them between the microscopic, quantum world and the macroscopic, classical one. A quantum mechanical model based on Planck's energy quantization rule and statistics for the electron and proton transfer in cell respiration and oxidative phosphorilation succeeded to explain the empirical allometric relationship connecting size to metabolism [1]. By a different approach, making use of the the low effective mass (m_{eff} = 13.6 eV) of water coherence domains (CDs) from the QED theory [2, 3] we previously proposed the evaluation of cell size by models based on water CDs Bose-type condensation (supercoherence), on CD translation in a spherical well, and on an isotropic oscillator consisting of two interacting CDs [4]. Although the results matched to relatively small and medium-sized bacteria, our initial models showed limitations with respect to larger cells, and approximated the various shapes of cells only to a spherical one. Here we present new models aiming to deal with larger spherical cells and with disk-like and rod-like cells.

Because the values of the maximum radius *a* of a spherical cell estimated by the models of spherical well (1.02 μm) and of isotropic oscillator (0.99 μm) showed an excellent agreement, we looked after a combined model – an isotropic two CDs harmonic oscillator enclosed in a spherical box with impenetrable walls, larger than that required only to accommodate the oscillator. The centre of mass of the oscillator of mass $2m_{eff}$ performs an independent translation, while the oscillator vibrates as a reduced mass $m_{eff}/2$. In a perturbational treatment, the unperturbed energy levels of translation in the box are shifted by the harmonic potential which acts as a small perturbation. Assuming that the difference between the perturbed first two levels exceeds thermal energy, a maximum radius *a* of the spherical cell of 3.21 μm at 310 K is obtained (volume 138.6 μm^3). The predicted size matches to larger prokaryotes like *Myxobacteria* (0.5 – 20 μm3), *Bacillus megaterium* (7 – 38 μm^3) and *Sphaerotilus natans* (6 – 240 μm^3), and also to the smallest eukaryotic cells like yeast, *S. cerevisiae* (14 – 34 μm^3), unicellular *fungi* and *algae* (20 – 50 μm^3), and the *erythrocyte* (85 μm^3). The disk-like and rod-like cells have in common the axial symmetry, and both can be approached by the model of a cylindrical potential box with impenetrable walls. Along the axis the problem reduces to a linear gap with infinite walls and length *a*, of energy levels E_n. Around the axis, we were interested only by the radial part of the solution, given by Bessel functions $J_l(r)$, with energy eigenvalues E_{lm}. The total energy is $E_{nlm} = E_n + E_{lm}$ with no immediate restriction to the values of *l*, *m* with respect to *n*. Because $J_l(\alpha r_o) = 0$, the maximum radius r_o is related to the roots x_{lm} of $J_l(\alpha r)$. In the case of the disk-like cell, we chose |110> (*n* = 1) as the ground state, and admit that the transition |110> --> |221> to a higher (*n* = 2) level is "biologically forbidden," or thermally unfavourable ($E_{221} - E_{110} \geq 3/2\ k_BT$). Using the x_{10} and x_{21} roots, we obtain for a thickness a = 1.15 μm, a radius $r_o \leq 3.8$ μm, while a *human erythrocyte* is 2 μm thick and has a 3.75 μm radius. For the rod-like cell, we postulate that biologically relevant transitions leave unchanged the axial translation energy E_n, $\Delta n = 0$. For $n = 1$, a thermally unfavourable, biologically forbidden transition |1*lm*> <--> |1*l'm'*> allows estimation of radius r_o. Choosing |102> ground state, and |102> --> |121> as a "life-forbidden" transition, and using x_{02} and x_{21} roots, a radius $r_o < 0.28$ μm is obtained for a length a = 1,02 μm. The dimensions r_o and *a* are roughly confirmed for typical and relatively small bacilli. The ratio $2r_o/a = 0.54$ of the cell shape fits very well, e.g.: *Brucella melitensis* (0.5-0.8), *Francisella tularensis* (0.3-0.7), *Yersinia pestis* (~ 0.5), *E. coli* (0.25-0.4). Comparable results are obtained with other couples of states, classified by an empirical "selection rule" for "biologically forbidden" transitions $\Delta(l + m) = 0, \pm 1$.

The results suggest that the dynamics of water CDs in the in the cell, which represent bound quantum systems, are an essential factor in determining the cellular size and shape. It is plausible that evolution selected the size and shape of cells such as to fit the form of potentials and of the CDs' wavefunctions. However, one can hope that quantum mechanics contains a vast conceptual provision, which could be applied in further water CD models to account for other ultrastructural features of cells.

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The Structures and Thermodynamics in (Paracrystalline) Polymorphism of Liquid Water

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This paper starts by detailing the extraordinary omission in thermodynamics and the phase rule, taught and used by most scientists for a century, which ignored all vector and tensor intensive variables beyond the scalar 'p' and 't'.

It then treats the parallelism between the two most abundant phases on the earth's surface: liquid H_2O and crystalline SiO_2. A parallelism slowly being accepted for their polymorphism in the many stable, and an almost infinite number of metastable, phase transitions. These are established for SiO2—as will be shown—and slowly being accepted for liquid water. The term 'paracystalline' is introduced, to replace the misleading use of the term clusters. The latter refers only to one part of the short range—and ignores the long range arrangements which exist in the liquid water phase.

This background is necessary to understand the evolution of the science of polymorphism, first in the liquid state generally, and then specifically in liquid H_2O. The data summarized by Chaplin and Stanley establish the real and putative existence of some dozens of polymorphs, but these are limited to the case where the intensive variables are only pressure and temperature. To these we must now add the enormous range of structural changes we have been able to effect in our laboratory by the use of polarized electric and magnetic fields and acoustic radiation as normal, albeit vector and scalar intensive variables. In addition, we have also demonstrated the role of the related phenomenon of epitaxy (at least) on various liquid structures which clearly change the p and t conditions for stability of a phase.

