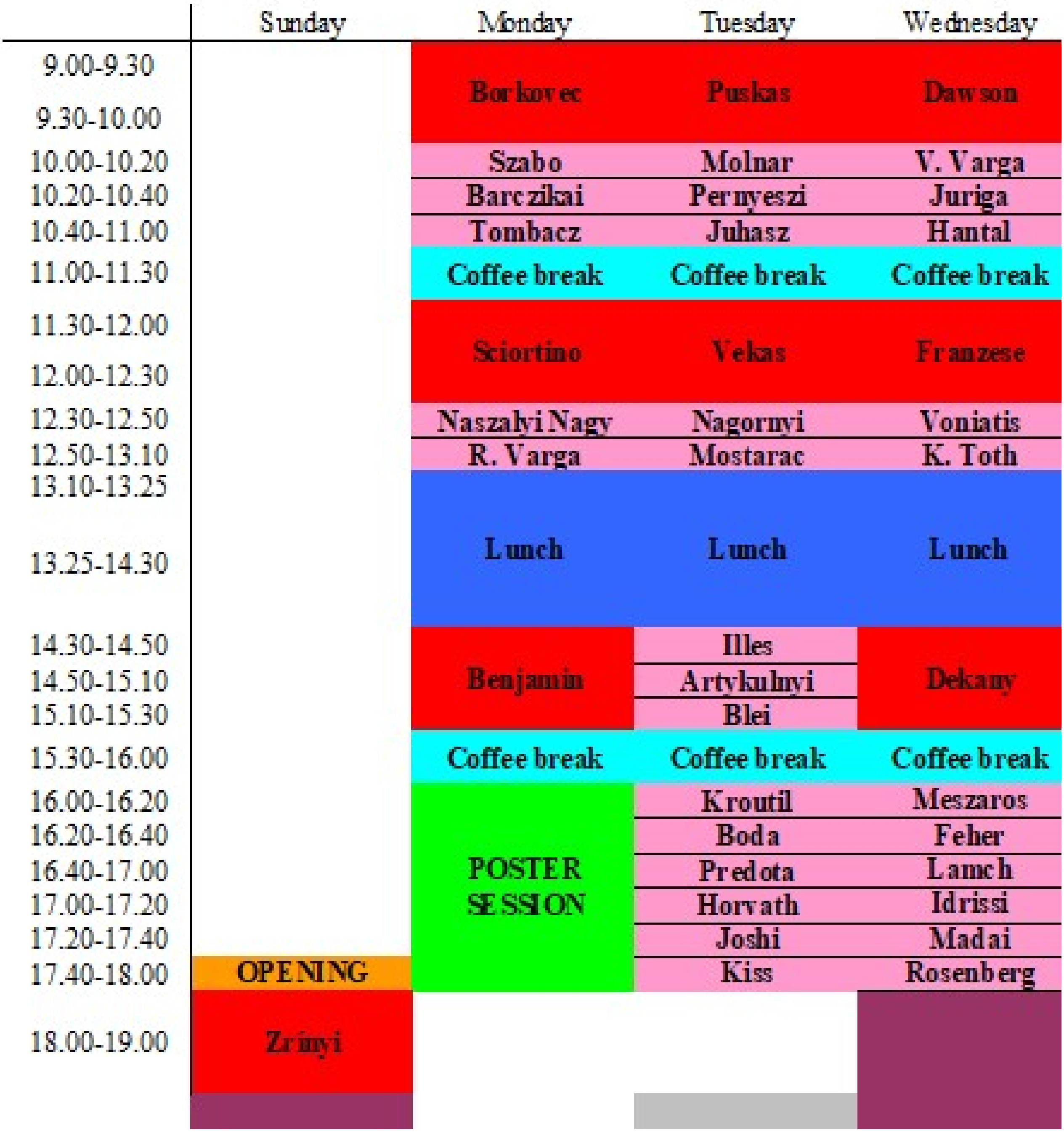
Chemistry, Physics and Biology of Colloids and Interfaces

2-6 June 2019, Eger, Hungary

CPBCI
2019

EGER 1774
ESZTERHAZY KAROLY UNIVERSITY

BOOK OF ABSTRACTS



	Sunday	Monday	Tuesday	Wednesday
9.00-9.30		Borkovec	Puskas	Dawson
9.30-10.00				
10.00-10.20		Szabo	Molnar	V. Varga
10.20-10.40		Barczikai	Pernyeszi	Juriga
10.40-11.00		Tombacz	Juhasz	Hantal
11.00-11.30		Coffee break	Coffee break	Coffee break
11.30-12.00		Sciortino	Vekas	Franzese
12.00-12.30				
12.30-12.50		Naszalyi Nagy	Nagornyi	Voniatis
12.50-13.10		R. Varga	Mostarac	K. Toth
13.10-13.25		Lunch	Lunch	Lunch
13.25-14.30				
14.30-14.50		Benjamin	Illes	Dekany
14.50-15.10			Artykulnyi	
15.10-15.30			Blei	
15.30-16.00		Coffee break	Coffee break	Coffee break
16.00-16.20		POSTER SESSION	Kroutil	Meszaros
16.20-16.40			Boda	Feher
16.40-17.00			Predota	Lamch
17.00-17.20			Horvath	Idrissi
17.20-17.40			Joshi	Madai
17.40-18.00	OPENING		Kiss	Rosenberg
18.00-19.00	Zrínyi			

Conference Program

Sunday, 2 June

17.40-18.00: Conference opening

Session 1 (chair: Angéla Jedlovszky-Hajdú):

18.00-19.00: **Miklós Zrínyi** (Budapest, Hungary): *Neutral colloidal particles and polymers in electric field*

19.00-21.00: Welcome reception

Monday, 3 June

Session 2 (chair: István Szilágyi):

09.00-10.00: **Michal Borkovec** (Geneva, Switzerland): *Forces between Colloidal Particles in Aqueous Solutions*
10.00-10.20: **Tamás Szabó** (Szeged, Hungary): *Semiconductor nanoparticle/graphene oxide composites for environmental applications*
10.20-10.40: **Dóra Barczikai** (Budapest, Hungary): *Biocompatible fibrous meshes incorporating silver nanoparticles for wound dressing applications*
10.40-11.00: **Etelka Tombácz** (Szeged, Hungary): *On the analogies and peculiarities of charging and colloidal stability of humic acids and graphene oxides*

11.00-11.30: Coffee break

Session 3 (chair: Sofia Kantorovich):

11.30-12.30: **Francesco Sciortino** (Rome, Italy): *Gels of DNA*
12.30-12.50: **Lívia Naszályi-Nagy** (Gent, Belgium): *DNA building block adsorption on SiO2@ZrO2 NPs*
12.50-13.10: **Rita Varga** (Budapest, Hungary): *Poly(aspartic acid) based nano gel fibers for tissue engineering*

13.10-14.30: Lunch

Session 4 (chair: Dezső Boda):

14.30-15.30: **Ilan Benjamin** (Santa Cruz, USA): *Surface-active molecules influence on charge transfer reactions at liquid interfaces*
15.30-16.00: Coffee break