Deviation from Identity of Macroscopic Properties of Enantiomers—via Water Chiral Preference

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The parity violation energy difference (PVED) between chiral isomers is of a tiny magnitude (<kT) which, in principle, can be expanded to a macroscopic detectable level under cooperative processes[1-3]. Recently, a series of findings have suggested that the hydration layers around chiral amino acids in water may differ for the enantiomers[3,4], which could support macroscopic chiral discrimination in rates of crystallization[5] and heat of solution[4]. Furthermore, for poly amino acids in water differences between L and D poly glutamic acid were observed in helix coil transition[6] , as well as in thermal stability and supra molecular structures7 . Surprisingly, when tested in D_2O under identical conditions these differences were markedly reduced[6,8], indicating a specific discrimination of H_2O molecules between chiral configurations. It has been proposed[3,6,8] that the spin isomers of water, i.e., ortho H_2O and para H_2O, prevailing at a 3:1 ratio respectively[9] , could account, at least in part, for this discriminatory power. In D_2O the spin isomers are much less pronounced[9] which may greatly attenuate such a putative chiral preference[6,8]. Chiral discrimination in water implies that partitioning of a racemic mixture into water may be followed by a transient optical activity at its initial phase. Such a yet unprecedented observation will be also presented. Together, the mentioned studies provides evidence to the assertion that water possess a chiral discriminatory power[3-6], which leads to violation

of chiral identity in aqueous solutions. It also provides new clues and a new investigation of water structure.

The main significance of our work is in the realm of the linkage and transfer of parity violation from level to level, beginning with the elementary particles and forces, to atoms molecules and more complicated systems, life itself.

Our work provides the experimental proof and the explanation how this linkage is done.

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Sunlight-Induced Structural Change of Liquid Water

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Sunlight irradiation induced structural change of liquid water to form clathrate-like the liquid water resulted in a change in the XRD pattern.[1] In addition to the peak at 2θ = structure, which was evidenced by XRD and IR spectroscopy. Irradiation of sunlight on 280 ($\sin\theta / \lambda = 1.6$ nm^{-1}) which was observed for a non-irradiated water, a peak at $2\theta = 12$ ($\sin\theta / \lambda = 0.7$ nm^{-1}) appeared on irradiation of sunlight and developed with the irradiation time. The peak continued to be intensified over a period of 1 h and more. Radial distribution function analysis of the diffraction pattern indicated that the ordering range expanded as the irradiation period was prolonged from 5 min to 1 h. Tetrahedral arrangement of non-irradiated water gradually changed to clathrate-like structure on irradiation of sunlight. Definite changes in IR spectrum of liquid water in the O-H stretching region were also observed on irradiation of sunlight at room temperature.[2] The spectrum shape in the range 2800 - 3800 cm^{-1} became trapezoidal on irradiation of the sunlight for more than 30 min under the sunlight strength of 3 MJ m^{-2}. The spectrum gradually changed to restore the original spectrum in 3 h when sunlight irradiation was shut off. These results indicate that the formation and elimination of a clathrate-like structure of water occurred reversibly at room temperature in response to irradiation and shutoff of the sunlight, respectively. The structural change induced by the sunlight irradiation occur red over a period of several minutes to hours. The structural change of liquid water implies that the physical properties of liquid water also change on sunlight irradiation. It is important to take into account the structural change in understanding the phenomena of nature associating with water.

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Why is it So Hard?

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Understanding molecular recognition in aqueous systems remains to be one of the most challenging problems in chemical biology. Why is it so hard, for example, to design ligands that bind tightly to proteins? The answer, in short, seems to be water. Understanding the role of water in molecular recognition would facilitate dramatically efforts in drug design and biomaterials research. Our efforts toward understanding water rely on a physical-organic approach: we combine synthesis, X-ray crystallography, microcalorimety, and computational efforts to shed light on water's crucial role in protein-ligand interactions in biology. Our results, in several cases, seem incompatible with widely accepted theories of the hydrophobic effect.

Interfacial Water Layers in Biolubrication

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Interfacial water layers attract increasingly attention in both biomedical engineering and material sciences. An actual Google search yields for ‘interfacial water’ a total of 20000 hits, PubMed 259. They exist in air and under water, with structures imposed by the polarity of the surfaces involved. Their importance consists in controlling a multitude of nanoscale processes, in particular related to lubrication and contact adhesion. Both processes are regulated by polarity contrasts. Access to a better understanding of these vital functions, for instance, the interaction of proteins with their immediate environment in a predominantly aqueous environment, emerges from new laboratory experiments shedding light on two static properties of interfacial water layers (order and surface stability) and two dynamic properties (speed of propagation and range). These intrinsic properties and their interplay have maximum relevance in biology.

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Liquid Water, the “Most Complex” Liquid: New Results in Bulk, Nanoconfined, and Biological Environments

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This talk will introduce some of the 63 anomalies of the most complex of liquids, water. We will demonstrate some recent progress in understanding these anomalies by combining information provided by recent experiments and simulations on water in bulk, nanoconfined, and biological environments. We will interpret evidence from recent experiments designed to test the hypothesis that liquid water may display "polymorphism" in that it can exist in two different phases—and discuss recent work on water's transport anomalies [1] as well as the unusual behavior of water in biological environments [2]. Finally, we will discuss how the general concept of liquid polymorphism [3] is proving useful in understanding anomalies in other liquids, such as silicon, silica, and carbon, as well as metallic glasses, which have in common that they are characterized by two characteristic length scales in their interactions.

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What Can We Learn From Plants About Water at Negative Pressures?

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Liquids, like solids, have tensile strength. Indeed, scientists have long known that plants exploit this strength to pull water out of the soil and up to their leaves with the pressures in the sap down to -100 atm (tensions up to 100 atm). Nonetheless, the metastable state of liquids under tension – beneath the binodal and above the spinodal – remains largely unexplored scientifically and completely unexploited technologically. In this talk, I will discuss the thermodynamics of transpiration in plants and present a bio-mimetic route to large tensions in the laboratory. Based on experiments with "synthetic plants", I will illustrate the surprising processes that are enabled by working in this regime. I will then discuss the origin of the limit of stability of liquid water in plants (natural and synthetic) and more generally. Finally, I will conclude with the presentation of opportunities to exploit this regime to gain insights into the fundamental character of the liquid water (e.g., the molecular origin of water's anamolies) and to address important technological challenges in the management of energy and natural resources.

Gurvitch Experiments Revisited

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One of the accepted paradigms is that molecules interact with target systems via various physicochemical forces. For instance, the action of a molecule involves interaction with its receptor, to trigger a cascade of biochemical events that activate biological functions. Within this paradigm, the presence of the molecule is necessary.

One question is whether a chemical reaction between for instance a protein and its receptor protein is needed, or whether this interaction does not require that the molecule actually come into physical contact to activate the receptor protein [1-3].

Other experiments related to non-chemical and non-contact communication between biological systems can be traced back to 1920 [4]. A. Gurvitch showed that onions kept closely together stimulate growth of each other's roots. He separated the roots by encasing them in different materials and showed that this was not simply a chemical influence. Further, the effects of growth stimulation occurred when quartz was used but not UV-opaque glass. Since then, there is an increasing body of evidence to suggest unconventional forms of intercellular communication. For instance, in 1992 G.Albrecht-Buehler observed that distant cells align themselves in culture media through cell to cell communication [5]. Together, these phenomena suggest the existence of non-chemical signal(s) that convey messages to or between cells.

New experimental studies related to distant non-chemical communication using different cells models will be presented. We will discuss the current state of knowledge and envision different hypotheses regarding the nature of these ‘'informational signals.’'

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Aquaphotomics

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Aquaphotomics (“all about water – light interaction”) is a new term, introduced to describe an area of science dedicated to enhance our understanding of water-light interaction at every frequency of the electromagnetic spectrum. In particular, VIS/NIR spectroscopy is considered as a new tool for water observation that provides immense information about water at molecular level and therefore, a better understanding of biological world. Water, as a natural biological matrix containing small molecules with a strong potential for hydrogen bonding, changes its absorbance pattern every time it adapts to physical or chemical change in biological systems or the environment. Therefore, its spectral changes permit measurement of small quantities or of structural changes in other molecules in the system, too. In other words, NIR light adds a new dimension to the water mirror effect caused by the visible light reflection from the surface of the water. Water becomes a “stereo, 3D” mirror on molecular level as, in addition to the reflection of the visible light from its surface, every frequency of the NIR light penetrates into the water and gets absorbed by each individual hydrogen bond in a unique way that could be described by the respective water absorbance pattern, WAP. This spectral pattern is indicative for other molecules surrounded by water, too, i.e. reflects the rest of the molecules in the water matrix.

Intrinsic Sustained Activity of Bicarbonate Aqueous Solutions

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Addition of Fe(II) salts ($FeSO_4$ or $FeCl_2$) in the range of concentrations of 10-50 mkM to bicarbonate artesian waters or aqueous bicarbonate solutions induces a wave of photon emission (PE) from them. Intensity of the wave is boosted in the presence of luminol, the probe for the reactive oxygen species (ROS). Induction by Fe(II) of luminol-amplified PE indicates that spontaneous chain reactions with ROS participation continuously flow in aqueous bicarbonate solutions. PE-waves in bicarbonate aqueous solutions can be induced in them by addition of Fe(II) in the presence of Luminol many weeks after their preparation provided that they are contacting with the air. Amplitudes of PE-waves decrease if a bicarbonate solution is kept in a sealed vessel. After its opening amplitude of PE-wave increases again indicating that contact with the air is needed for the persistence of processes responsible for PE. However, addition of H_2O_2 in sub-millimolar concentrations to 1-5 mM Na/K-bicarbonate solutions initiates in them a peculiar process accompanied with spontaneous low-level photon emission amplified with luminol. The process may proceed in hermetically closed test-tubes and in the darkness for many months without decay. The process exhibits extremely high sensitivity to the action of physical and chemical factors of ultra-weak intensity. Monthly and circadian rhythms of PE are observed. Amplitude of PE intensity from test-tubes filled with active solutions increases 2-3 fold on periods coinciding with the eclipses of Moon and Sun. Preparations of water-soluble fullerenes in dilutions equivalent to their concentrations 10^{-13}, 10^{-15} and 10^{-19}-10^{-20} M increased photon emission 2-3-fold while intermediate dilutions affected it much weaker. We suggest that addition of H_2O_2 to aqueous bicarbonate solutions initiates in them cyclic chain reactions in which water is oxidized with oxygen. Bicarbonate may stabilize these cyclic reactions due to its ability to participate in free radical reactions. Extremely long-lasting photon emission (high density electromagnetic energy) from activated bicarbonate solutions indicates that they reside in stable non-equilibrium (excited) state supported presumably by continuous efflux of low density (electromagnetic) energy from the environment. Thus such systems are able to transform low grade energy into high grade energy. It is notable that bicarbonate is the necessary constituent of cytoplasm of aerobic cells and of important biological liquids, in particular of blood plasma. Normal and healing drinking waters also usually represent bicarbonate solutions. Steady activity of bicarbonate aqueous solutions induced by rather weak factors may represent a property important for many vital functions of individual living systems as well as for the natural environmental processes.