16.00-18.00: POSTER SESSION

Tuesday, 4 June

Session 5 (chair: Tamás Szabó):

09.00-10.00: **Judit Puskas** (Akron, USA): *Folic acid conjugated polymeric nanocarrier for targeted cancer detection in hepatocellular carcinoma*
10.00-10.20: **Kristóf Molnár** (Budapest, Hungary): *Biocompatible, biodegradable and implantable poly(amino acid) based fibrous networks*
10.20-10.40: **Tímea Pernyeszi** (Pécs, Hungary): *Use of microorganisms in environmental bioremediation*
10.40-11.00: **Ákos Juhász** (Budapest, Hungary): *Creating electrospun 3D artificial matrices for biomedical purposes*

11.00-11.30: Coffee break

Session 6 (chair: Etelka Tombácz):

11.30-12.30: **Ladislau Vekas** (Timisoara, Romania): *Magnetically controllable fluids - tuning the composition, colloidal stability, magnetic and flow properties to the requirements of applications*
12.30-12.50: **Anatolii Nagornyi** (Dubna, Russia): *Structural characterization of aqueous magnetic fluids stabilized by sodium oleate*
12.50-13.10: **Deniz Mostarac** (Vienna, Austria): *The impact of structural inhomogeneities, superparamagnetism and central attraction, on the equilibrium structure of magnetic filaments*

13.10-14.30: Lunch

Session 7 (chair: Milan Předota):

14.30-14.50: **Erzsébet Illés** (Szeged, Hungary): *Multifunctional PEG-carboxylate copolymer coated nanomagnets for biomedical application*
14.50-15.10: **Oleksandr Artykulnyi** (Dubna, Russia): *Impact of poly (ethylene glycol) concentration and molecular mass on the structure and interaction parameters of anionic surfactant micellar solutions*
15.10-15.30: **Michael Bley** (Freiburg, Germany): *Molecular Simulation of Thermodynamic Properties with the Osmotic Equilibrium Approach: Accessing Activities in Complex Concentrated Liquid Phases*

15.30-16.00: Coffee break

Session 8 (chair: George Horvai):

16.00-16.20: **Ondrej Kroutil** (České Budějovice, Czech Republic): *VSFG spectrum prediction from classical molecular dynamics simulations*
16.20-16.40: **Dezső Boda** (Veszprém, Hungary): *Ionic transport through nanopore devices: diodes, transistors, sensors*
16.40-17.00: **Milan Předota** (České Budějovice, Czech Republic): *Simulations of ions and oxalic acid on rutile and quartz surfaces*
17.00-17.20: **Réka Horváth** (Budapest, Hungary): *Investigation of methylamine at aqueous surfaces by computer simulation methods*
17.20-17.40: **Gargi Joshi** (Nomi, Japan): *Controlling the Oriented Deposition of LC Polysaccharide at Evaporative Interface in a Confined Geometry*
17.40-18.00: **Bálint Kiss** (Lille, France): *Investigation of the thermodynamic properties and the liquid-vapor interface in formamide-water systems*

19.00-22.00: Wine tasting (optional event)

Wednesday, 5 June

Session 9 (chair: Angéla Jedlovszky-Hajdú):

09.00-10.00: **Kenneth Dawson** (Dublin, Ireland): *Nanotherapies, Risk and Opportunity; Interaction of Nanoscale Objects with Living Organisms*
10.00-10.20: **Viktória Varga** (Szeged, Hungary): *Investigation of different human serum albumin-based composites for kynurenic acid drug delivery*
10.20-10.40: **Dávid Juriga** (Budapest, Hungary): *Poly(aspartic acid) hydrogels: potential scaffold for tissue engineering*
10.40-11.00: **György Hantal** (Vienna, Austria): *On molecular mechanisms of general anesthesia*

11.00-11.30: Coffee break

Session 10 (chair: Róbert Mészáros):
11.30-12.30: **Giancarlo Franzese** (Barcelona, Spain): *From Nanomaterials to Perspectives for Brain Cancer Treatments*
12.30-12.50: **Constantinos Voniatis** (Budapest, Hungary): *Poly(vinyl alcohol) as a potential material for new surgical meshes*
12.50-13.10: **Krisztina Tóth** (Budapest, Hungary): *Characterization of dopamine containing fibrous polymer-drug conjugates*

13.10-14.30: Lunch

Session 11 (chair: Imre Varga):

14.30-15.30: **Imre Dékány** (Szeged, Hungary): *Protein/ polyelectrolyte/ gold self-assembled structures: drug delivery and sensor applications*

15.30-16.00: Coffee break

Session 12 (chair: Oleksandr Tomchuk):

16.00-16.20: **Róbert Mészáros** (Komarno, Slovakia): *Effect of Added Surfactant on the Poly(Ethyleneimine)-Assisted Gold Nanoparticle Formation*
16.20-16.40: **Bence Fehér** (Budapest, Hungary): *Structural Investigation of Red Fluorescent Bovine Serum Albumin-Gold Complexes*
16.40-17.00: **Łukasz Lamch** (Wrocław, Poland): *NMR studies upon aggregation behavior of hydrophobically functionalized poly(4-styrenosulfonic-co-maleic acid)*
17.00-17.20: **Abdenacer Idrissi** (Lille, France): *Self-association process in urea, acetone, acetamide and choline chloride aqueous solutions: Vibartion spectroscopy and molecular dynamics simulation*
17.20-17.40: **Eszter Mádai** (Darmstadt, Germany): *Using nanopores as sensors: The effect of the charge pattern from symmetric to asymmetric leading to a dual-response device*
17.40-18.00: **Margaret Rosenberg** (Vienna, Austria): *Self-assembly of hollow colloidal silica cubes*

18.00-22.30: Conference Banquet

Thursday, 6 June

Session 13 (chair: Pál Jedlovszky):

09.00-09.30: **George Horvai** (Budapest, Hungary): *Deeper insight into the surface tension of common solvents and of the aqueous solutions of common surfactants*
09.30-10.00: **Sofia Kantorovich** (Vienna, Austria): *In-silico study of randomly crosslinked nanogel*
10.00-10.20: **Balázs Fábián** (Prague, Czech Republic): *Investigation of the dynamics of fluid interfaces*
10.20-10.40: **Andrew Milne** (Glasgow, UK): *Polarisation Corrections and the Hydration Free Energy of Water*
10.40-11.00: **Martin Kaiser** (Vienna, Austria): *Self-propelled Dipolar Nanocubes*

11.00-11.30: Coffee break

Session 14 (chair: Abdenacer Idrissi):

11.30-12.00: **István Szilágyi** (Szeged, Hungary): *Co-immobilization of superoxide dismutase and horseradish peroxidase on polyelectrolyte-functionalized layered double hydroxide particles*

12.00-12.30: **Oleksandr Tomchuk** (Dubna, Russia): *Fractal aggregation in tetraethoxysilane/ethanol/water solutions by SANS*