Giant DNA in Water: Conformational Transition and Radiosensitivity

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During the last decade, based on the methodology of single DNA observation in water environment, it has been confirmed [1] that individual giant DNA molecules, larger than several tens of kilo base-pairs, undergo a large discrete transition in their higher-order structure. The fundamental characteristics of the transition are summarized as follows: 1) The structural transition between elongated coil and packed compact states in giant DNA is all-or-none on individual DNA molecules, whereas it seems continuous on the level of the ensemble of DNA molecules. 2) The discrete nature of the transition is rather general regardless the change of the mechanism of compaction by using different condensing agents, such as polyamine, hydrophilic polymer, cationic surfactant, etc. 3) When the degree of the charge neutralization is insufficient, intra-molecular phase segregation is generated, i.e., elongate and compact states coexist along a long DNA molecule.

In the present paper, we will show the results of our recent measurements on double-strand breaks on giant DNA caused by γ-ray irradiation. It is shown that double-strand breaks are significantly protected for the tightly compact DNA, whereas there is no apparent decrease on the damage for loosely aggregated DNA molecules. These results indicate the importance to explore the difference in the higher-order structure among 'DNA condensation' in relation to their biological properties.

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Six Ways to Probe Interfacial Nondestructively

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The traditional techniques for studying the structure of interfacial water layers, such as molecular dynamics simulations, neutron and X-ray diffraction, have been recently extended by a number of new techniques, such as sum-frequency vibrational spectroscopy, ultrafast laser pulses combined with time-resolved electron crystallography, or atomic force microscopy. The deviation from the mainstream technique promised new insights into the structure of interfacial water layers. Indeed, the new techniques showed an enormous potential for the study of the subject, which is extremely sensitive to observation. Clearly, information extracted from probing interfacial water layers with one single tool is critical: Valuable information, such as dynamic structure, interfacial residence time, or bond stability might return in a distorted form. Therefore, we focused on dual techniques allowing us to systematically investigate the structure of interfacial water layers: one tool only to induce a change into the system, and another tool to independently monitor the responses of the system. The complementary technique offered unprecedented insight into the structure interfacial water layers. We report on six variation of the dual technique. The synoptic perspective emerging from the dual analysis of interfacial water layers is, however, not only that we know a little more about their structural properties, but more importantly, that we know how to practically influence and modulate their structure.

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Poster Abstracts

(alphabetical by author)

Sonoluminescence and Quantum Optical Heating

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We discuss a quantum optical heating mechanism which might contribute substantially to the sudden energy concentration in sonoluminescence experiments. We emphasize the role of the noble gas atoms inside the bubbles. Although predominantly in their ground state, they act like catalysers and facilitate the creation of phonons at a very high rate. Our model is based on a quantum optical approach which is routinely used to describe the laser cooling of tightly trapped ions.

The Structure and Function of Quinones in Photosynthesis: High-Frequency EPR Spectroscopy Studies of Substituent and Solvent Effects on the g-Tensors of Benzoquinone Models*

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Photosystem II (PSII) is a multi-subunit membrane protein that catalyzes the oxidation of water to dioxygen and reduction of plastoquinone to plastoquinol. Quinones are utilized as electron transfer cofactors in photosynthetic proteins that are essential to life. In PSII, the electron transfer involves two plastoquinones, the primary and secondary quinone acceptors (QA and QB). The versatility of quinones and the wide variation in their function is due to their diverse redox potentials, which are controlled by substituent effects and by interactions within the protein binding pocket. To understand the substituent and solvent effects on quinone molecules, we are studying an extensive library of model benzoquinones in protic and aprotic solvents using high-frequency electron paramagnetic resonance (HF EPR) spectroscopy. At high magnetic fields, increased electron Zeeman interaction leads to better resolution of spectral features arising from the different g-tensor components. Our studies suggest that the g-tensor of the semiquinone anion radicals is influenced by the spatial distribution of the orbital carrying the unpaired electron and is strongly influenced by the π-spin densities at the carbonyl oxygen atoms, which have a much larger spin orbit coupling constant compared to carbon atoms. Thus, a detailed study of the change in the g-values of model benzoquinones in different solvents highlights the effect of the solvent and substituent effects on the π-spin densities at the carbonyl oxygen of the benzoquinones.

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The Extra- and Intracellular Water as a Target for Non-Thermal Biological Effect of Millimeter Waves

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The phenomenon of non-thermal biological effect of low intensity Millimeter Waves (MMW) has been known for several decades and it is more and more widely used in alternative medical treatments of a variety of diseases. However, the physicochemical mechanisms through which the non-thermal effect of MMW on cells and organisms is realized still remain unclear.

Since water is the dominant component of the cell, which has higher absorption properties for MMW, it is suggested as a main target through which the biological effect of MMW on cell is realized.

For testing this hypothesis, the effects of 5mW/cm^2 MMW on physicochemical properties of physiological solution (PS) (specific electrical conductance, heat fusion, specific absorption rate, gases solubility, reactive oxygen species) and the effect of direct MMW radiation and MMW-pretreated PS on functional activity of isolated single neurons, heart muscle and brain tissue of rats were studied.

Through the study of the effect of MMW dependency on physicochemical properties of PS on frequency of modulated field it was shown that there are frequency “windows” (4 and 8Hz) at which the MMW modulation has more pronounced effect on physicochemical properties of PS. The heat fusions of PS pretreated by 4 and 8 Hz modulated MMW were higher by 8,6 % and less by 6,8 %, correspondingly, compared with non-treated PS. The concentration of H_2O_2 in PS was increased by 10 min 4 Hz modulated MMW irradiation from 3,03 to 3,24 nM. It is suggested that MMW-induced vibration of water dipole molecules brings to the increase of water molecules dissociation, the interaction product of which with oxygen brings to the formation of H_2O_2.

To find out whether the MMW-induced elevation of H_2O_2 in PS serves as a messenger through which the non-thermal biological effect on cells and organisms are realized, the comparative study of MMW-treated PS and 5x10^{-9} M H_2O_2 -containing PS on snails single neurone volume and electrical activity, heart muscle hydration and contractility and rats brain tissue hydration was performed.

The obtained data shows that both MMW-pretreated PS and H_2O_2-containing PS have dehydration effect on snail neurons, hearth muscle, brain tissue and depressing effect on the neuronal activity and heart muscle contractility. These data are strong evidence of the fact that water molecule dissociation, which determines its physicochemical properties, could be changed by energy, which is far from thermal threshold and could have a biological effect on cells and organisms. So the “KT paradox “could not be a barrier to recognize the existence of non-thermal biological effect of MMW.

Dramatic Difference in Freezing of Water on Positively and Negatively Charged Pyroelectric Surfaces

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Dramatic differences in the freezing temperature of super-cooled water (SCW) were recorded on the positively and negatively charged surfaces of pyroelectric $LiTaO_3$ crystals. Using a specially designed setup, the very same surface of a pyroelectric crystal can be charged either positively or negatively or kept neutral due to cooling or heating. We present here that drops of SCW freeze on the uncharged reference surfaces at -12.5±3°C, on the positively charged surface at -7±1°C, whereas on the negatively charged surface as low as at -18±1°C. Furthermore, drops of water cooled down on a negatively charged surface and remained liquid at -8°C were frozen immediately by heating this surface to -6°C, as a result of the replacement of the negative surface charge by a positive one. Specular X-ray powder diffractions, including rocking curve analysis, indicate that ice grows on the non-charged surfaces as (001) oriented crystals perpendicular to the solid surface. On the positively charged surfaces, (100) oriented ice-like clusters are formed and then trigger secondary random nucleation. In contrast, nucleation near the negative charged surfaces is suppressed and the ice crystals grow from air/water interface in the (001) direction perpendicular to the water drop surface. We have also observed similar influence of the surface charge on the freezing points of SCW using pyroelectric non-crystalline (so-called quasi-amorphous) films of $SrTio_3$. These results imply that the (100) ice-like clusters are stabilized in the vicinity of a positively charge surface, whereas the clusters stabilized by a negatively charged surface have a structure which is non ice-like.

Interaction Energy of Model Lipid Membranes with Water

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The Langmuir-Blodgett/Schaefer (LB/LS) method and contact angle measurements were used to investigate interaction energy of lipid films with water. Membranes were constituted of single-component or binary systems formed by phospholipids: saturated 1,2-dipalmitoyl-*sn*-glycero-3-phosphocholine (DPPC), unsaturated 1,2-dioleoyl-*sn*-glycero-3-phosphocholine (DOPC) and cholesterol (Chol) or their mixture DPPC/DOPC and DPPC/Chol with different DOPC or Chol molar ratio. The surface free energy for single and binary lipid mono- and bilayer systems was evaluated from the advancing and receding contact angles of water using the contact angle hysteresis (CAH) model. Taking into consideration an area occupied by one molecule in packed monolayer, the obtained surface free energy values allow calculation of the interaction energy of one lipid molecule with water and then of one mole of lipids molecules. Saturated DPPC mono- and bilayers exhibited much lower surface free energy than unsaturated DOPC one, probably due to the differences in packing of the molecules. Pure Chol cannot form stable mono- and bilayers. In the case of mixed DPPC/DOPC layers an increase in the total surface free energy is observed, being an effect of the changes in packing and ordering of the molecules, and for DPPC/Chol system the energy changes are due to complex DPPC/Chol formation and/or patched film occurrence, especially in the mixed systems containing more Chol than DPPC. In the mixed DPPC/Chol system a strong cohesive force acts between molecules, especially when Chol molecules are surrounded by DPPC molecules (complex formation), but at the higher surface pressure the patched film may form. These studies provided a fundamental framework for better understanding of the interactions occurring in the biological lipid systems, and changes in their wettability by water.

TE and Water Uptake Kinetics:

Relation with Yield Components in Peanut (*Arachis hypogaea* L.) Under Drought

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Transpiration efficiency (TE) is an important trait for drought tolerance in peanut (*Arachis hypogaea* L.). The variation in TE was assessed gravimetrically using a long time interval in nine peanut genotypes (Chico, ICGS 44, ICGV 00350, ICGV 86015, ICGV 86031, ICGV 91114, JL 24, TAG 24 and TMV 2) grown in lysimeters under well-watered and drought conditions. The transpiration was measured by regular weighing of the lysimeters whose soil surface was mulched with a 2-cm thick layer of polythene beads. TE studied varied from 1.4 to 2.9 g kg^{-1} under well watered and 1.7 to 2.9 g kg^{-1} under drought conditions, showing consistent variation for TE among the nine genotypes. A higher TE was found in ICGV 86031 in both well-watered and drought conditions and the lower TE was found in TAG 24 under both the water regimes. Although the total water extraction differed little across the genotypes, the pattern of water extraction from the soil profile varied among the genotypes. High water extraction within 24 days following stress imposition was negatively related to pod yield ($r^2 = 0.36$), and negatively related to water extraction during a subsequent period of 32 days ($r^2 = 0.74$). By contrast, the latter, i.e. water extraction during a period corresponding to pod filling (between 24 and 56 days after flowering) was positively related to pod yield ($r^2 = 0.33$). TE was significantly and positively correlated with pod weight ($r^2 = 0.30$) under drought condition. Our data showed that under the intermittent drought regime, TE and water extraction from the soil profile during a period corresponding to pod filling appeared to be most important traits contributing to higher pod yield in the nine groundnut genotypes tested.