12.30-12.50: **Imre Varga** (Budapest, Hungary): *A novel method for surfactant binding isotherm measurements of polyelectrolyte/surfactant mixtures validated by neutron reflectivity data*

12.50-13.10: **Ildikó Tóth** (Szeged, Hungary): *Wetting and evaporation properties of carbon nanotube buckypapers doped by hydrophilic nanowires*

13.10-13.25 Conference closing

13.25-14.30: Lunch

List of Posters

1. **Krisztina Bali** (Budapest, Hungary): *Oppositely charged polyelectrolyte/surfactant assemblies as emulsion stabilizing agents*
2. **Zuzana Benková, Peter Čakánek** (Bratislava, Slovakia): *Interactions of peptides with poly(ethylene oxide) grafted onto carbon nanotubes*
3. **Denys Biryukov** (České Budějovice, Czech Republic): *A General Tool for Zeta Potential Predictions from Molecular Simulations*
4. **Dezső Boda** (Veszprém, Hungary): *A scaling behavior of the transport of multivalent ions through rectifying nanopores*
5. **Joanna Feder-Kubis** (Wrocław, Poland): *Ionic liquids with natural terpene derivative as an effective fungicidal and protective preparation for the preservation of historical paper*
6. **Máté Gulácsi** (Budapest, Hungary): *Optical properties of hydrogel fiber membranes*
7. **György Hantal** (Vienna, Austria): *Chemistry and water dynamics at the surface of hydrated magnetite*
8. **Anna Harsányi** (Budapest, Hungary): *Preparation of Poly(N-isopropylacrylamide-co-4-vinylimidazole) microgel particles*
9. **ZoltánHató** (Veszprém, Hungary): *Molecular simulation of kaolinite layer curling*
10. **Kevin Herman** (Szeged, Hungary): *Heterocoagulation assisted synthesis of zirconia/graphite oxide nanocomposites*
11. **George Horvai** (Budapest, Hungary): *Selective adsorption of basic compounds from aprotic solvents onto acidic polymers*
12. **Erzsébet Illés** (Szeged, Hungary): *Tuneable magnetic hyperthermia properties of pristine and mildly reduced GO/MNP nanocomposites*
13. **Attila Kardos** (Budapest, Hungary): *Synthesis of chemically modifiable p(HEMA)-b-PEG block copolymer*
14. **Łukasz Lamch** (Wrocław, Poland): *Synthesis and biological properties of new mild amidebetaine and amidesulfohydroxybetaine-type amphotheric surfactants*
15. **Lydie Plačková** (České Budějovice, Czech Republic): *Dynamic properties of aqueous solutions of atomic and molecular ions – effect of scaled charges*
16. **Csaba Róth** (Budapest, Hungary): *Preparation of multilayer "smart" nanocapsules*
17. **Evelin Sipos** (Budapest, Hungary): *Damage formation in weak planar fiber texture*
18. **Ildikó Tóth** (Szeged, Hungary): *Wettability characterization of carbon cloth type gas diffusion layer via infrared thermography and contact angle analysis*
19. **Mónika Valiskó** (Veszprém, Hungary): *Modeling of pH tunable nanodevices*
20. **Tamás Veres** (Budapest, Hungary): *Electrospun magnetic scaffold for theranostics*

Invited lectures

Surface-active molecules influence on charge transfer reactions at liquid interfaces

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ABSTRACT

Charge transfer reactions such as electron and ion transfer as well as reactions with significant difference in charge distribution between the reactants and products (such as S_N2 and ionization reactions) are very sensitive to the solvent polarity. The dynamics and thermodynamics of these reactions are strongly influenced by the heterogeneous character of the liquid/liquid and liquid/vapor interfaces where the polarity of the media changes rapidly over a sub-nanometer length scale and by surface density fluctuations. Surface active molecules that are adsorbed at the interface and interacts with the reactants can provide a local reaction environment whose polarity is further distinguished from that of the neat interface. We examine how these surface active molecules affect reactivity and how their effect is influenced by the local structure and dynamics of the interface.

Forces between Colloidal Particles in Aqueous Solutions

Michal Borkovec

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ABSTRACT

Numerous phenomena involving colloidal particles are governed by particle-particle or particle-substrate interactions. Examples include stability and rheology of colloidal suspensions, formation of colloidal crystals, or particle deposition. While the importance of such interaction forces has been appreciated for a long time, measuring such forces directly remained a considerable challenge until quite recently. Presently, however, various techniques are becoming available for direct force measurements, but my view is that the colloidal probe technique based on the atomic force microscope (AFM) is emerging as the most promising and versatile one.

The present talk will discuss the use of the colloidal probe technique to measure forces between colloidal particles. In particular, I will demonstrate that interactions between similar as well as dissimilar particles are principally controlled by electrostatic double-layer and van der Waals forces as already suggested by the classical theory of Derjaguin, Landau, Verwey and Overbeek (DLVO). The talk will further highlight the nature of forces acting between charged colloidal particles in the presence of multivalent ions and polyelectrolytes. While forces in these systems remain DLVO-like and are mainly controlled by charge reversal, additional attractive non-DLVO forces come into play. Additionally, two novel phenomena will be highlighted as well. First, charge regulation effects can become very important for dissimilar particles. Second, double layer forces can become strongly non-exponential in the presence of multivalent coions or like-charged polyelectrolytes.

Nanotherapies, Risk and Opportunity; Interaction of Nanoscale Objects with Living Organisms

Kenneth Dawson

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ABSTRACT

Man-made nanostructures are of the size and nature that they gain access to new biological (intracellular and other) compartments, and there are potentially endogenous energy dependent mechansims to lead them there. We summarise the foundations and progress to date in this arena. In particular we clarify the range of nanoscale (surface, shape etc) control parameters that may determine the biological outcomes. These considerations suggest an enduring potential to target substances to specific locations, for benefit of therapeutics, and the progress to date is summarized.

In the (typical) absence of exquisite control of the nansocale structures (and thereby processes) *in vivo,* nanoscale materials are (guided by biomolecular coronas derived from the biological environment) incorporated and ultimately processed within endogenous intra-, trans- and cellular trafficking and processing pathways. There they may persist for extended periods of weeks, months (or longer) potentially either leading to persistent dis-regulation of signaling and other biological processes, or slow degradative production of secondary (and other downstream) metabolites not commonly observed in other situations. The absence of much in depth understanding of the long term effects represents the most obvious risk in the arena.

It is clear that new future dimensions are opening up at the nanoscale, involving convergent outcomes between the nanoscale structures, gene editing, and other forms of biological intervention. These areas are in their infancy, but one can already see many of the key issues for the future.

As a community, and a society, our management of these arenas was dedicated, and sincere and quite effective, but we confronted new questions and issues, without the tools early on to deal with them. What we learned from responsible management of ‘risk’ issues (in the larger sense) may be useful for future generations of risk managers in other arenas.