Thermodynamic Integration Based on Molecular Dynamics Simulation Combined with 3D-RISM Theory

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Recently, we proposed a combination of molecular dynamics (MD) simulation with the three-dimensional reference interaction site model (3D-RISM) theory, i.e., MD/3D-RISM method. In this study, we extend this combination method to a thermodynamic integration method to calculate the free energy differences between different states in solution. Regarding this extension, we develop two computational tools: i.e., we introduce either (1) the reaction coordinate or (2) the coupling parameter, where the latter is the parameter for switching the interaction potentials. We will present a basic formalism and an application of this method to the cation recognition by crown ether 18C6 in aqueous solution as one of the simplest examples.

Biosolids Dewatering Using Super Absorbent Polymers (SAPs)

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Super absorbent polymers (SAPs) have the ability to absorb water from several tens to several hundreds times their own weight. They play an important role in a variety of applications such as water seepage control in agriculture and

diapers. Biosolids are 95% water. Treatment and disposal involve several operations such as thickening, digestion dewatering and transport. Most of the biosolids treatment operations highly depend on solid content. Some processes are energy intensive e.g. centrifugation. Thus efficient management is required to control such intricate treatment process. This work describes the potential role for SAPs in developing more efficient biosolids processing using Milorganite surrogates and real biosolids obtained from the Metropolitan Reclamation District of Greater Chicago (MWRDGC). Work consists of separating solids from biosolids suspension using SAPs through a membrane. Preliminary results showed significant increase in solid content of a Milorganite surrogate of 5% solid content. Depending on the preparation method and surrogate type this solid content increase ranged between 50 to 100 %; i.e., final solid content ranged from 7-11%. Results are justified with real post digested biosolids samples. Furthermore SAPs recycling is possible and was reused for up to 20 times when tested on pure gelated body.

Oscillations of the Ortho/Para Ratio of Liquid Water and the Ultradian Oscillator of the Cell's 24 h Biological Clock

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The Morré laboratories have described an ultradian oscillator of the cell's biological clock. The protein is a cell surface oxidase which oscillates with a regular period length of 24 min (oscillates 60x/24 h circadian day). The activity requires bound copper and is recapitulated in solution by aqueous copper salts. Period lengths of both the ENOX1 proteins and of the copper II oscillations in D_2O are increased from 24 min to 30 min in keeping with the 30 h circadian day of organisms grown in D_2O. Mutant proteins with period lengths of 22, 36 or 42 min transfected into mammalian COS cells yielded circadian periods of 22, 36 or 42 h. Our most recent findings (Morré, Orczyk, Hignite and Kim, 2008 *J. Inorg. Biochem.* 2002:260-267) demonstrate that the oscillatory behavior is related to the equilibrium dynamics of the ortho/para hydrogen spin-isomers of the copper (II)-associated six water molecules. The phenomenon involves two separate levels of rotational energy, one for ortho and one for para. Interconversion between ortho and para isomers is rare as the Pauli Principle requires that the overall wave function of the molecule must change signs with particle interchange. The interconversion that does take place does so in a harmonic fashion with the ratio of ortho and para spin-isomers range from 2.83 to 3.17 over an 18 min period, the intrinsic period length in the absence of metals. The changing ortho to para ratio affects the auto-oxidation of NADH as maxima in oxidation activity occur when the ratio of ortho to para spin-isomers of water is the highest. In the presence of copper II chloride, NADH oxidation activity occurs on a 24 min period. Copper II chloride, acting as a nuclear paramagnetic center, affects the ortho/para interconversion process resulting in a longer period of harmonic oscillations in the ortho/para spin-isomer ratio. It is hypothesized that copper II hexahydrate serves as the catalytic center for cell surface NADH oxidase (ENOX1), which serves as a molecular timekeeper that regulates the cell's 24 h biological clock through regulating ortho/para interconversion. An equation, empirically derived from equations describing harmonic motion, has been fitted to infrared data which describes the ortho/para ratio in liquid water. Currently, a need exists to ground the empirical equation on a theoretical foundation.

Investigating the Relationship Between Slip Length and Interfacial Viscosity on OTS Mica and HOPG

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The properties of nanoconfined water are crucial to the understanding and of biological systems and the design of many engineering systems such as nanofluidics, and nano filtration devices. Atomic Force Microscopy (AFM)-a versatile tool for imaging, measuring and manipulating matter at the nanoscale-was used to probe the nano-confined behavior of water at the interface of three different substrates, with varying wettability and surface roughness. Classical fluid dynamics assumes that liquid at the interface of a solid surface adheres to the surface and does not flow, known as the no-slip (zero velocity), boundary condition. Although valid in macroscopic flows, recent studies show that this condition no longer holds on the micro/nano scale as surface properties such as wettability and surface roughness have a strong effect on the overall flow at reduced dimensions, thus slippage is possible. Here we report an experiment where a hydrophilic AFM tip approached a hydrophobic nanometer-smooth Octadecyltrichlorosilane (OTS) SAM deposited on silicon, hydrophilic nanometer-smooth silicon, atomically-smooth muscovite mica as well as Highly Ordered Pyrolytic Graphite (HOPG), all performed in ultrapure water. While normally approaching, the AFM tip was also laterally oscillated, by means of a Lock-in Amplifier, allowing the direct measurement of the (interfacial) viscous lateral force, as a function of tip sample distance. The data suggests the intrinsic viscosity and the slip length depend on the hydrophobicity of the substrate, with more slippage on the hydrophobic surfaces than the hydrophilic surfaces.