Protein / polyelectrolyte / gold self-assembled structures: drug delivery and sensor applications

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An important representative of the biocolloids like albumin proteins (e.g., BSA, HSA) have a variety of conformational properties depending on the pH of the medium [1]. Synthetic polyelectrolytes have similar properties and the two polymer chains in the same pH medium can have the opposite charge. It is an excellent property of proteins to form stable colloidal solutions at high electrolytes concentrations and they can be used as a stabilizer in electrolyte medium, e.g.in physiological conditions. When the noble metal nanoparticles (silver and gold) are prepared, they coagulate in this electrolyte medium without polymer stabilizer while the adsorption of proteins on the nanoparticle surface shows a steric stabilization effect.

Self-assembled structures having opposite charged polyelectrolytes/proteins are capable closing drug molecules in a core-shell particles, which exhibiting controlled drug delivery properties. The present lecture we describe the preparation of these polyelectrolyte/protein systems, the structural characterization of the composites (particle size, surface charge etc.) and the measurement release kinetics of the incorporated drug molecules in physiological conditions. For exact determination of the protein-drug interaction can also be implemented using two dimensional (so called surface plasmon resonance (SPR) techniques. Knowing the temperature dependence of the biopolymer/drug ligand interaction, we have calculated the thermodynamic potential functions characteristic for the binding energy and the kinetic data for drug release. The interactions were also followed by fluorescence measurements when the thermodynamic data (e.g. binding constants) were also calculated according to the Stern-Volmer formula. When AuNPs are stabilized with proteins, plasmonic properties can be tuned as a function of the Au/protein ratio [2]. Depending on the physiological changes in the environment, various optical properties can be measured and the gold/protein system can also be used as an optical sensor to detect various drug molecules and biologically active substances.

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From Nanomaterials to Perspectives for Brain Cancer Treatments

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ABSTRACT

The Blood-Brain-Barrier (BBB) is the tight membrane that protects our brain and represents the major hindrance to the use of chemotherapeutic agents for brain tumors. Recent *in vitro* and *in vivo* studies show that it is possible to increase the ability to cross the BBB for engineered nanoparticles (NPs) carrying a loose layer of proteins [1]. Nevertheless, the NP-protein corona composition – and, as a consequence, the cellular biological response to the NP – change over time as a consequence of the competition among the plasma proteins once the NP is in the blood stream [2]. In collaboration with experimental groups, we develop a multiscale approach for the study of bio-membranes, proteins, NPs and nanomaterials in aqueous solution oriented to applications to the BBB crossing for oncological treatments. We model the kinetics of NP interaction with proteins [2-4], of proteins with water [5-10], and of water with membranes and nanomaterials [11-15], with the aim of finding how to optimize the NP-protein corona formation to cross the BBB. We will describe our recent results by all-atom simulations and coarsegrained models, e.g. showing that the water-membrane interface has a structural effect at ambient conditions that propagates further than the often-invoked 1 nm length scale and that the translational and rotational dynamics of water molecules is strongly determined by their local distance to the membrane so that we can identify the existence of an interface between the first hydration shell, partially made of hydration water bound to the membrane, and the next shells entirely made of unbound hydration water. These results could drastically affect the kinetics of the protein-corona, determining the fate of NPs during the BBB crossing [16].

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[16] The authors acknowledge funding from the Spanish MINECO Grants No. FIS2015-66879-C2-2-P, and the ICREA Foundation.

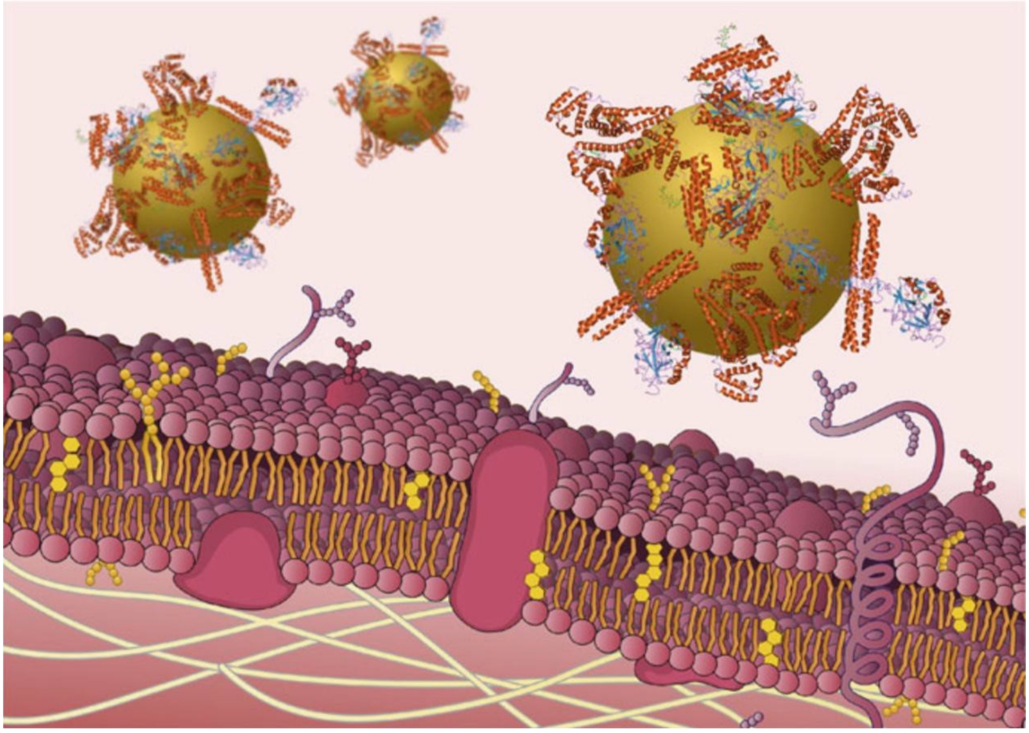

Figure 1. Cartoon of NP-Protein corona complexes near a cellular membrane [4].

Folic acid conjugated polymeric nanocarrier for targeted cancer detection in hepatocellular carcinoma

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ABSTRACT

Targeted therapies provide increased efficiency for detection and treatment of cancer with reduced side effects. Folate receptor (alpha-subunit) is overexpressed in multiple tumors including liver cancer. In this study, we evaluated the specificity and toxicity of a new folic acid containing drug delivery vehicle (DDV) in a hepatocellular carcinoma (HCC) model. DDV was prepared with two units each of folic acid (FA) and fluorescein isothiocyanate (FITC) molecules and conjugated to a central poly(ethylene glycol) (PEG) core via a chemo-enzymatic synthetic process. Rat hepatoma (N1S1) and human monocytic (U937) cell lines were used for cell culture-based assays and tested for DDV uptake and toxicity. Folate receptor expressions in liver tissues and cell lines were verified using standard immunohistochemistry techniques. Rat HCC model was used for *in vivo* assessment. DDV was injected via intra-arterial or intra-venous methods, and imaged with an *in vivo* imaging system. Strong signals of FITC in the liver tumor region correlated to targeted DDV uptake. The use of PEG enhanced water-solubility and provided flexibility for interaction of FA ligands with multiple cell surface receptors that resulted in increased specific uptake. Our study suggested that PEG incorporation and folate targeting via intra-arterial approach is an efficient strategy for targeted delivery in HCC therapy.