Possible Optical Enhancement of the Energy Concentration in Sonoluminescence

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We propose to manipulate the confined noble gas atoms inside the sonoluminescing bubble with the help of an external laser field. Such a laser would create a coupling between the quantized motion and the electronic states of the atoms similar to the coupling created by a weak but highly inhomogeneous electric field.

Depending on its laser frequency with respect to the relevant noble gas transition, it is therefore expected to either enhance or inhibit the sonoluminescence phenomenon.

Drinking Water Production: Formation of Reproducible Biofilm Communities on RO Membranes in a Test Cell

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One of the major problems during the operation of reverse osmosis membrane plants is biofouling due to microbial biofilms forming on the spacers and the membranes in the system. Biofilms growing in these environments can vary strongly in their appearance, characteristics and composition of the microbial communities. Aim of this study was to set up a simple method to produce comparable biofilms for study of biofilm formation in reverse osmosis (RO) drinking water production systems. Biofilms were grown in a laboratory scale RO-membrane test cell system. During these experiments only the flow rate was changed, nutrient dosing and water temperature were controlled. Denaturing gradient gel electrophoresis (DGGE) analysis was used to show the comparability of the resulting mixed species biofilms. Single organisms were extracted by plating techniques and subsequently sequenced (16S RNA); pieces of the membrane and spacer were prepared for examination in scanning electron microscopy (SEM). The DGGE results show a stable biofilm community, the major bands stayed the same throughout the study. The sequenced single strains (16S RNA) turned out to be organisms known to grow in these environments. SEM analysis of the grown biofilms show well formed mature microbial communities grown on the spacer and the membrane in the used system. The method presents a simple way to study reproducible biofilms and their behavior in RO-membrane systems under varying conditions. This system can be of use for future studies in the field of biofilm communities in RO drinking water production systems.

Hydrogen Bonding in Water During Hard vs. Soft Confinement

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Molecular motions and properties of water depend on the degree of hydrogen bonding. In this study, IR bands of water (ν-OH, δ-OH, and $\nu_2+\nu_3$) were analyzed to quantify the kinetics and thermodynamics of hydrogen bonded (HB) and non-hydrogen bonded (NHB) populations of water molecules at cryogenic temperatures in hard vs. soft confinement. In the first part of the study, water was confined in a nanoporous SiO_2 matrix (hard confinement), which allowed to explore liquid-liquid and liquid-glass transitions during cooling down to -180°C. The fragile to strong transition and the glass transition of water was detected at -51°C and -135°C, respectively. These transitions were observed as changes in the growth of the HB population with temperature. In the second part of the study, a kosmotropic agent (e.g., trehalose) was mixed with water in different mass ratios (φ = 10 to 43% w/w) to explore the changes in water HB populations during supercooling (soft confinement). The presence of trehalose increased the HB population of water and the spectroscopy analysis revealed the presence of two different water clusters in aqueous trehalose solutions: (1) water molecules directly associated with the carbohydrate, forming its hydration layer(s); and (2) water molecules that are involved in

water-water small clusters. The latter showed characteristics of water in hydrophilic confinement.

Effects of Static Magnetic Field on Water and Electrolyte Solutions Properties

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Although changes caused by magnetic field depend on many factors and are still somewhat controversial, influence of static or alternating magnetic and electromagnetic fields on the physicochemical properties of water or aqueous solutions and suspensions has attracted much interest. These effects lasted even up to many hours since the field has been removed and this phenomenon is called 'memory effect'.

Water and electrolytes solutions were exposed for 5 or 20 min to a weak static magnetic field at dynamic condition and their conductivity and amount of evaporated water were then measured as a function of time. Simultaneously, these quantities were determined for magnetically untreated samples, as the reference systems. It was found that magnetic field increases the amounts of evaporated water and influences conductivity of examined solutions. For the electrolyte solutions containing water structure-disordering ions these effects depend on the thermodynamic functions of the ions hydration. Roughly, linear change in the conductivity versus 'scaled' these functions were obtained. On this basis it can concluded that magnetic field causes changes in the hydration shell of the ions.

Natural Bond Orbital Analysis of Small Water Clusters: A Decrease in Charge Transfer Blocks Tetrahedral Structure from Predominating in Liquid Water

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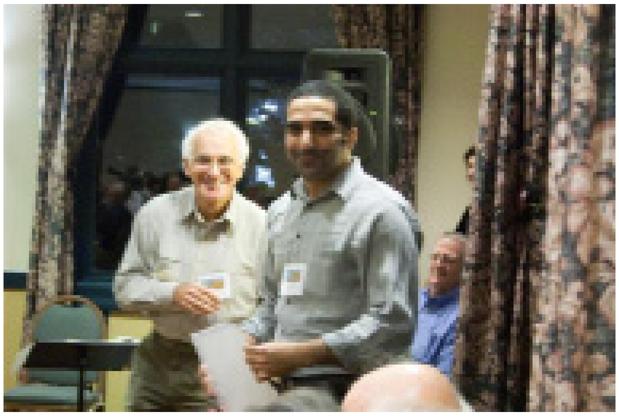
Recent studies have broadened our view of water structure and dynamics. Establishing a predictive model of water is at the central position in the field of drug design, for example. While the tetrahedral structure model remains a standard, the structure of water has been a subject of intensive debate since Wernet and coworkers challenged our traditional view of water structure in 2004 by suggesting water molecules from linear structures instead of tetrahedral networks. We have studied hydrogen bonding in a series of small water clusters (trimer ~ pentamer) using ab initio calculations. The results from natural bond orbital (NBO) analysis indicate that the tetrahedral structure of water is energetically disfavored in these small clusters due to a significant decrease in the extent of water-to-water charge transfer (CT) compared to chain structures. We provided explanations for the fact that most classical water models generate tetrahedral structures of water and we also suggest strategies to develop future classical models that take into account the CT effect in order to better represent the structure of water.