Gels of DNA

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ABSTRACT

DNA oligomers can nowadays be assembled to produce a large variety of nanometric constructs, via a cascade of self-assembly processes, each one guided by the length of complementary sequences of distinct DNA strands. In the lecture I will show that it is possible to build bulk quantities of DNA-made nanoparticles that closely match idealized colloids, transferring modern in-paper and in-silico intuitions into experimental realizations. I will show how unconventional collective behaviors, recently explored theoretically and numerically, can indeed be reproduced in the lab. Specifically I will discuss: (i) how to exploit limited valence interactions to suppress phase separation[1,2], enhancing the stability of the equilibrium gel phase [3-5]; (ii) how to exploit competing interactions to generate a material that is fluid both at high and at low temperatures and a solid-like disordered open network structure in between [6-8] and (iii) how to exploit bond-swap dynamics to create an all-DNA vitrimer [9-10].

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Magnetically controllable fluids-tuning the composition, colloidal stability, magnetic and flow properties to the requirements of applications

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ABSTRACT

Particle size distribution and magnetic field induced particle aggregation are essential features both of ferrofluids and magnetorheological fluids. The extremely bidisperse ferrofluid based MR fluids come into play with completely new features in what concerns particle structure formation and yielding behavior depending on the composition adjusted on two hierarchical levels. By carefully tailoring the composition and structure at nano and micro level the characteristics of magnetizable fluids are adapted to a wide range of requirements, from high colloidal stability, practically agglomerate-free concentrated ferrofluids for leakage-free rotating seals to high kinetic stability MR fluids designed, among others, for semi-active MR dampers in earthquake protection systems . There will be summarized results of comprehensive analyses combining electron microscopy, X-ray photoelectron spectroscopy, attenuated total reflectance Fourier transform infrared spectroscopy, vibrating sample magnetometry, small-angle X-ray and neutron scattering, dynamic light scattering and magneto-rheometry revealing the behavior of ferrofluids and magnetorheological fluids designed for various applications.

Neutral colloidal particles and polymers in electric field

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ABSTRACT

All neutral particles experience forces and torques when subjected to electric fields. Especially strong field-particle interactions characterize colloidal particles showing dielectric properties. In the presence of electric field, dielectrophoretic forces and torques acting on particles result in locomotion and structure formation. If the particles are dispersed and stabilized in liquids the rheological behaviour of these fluids (electrorheological fluids) is strong function of imposed field. If colloidal particles with special electric properties are built into flexible polymer matrix, electric field sensitive polymer gels or elastomers are obtained. The particles couple the shape of the gel (or elastomer) to the external fields. Shape distortion and locomotion occur instantaneously and disappears abruptly when electric field is applied or removed, respectively. This kind of change in the material properties can be applicable to a variety of fields as a new driving mechanism. Controllable rotation of electroactive polymer (EAP) has relevance to a range of practical applications, for example in micro-motors and in micro-fluidics. A novel principle has been proposed for realization of a colloidal micromotor, based on the electrorotation (Quincke rotation) phenomena. 2D biocompatible scaffold for tissue engineering has been prepared under high electric field and unidirectional strain-controlled experiments on fibrous mat has been studied. The experiments evidenced that damage evolution is a consequence of strain induced random events. The frequency distribution of the number of damages as well as the magnitude of rupture force were determined. The results provide a better insight into damage tolerance and complex nonlinear tensile properties of weak electrospun networks.

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Keynote lectures

Deeper insight into the surface tension of common solvents and of the aqueous solutions of common surfactants

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ABSTRACT

We have demonstrated how intrinsic surface analysis methods can provide a deep insight into the thermodynamics of fluid surfaces, by calculating the tangential pressure profile across the liquid−vapor interface of five molecular liquids, characterized by markedly different intermolecular interactions [1]. Because the value of the surface tension can be obtained by integrating the tangential pressure profile, this profile provides direct information on how the surface tension is distributed along the interface normal axis. Our results show a surprising insensitivity of this distribution of the surface tension to the type of intermolecular interactions acting in the liquid phase. Thus, in every case at least 85% of the surface tension comes from the first molecular layer, while, with the exception of methanol, the second layer contributes roughly 10% to the surface tension.

We have also analyzed the contribution of the different atoms and groups to the surface tension in various surfactant solutions in water, corresponding both to unsaturated and saturated surface coverages, through the calculation of the contribution of these species to the lateral pressure profile of the system. The type of the headgroup plays a much more important role in this respect than the length of the apolar tail. In the case of alcoholic surfactants, the surface tension contribution of the OH headgroups turns out to be negligible. The most important finding of this study is the key role the counterions play in contributing to the surface tension in the case of the ionic surfactants. This role seems to be related to the "hardness" of these ions according to the Hofmeister series, and hence to their surface affinity. On the other hand, there is a strong compensation between the surface tension contribution of the counterions and ionic surfactant heads.

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In-silico study of randomly crosslinked nanogels

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ABSTRACT

Colloidal gel particles, known as nanogels or microgels depending on their characteristic size, are nowadays one of the most important building blocks of soft responsive materials, as they combine a flexible and porous polymer network structure with strong mechanical response to external stimuli [1]. Despite their relevance and the diversity of available experimental synthesis techniques, the complexity of these systems still represents a challenge for their theoretical modelling and makes unavoidable the use of coarse-grained approaches [2,3].

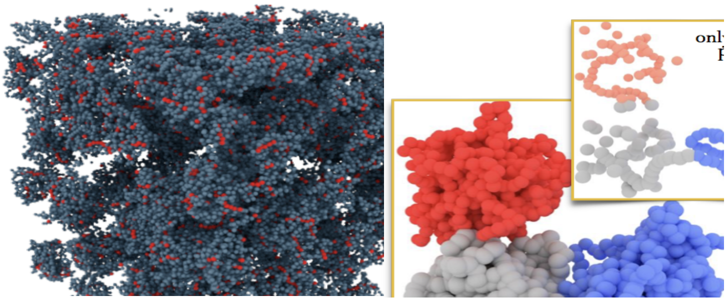

Figure 1. The system of magnetic nanogels (left). Zoomed in cluster formed by three magnetic nanogels and the magnetic particles (upper left) responsible for self-assembly.

Recently, we introduced a bead-spring computer model for colloidal gel nanoparticles, as the ones synthesized by random crosslinking of polymers confined in emulsion nanodroplets [4]. With this model we study in simulations the effects of crosslinks and magnetic particle distribution on the internal structure of the nanogel particles, as well as their swelling/deswelling behaviour. We also present results of the self-assembly behaviour of nanogels loaded with ferromagnetic nanoparticles in dispersions with moderate concentration (Figure 1). The self-assembly in this system is governed by magnetic forces.

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Co-immobilization of superoxide dismutase and horseradish peroxidase on polyelectrolyte-functionalized layered double hydroxide particles

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ABSTRACT

Oxidative stress caused by reactive oxygen species (ROS) induces several diseases by damaging cell constituents. Antioxidant enzymes including superoxide dismutase (SOD) and horseradish peroxidase (HRP) are the primary defense systems against ROS. However, their supplementation to living organisms is limited due to their high sensitivity to the environmental conditions such as pH, ionic strength and temperature. To overcome this challenge, enzyme immobilization on biocompatible nanomaterials is a promising way to obtain composites of antioxidant activity. The solid supports are required to provide functional stability for the enzymes. These delivery systems must also possess high colloidal stability to avoid aggregation once dispersed in bio-fluids such as blood. In this presentation, the development of an antioxidant hybrid consisting of SOD and HRP as well as polyelectrolyte-functionalized layered double hydroxide (LDH) nanoparticles is discussed.

Accordingly, 2-dimensional LDH nanoparticles of narrow size distribution were synthesized by a hydrothermal method. Surface functionalization was carried out with heparin (HEP) polyelectrolyte via electrostatic interactions. Due to the precise optimization of the experimental conditions during preparation, stable LDH-HEP dispersions were obtained, which possessed extremely high resistance against salt induced aggregation. Immobilization of SOD and HRP was carried out by physical adsorption. Both LDH-SOD-HEP and LDH-HEP-HRP composites showed high activity in decomposition of superoxide radicals and hydrogen peroxide, respectively. To mimic the cellular environment, the enzymes were co-immobilized using the sequential adsorption method in the LDH-HEP-HRP-PLL-SOD-HEP order, where PLL refers to polylysine. The experimental conditions were refined in the synthesis that the multicomponent material formed highly stable colloid. More importantly, the developed enzymatic cascade system has proven as an efficient antioxidant in biochemical assays and it protected living cells against oxidative stress.

Acknowledgement: This research was supported by the Ministry of Human Capacities, Hungary through the project 20391-3/2018/FEKUSTRAT.

Fractal aggregation in tetraethoxysilane/ethanol/water solutions by SANS

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ABSTRACT

The study of the structure of branched polymeric materials is of current interest because of its great role in modern technologies. The classical material most widely used to produce silicon-based branched polymers is silicon tetraethoxide (TEOS). After hydrolysis in alcohol-water solutions it forms clusters, which results in a wide class of different structures depending on the number of parameters like pH, H_2O/TEOS molar ratio (*w*), total TEOS concentration *etc*. [1-2].

In present research, small-angle neutron scattering with the contrast variation (H/D substitution) was applied to fractal aggregates in hydrolyzed solutions of TEOS in ethanol. Obtained data indicate that the structure of clusters does not contain closed hydroxyl groups. Thus, the overwhelming majority of the hydrolyzed bonds participate in the condensation reaction to form Si-O-Si structure units. The temporal dependence of cluster growth was investigated together with the dependence of the structure of a liquid nanosystem under study on the parameters of synthesis.

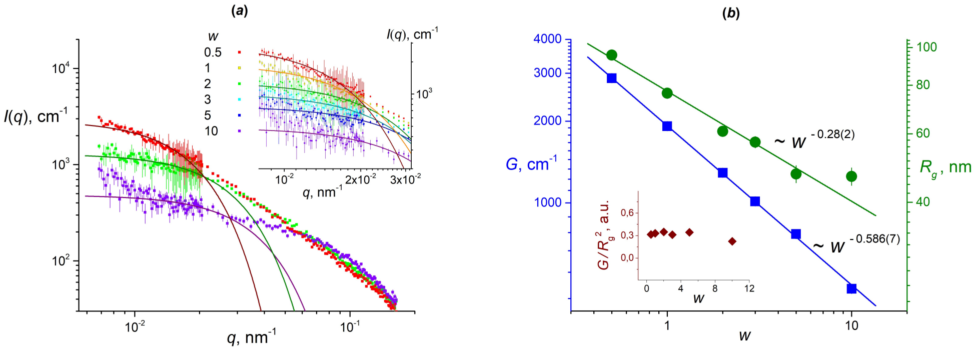

Fig. 1. w-dependent small-angle neutron scattering: experimental spectra (*a*) and Guinier analysis (*a*), (*b*).

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Oral contributions

Impact of poly (ethylene glycol) concentration and molecular mass on the structure and interaction parameters of anionic surfactant micellar solutions

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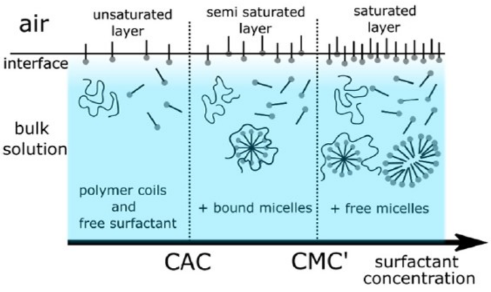
ABSTRACT



Micellar systems of anionic surfactants such as sodium oleate (SO) and dodecylbenzene sulphonic asid (DBSA) are widely used for double layer sterically stabilization of magnetic nanoparticles in aqueous ferrofluids. The physicochemical properties of micellar buffer solution directly influence on the structural organization of ferrofluids and necessarily taken into account in the synthesis protocol [1].

Water-soluble neutral polymer poly (ethylene glycol) (PEG) is actively used in aqueous ferrofluids to increase its biocompatibility [2]. Also it was shown the final ferrofluids properties depend on PEG molecular mass and concentration. The present work is dedicated to the investigations of structural and interaction parameters of SO and DBSA micellar systems under effect of addition of PEG. Small-angle neutron scattering (SANS) together with the surface tension study allowed us to determine a number of micelle parameters including the aggregation number, degree of ionization, axial ratio of micelle shape and inverse screening length for various compositions of the mixed solutions [2,3]. It was shown that different substance concentration ratio and polymer molecular mass leads to quantitative and qualitative changes of studied parameters due to complex, multi-step process of polymer-surfactant interaction (see schematic figure), namely, formation of bounded micelles onto polymer chain before he appearance of regular micelles.

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Biocompatible fibrous meshes incorporating silver nanoparticles for wound dressing applications

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Poly(amino acids) and their derivatives are a promising new class of biomaterials, but one of their drawbacks is their relatively difficult synthesis and functionalization. Using polysuccinimide this issue can be solved, since polysuccinimide (PSI) is prone to react with nucleophiles under mild conditions therefore resulting in the water soluble poly(aspartic acid) (PASP) and its derivatives. Electrospinning is an efficient method for polymer processing, that allows the formation of non-woven fibrous polysuccinimide meshes which could be then used as wound dressings. Due to their broad spectrum of antibacterial activity, incorporation of silver nanoparticles (AgNP) could provide antibacterial properties to the fibrous system [1,2]. Minimizing pain and inflammation could also be achieved by encapsulation of small-molecule drugs such as paracetamol.

The aim of our research was developing a one-pot method for the synthesis of AgNPs in the presence of a biocompatible poly(amino acid) derivative and small-molecule drugs, subsequently creating a novel antibacterial wound dressing system and finally investigating its antimicrobial properties, release profile and hydrolitical stability.