SR-FTIR Spectromicroscopy of Interfacial Exclusion Zones

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The dynamics of water at interfaces is of critical importance to biology, chemistry, and geoclimatic processes. The existence and characteristics of exclusion zones at many common interfaces is becoming increasingly well known. However, the underlying mechanism by which such zones form is not clearly understood. FTIR spectroscopy is a well-established technique for the determination of chemical structure and more recently for examination of the intermolecular environment. Small changes in the structure of a molecule or the degree of hydrogen bonding occurring between molecules are easily detectable. The observed red shift ($3404\ cm^{-1}$ to $3280\ cm^{-1}$) in the principal OH stretching band (v_1) as liquid water freezes into ice illustrates this point well. If the water molecules within exclusion zones are more strongly hydrogen bonded than bulk water, a similar shift is expected. For this study we combine the high brightness of synchrotron radiation, the chemical sensitivity of FTIR spectroscopy and infrared microscopy to produce high resolution one- and two-dimensional maps of exclusion zones. Experiments were carried out on beamline 1.4.4 at the Advanced Light Source, Lawrence Berkeley National Laboratory. Thin sections of excluding (e.g., Nafion, polyHEMA, boron doped silicon) and non-excluding (e.g., Teflon, exhausted Nafion, nitrogen doped silicon) materials were spectroscopically sampled with diffraction limited spatial resolution between 1 and 10 microns. The constructed maps revealed differences in the IR active molecular oscillators of water as a function of distance from the nucleating surface. Changes in the centroid position of the primary OH stretch band is small and there is only slight broadening indicating that Exclusion Zone water is not a stable crystalline structure. The first combined harmonic overtone at $5260\ cm^{-1}$ is red shifted by ~14 wavenumbers which indicates that the overall motion of the molecular oscillators are damped. The combined v^2+L^2 mode at $2150\ cm^{-1}$ did show a very slight blue shift of about 4 wavenumbers. These changes are not observed when a non-excluding polymer control is used. Furthermore, no CF stretch is observed outside of the polymer which rules out any polymer brush involvement in Exclusion Zone formation. The results indicate that Exclusion Zones are not a static phenomenon characterized by aligned dipoles in a quasi lattice with anomalously long hydrogen bond lifetimes. Most likely these regions represent a shift in the steady state equilibrium that inherently exists within liquid water. Exlcusion Zones are the result of long-range changes in the dynamic fluctuations of liquid water in response to the presence of certain types of surfaces.

The Structure and Function of Quinones in Photosynthesis: Differential Pulsed Voltammetry and cw EPR Spectroscopy Studies of Substituent Effects on the Electronic Properties of Benzoquinone Models[*]

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Quinones serve as electron carriers in electron-transport proteins that are essential to photosynthesis and cellular respiration. The versatility of quinones and the wide variation in their use stems in part from their diverse redox potentials, which are controlled by substituent effects and by 'smart matrix effects' of the protein binding pocket. In order to develop a systematic understanding of substituent effects on the electronic structure of quinones, we have performed a study of a series of 1.4 benzoquinone models. We measure the redox potentials of the model quinones by differential pulse voltammetry (DPV). We correlate the redox potentials

of the quinones to the isotropic hyperfine components of the ring proton and methyl group proton hyperfine couplings that are obtained from continuous-wave electron paramagnetic resonance (EPR) spectra. The correlation of the changes in the redox couple of the quinones with the electron spin density provides insight on the distinct influence of substituent groups on electronic structure of the respective quinones.

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Effect of Solvent Ionic Strength on Molecule-Surface Interactions in Aqueous Colloids

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The molecular adsorption processes of a hydrophobic ion Malachite Green (MG) on colloidal and biological membrane surfaces under different salt species and concentrations in aqueous solutions have been characterized by using a nonlinear optical technique- Second Harmonic Generation. This colloidal system serves as a model for understanding the effect of solvent ionic strength on the interactions between molecules and particle surfaces in a colloidal environment. Adsorption isotherms of MG onto the surfaces of polystyrene sulfate (PSS) particle, polystyrene carboxyl (PSC) particle, Escherichia coli cell, and Murine Erythroleukemia (MEL) cell have been measured for the determination of the maximum adsorption densities (Nmax) and adsorption equilibrium constants (K) under various salt species/concentration conditions. The effects of several chloride salts (NH4, Cs, K, Na, Ca, Mg, Al) on the adsorption characteristics (Nmax and K) have been found to correlate with the Hofmeister series. These observations indicate that direct ion-polymer/ion-biomolecular interactions are largely responsible for the Hofmeister phenomenon in protein aggregation.

Effect of the Ordered Water on Protein Folding studied by an Off-Lattice Go-Like Model

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Recent experiments and numerical simulations have shown that the water molecules confined on the surfaces of some substrates, including the surfaces of cellular components in tissues and cells, form icelike ordered structures. If a protein folds in an environment with those icelike ordered water molecules, its behavior may be different from that in bulk water. In this poster, the effect of this ordered water environment on protein folding is studied by using an off-lattice Gō-like model. In our simulation system, the protein is confined in two hard parallel plates, and the effect of the ordered water is described by the reduction of the random force since the experiment shows that the ordered water has a low mobility compared with bulk water. The simulation results show that the native structure of the protein, which is the required three-dimensional structure by the cellular function of the protein, is significantly improved in the environment with ordered water. The folding rate of the protein from a random coil to this native state is also greatly speeded up in the environment with ordered water. Moreover, it is found that both the stability and the folding rate with respect to the size of the confined space can be characterized by negative exponential laws with close exponential parameters for different proteins.

References

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