AgNPs were synthesized by chemical reduction method in the presence of PSI then the resulting nanoparticles were characterized with DLS and UV-VIS spectroscopy. By changing the synthesis and electrospinning parameters, the procedure was optimized for both the nanoparticle synthesis and the mesh fabrication. The fibrous structure of the meshes was examined by SEM. For the evaluation of antibacterial properties disc diffusion tests were carried out using *E.coli*. Release kinetics of paracetamol was studied using UV-VIS spectroscopy.

Synthesis and fabrication was successfully performed with the optimized parameters resulting in drug-loaded electrospun PSI fibers containing AgNPs. The antibacterial studies confirmed that silver-content hinders the colonization of the meshes by E. coli. Based on the release kinetics study, the synthesized antibacterial meshes proved to be suitable for prolonged drug-release as well.

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MINISTRY OF
HUMAN RESOURCES

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Molecular Simulation of Thermodynamic Properties with the Osmotic Equilibrium Approach: Accessing Activities in Complex Concentrated Liquid Phases

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ABSTRACT

Thermodynamic properties such as activities of complex concentrated liquid phases are a key parameter for describing chemical equilibria by means of mass action law. The mass action law and the equilibrium constant provide a measure for the direction of any chemical equilibrium. Equilibrium constants calculated from the activities of all compounds involved in a given equilibrium process are for example crucial for understanding and improving solvent extraction systems used in separative approaches for waste management of rare earth elements and spent nuclear fuels. The osmotic equilibrium approach has been developed for accessing activities for a huge bandwidth of complex liquid systems up to high solute concentrations [1,2,3]. Starting from Molecular Dynamics (MD) simulations of vapour-liquid interfaces using explicit polarization for all compounds simulated provides a direct access to the activity by comparing the mean amount of evaporated molecules of a given species in the vapour phase for a mixture and for the pure species, respectively. The evaporating molecules are usually sufficiently volatile solvents such as water or smaller organic molecules such as ethanol or n-heptane. Activities and activity coefficients of the non-evaporating solutes species are calculated by using extended Debye-Hückel theory in the case of ionic solutes and via excess Gibbs energy models in the case of non-ionic systems. Obtained structures and thermodynamic properties showed a very good agreement with previous experimental and theoretical studies on various aqueous electrolyte solutions and organic solvent phases [1,2,3]. The observed statistics of the evaporation process are used for calculating the error resulting from this methodology and they allow calculating the time scale required for a given precision and selectivity. Ongoing work on this method covers the investigation of the influence of aggregate structures such as micelles and their structure and shape on the resulting thermodynamic properties. Increased simulation times can reduce the error of the method and increase the selectivity for very similar compounds such as the series of the lanthanide nitrate salts.

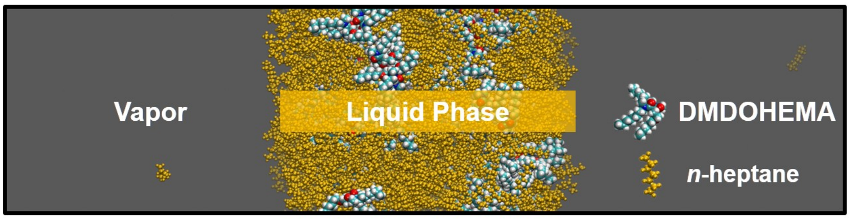

Fig. 1.: Snapshot of a simulation of a mixture containing an extractant (DMDOHEMA) and an organic diluent species (n-heptane). The liquid phase (orange) is in equilibrium with the adjacent vapour phase (gray). Two evaporated n-heptane molecules are found in the vapour phase.

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Ionic transport through nanopore devices: diodes, transistors, sensors

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ABSTRACT

Computer simulation results for ionic transport through synthetic nanopores is presented. Nanopores serve as the core units of various nanodevices such as diodes [1,2], transistors [3], and sensors [4,5]. We study how the output signals given by the devices as responses to input signals (device functions) depend on the properties of nanopores. The device functions are rectification, switching, selectivity, and sensitivity of sensing. Also, we study these systems in a multiscale approach using models of various resolutions computed by the suitable simulation methods. We are interested in the question of what molecular details need to be included in the model in order to reproduce the device behavior. We investigate the applicability of reduced models and study what degrees of freedom should be included in the model and what degrees of freedom can be omitted. We show results of molecular dynamics (MD) simulations for all-atom models, Monte Carlo simulations for reduced models, and a mean-field continuum theory (Poisson-Nernst-Planck) for point ions. The parameters of the reduced models can be fitted either to MD data or experimental data. We will show examples for both.

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Investigation of the dynamics of fluid interfaces

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ABSTRACT

Interfaces are ubiquitous in nature, and play a paramount role in a wide variety of physical, chemical, and biochemical processes. Lately, astonishing developments of both experimental and theoretical methods provided an unprecedented insight into the molecular structure and properties of liquid interfaces. Despite these advances, the analysis of liquid surfaces is still far from trivial: the surfaces are corrugated by thermal fluctuations in the form of capillary waves. Although the importance of advanced methods[1,2,3] capable of treating these systems is already well known, they are yet to be routinely applied.

In our work, we investigated the interfacial properties of various liquid-vapor and liquid-liquid systems by means of the Identification of the Truly Interfacial Molecules (ITIM) method[3]. The molecules used in this study, namely water, acetone, acetonitrile, methanol and carbon-tetrachloride, range from apolar through aprotic dipolar to hydrogen bonding. The dynamical behavior of the surface molecules was explored by calculating their mean residence time, hydrogen-bond survival time, mean squared displacement and velocity autocorrelation functions[4].The obtained results show a 2 to 4-fold increase in mobility of the interfacial molecules. This in turn suggests a picture of a much more fluid surface layer, sharing some traits with those of rarefied fluids in the case of non-hydrogen-bonding liquids, which can have important implications for diffusion-limited reactions occurring at the surface of liquid phases.

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Structural Investigation of Red Fluorescent Bovine Serum Albumin-Gold Complexes

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ABSTRACT

Bovine Serume Albumine (BSA) is a transport protein with 35 Cystein and 66 aromatic amino acid residues. It has 5 reversible conformations in five different pH ranges [1]. It has been demonstrated recently [2] that when $HAuCl_4$ is added to BSA and the pH of the mixture is adjustment to 12, red fluorescence BSA-Au complexes are formed in about two days. These fluorescent complexes gained significant interest in the literature due to their potential application in bioimaging. Originally it was claimed by Xie et al [2] that in the BSA-Au systems the Au^{+3} ions are reduced to Au^0 by the tyrosine residues at pH=12 and nanocluster of 25 gold atoms are formed, which gives rise to the fluorescent properties of the complex. However, Dixon and Egusa questioned this interpretation in their work [3], where they show the presence of Au^{+3} in the complex and demonstrate that the change of the optical properties is related to the conformational changes of the BSA. They have also shown that the fluorescence intensity has a maximum at 1:26 BSA:Au ratio. At the same time several questions remains open: e.g. the fluorescence intensity of BSA-Au complexes are determined typically after two days but the evolution of the fluorescent and structural features are not investigated at long time scale (weeks). A further question is that though the conformational changes of BSA were found reversible for pH changes, it has not been investigated if this reversibility is preserved in the presence of gold(III) ions and if the fluorescent properties of the complex developed at high pH is affected by pH changes. Finally, though the fluorescent intensity of the BSA-Au complexes was investigated in the function of gold(III) concentration, these results are not correlated either with the conformational or structural changes of the BSA. To provide answers for these questions, we investigated the structural, conformational and fluorescent characteristics of the BSA-Au mixtures in long timescale with Circular Dichroism (CD), Small Angle X-Ray Scattering (SAXS) and fluorescent measurements. Our results imply that the diminishing fluorescent intensity of BSA-Au complexes may be related to the slow formation of gold nanoclusters.

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On molecular mechanisms of general anesthesia

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ABSTRACT

Anesthesia has been commonly employed in the surgical practice for more than a century. Although it was understood almost a century ago that anesthetics act in the cell membrane, a general rationalization of the anesthetic mechanism is still missing. Such a mechanism should account for two major observations: 1) chemically very different molecules can act as anesthetics (e.g. xenon, chloroform or diethyl ether) and 2) anesthetic effect can be reverted by applying pressure. Two widespread explanations have been proposed, but so far neither of them has been unequivocally proven right. One popular hypothesis puts forward possible interactions of anesthetics at some active sites in the transmembrane domain of certain membrane-bound proteins. However, this assumes specific substrate-protein interactions, which might not be a general enough scenario. Other popular theories explain anesthesia as an indirect effect: anesthetics substantially change the structure and dynamics of the lipid molecules and this induces conformational changes of transmembrane proteins.

In this presentation, I will outline a recent study we designed to shed some light on the molecular mechanism of anesthesia. In particular, we performed classical all-atom MD simulations of model lipid membranes of very different compositions (both phosphatidylcholine and sphingomyelin based bilayers with and without cholesterol) at low and high pressure. The induced changes upon addition of two different anesthetic molecules in the properties of the lipid bilayers as well as in the lateral pressure profiles across the membrane are correlated with the distribution of anesthetics. Effects fulfilling the two above conditions (generality and pressure reversion) are hypothesized to be responsible for the anesthetic effect.

Investigation of methylamine at aqueous surfaces by computer simulation methods

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ABSTRACT

Methylamine is already known for its relative atmospherical and interstellar abundance among amines, therefore many theories assume a special role of it in the prebiotic evolution as well as in several reactions included in the nitrogen cycle of the Earth. According to *ab initio* calculations and experiments, aqueous surfaces have a catalytic effect on these reactions through their interaction with methylamine. For examination of the behavior of methylamine at icy surfaces and at the liquid-vapor interface of water-methylamine mixtures, computer simulations were performed.

Related to the panspermia hypothesis, the adsorption equilibrium of methylamine was investigated on the surface of amorphous ice, which is characteristic to the interstellar medium, by grand canonical Monte Carlo simulation method at five different temperatures ranging from 20 K to 200 K. We demonstrated the strong tendency of methylamine molecules for being adsorbed at the surface of amorphous ice, including their ability for multilayer adsorption. Our analyses revealed that the methylamine prefers to be in all the orientations where the carbon-nitrogen bond axis lays parallel with the macroscopic ice surface, and also that at low chemical potential values methylamine tends to form up to three hydrogen bonds with the surface water molecules of the amorphous ice. The liquid-vapor interface of aqueous methylamine solutions of several different, finite concentrations was also investigated by molecular dynamics simulation method. Our results indicated that methylamine molecules show a tendency to be accumulated in the first molecular layer; however, they do not show considerable self-association at the surface of their aqueous solutions. Surface methylamine molecules strongly prefer the alignment in which the apolar CH_3 group points straight to the vapor phase. The presence of methylamine accelerates the exchange of methylamine and water molecules between the surface layer and the bulk phase; furthermore, methylamine molecules slow down the lateral diffusion of each other and immobilize the water molecules within the surface layer.

Summarizing, we have seen that methylamine could indeed play a special role in the prebiotic evolution as it is described in the panspermia hypothes. Further, based on our results, it is also possible that methylamine might participate in atmospherical reactions.

Self-association process in urea, acetone, acetamide and choline chloride aqueous solutions: Vibartion spectroscopy and molecular dynamics simulation

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ABSTRACT

The balance of the intermolecular interactions (solute-solute, solute-water and water-water) is a key issue in the understanding of the structure of aqueous solutions, in particular the self-association behaviour of solution components resulting from the preference of like-molecule interactions (solute-solute and water-water molecules). Aqueous solutions are certainly an attractive field within this context since the balance between van der Waals interactions and the hydrogen bonds provides an additional complexity to these solutions, who nature remains a challenging area of research. In this perspective, we would like to put forward a property that seems important in aqueous solutions, namely the solute self-association. The predictions concerning the existence or not, and the extent of the self-association of a solute as well as the effect of the solute on the structure of water remain controversial. Particularly in mixtures where the full miscibility is achieved at the macroscopic level, at the microscopic level the solute molecules are inhomogeneously distributed, or self-associated. The quantification of the self-association using classical molecular dynamics simulation is not straightforward since an accurate parameterisation of the interaction potential model of the components of the mixture does not guarantee the proper description of the local structure of the mixture.

We investigate the self-association in urea, acetone, acetamide and choline chloride aqueous solutions at different mole fractions of the solute via vibration spectroscopy and classical molecular dynamics simulations. These solutes are iso-electronic, have the same Y-shape, and the hydrophobic contribution (number of methyl groups) gradually increases from urea to acetone. Aqueous urea has intriguing properties at high urea concentrations, such as favouring protein denaturation, increasing the solubility of hydrocarbons and slowing down the micellar aggregation. Although it is practically certain that the competition of the hydrogen bonding between the two species plays an important role in the above mentioned properties, the characterisation of the hydrogen bond network in a convincing physical picture is still a challenge already in pure water, let alone the mixtures. We quantify the degree and characteristics of self-association of these solutes in water through the use of the concept of infrared excess molar absorption of a given vibrational mode as an observable which contains all the information on the collective interactions in the mixture and in MD simulations by the evaluation of statistical functions which are calculated over the nearest-neighbour volumes such as the nearest-neighbour radial and orientational distributions, the distribution of the topological parameters of the Voronoi polyhedra as well as using a density-based approach in order to characterise the domains of the inhomogeneity distribution of the solute molecules.

Multifunctional PEG-carboxylate copolymer coated nanomagnets for biomedical application

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ABSTRACT

Hydrophilic magnetic nanoparticles (MNPs) designed for diagnostic or therapeutic applications (e.g. MRI, hypertermia, drug-delivery) are in the focus of scientific interest last decades. A protective layer is needed to prevent the aggregation, to stabilize the dispersion and to hinder the chemical and biological degradation of nanomagnets. Recently the PEGylation, i.e. the covering nanoparticles by polyethylene glycol (PEG) (called also as polyethylene oxide (PEO)), is the most favoured way to ensure their biocompatibility. In this work, we combine the high hydrophilicity of coating provided by PEG chains with the strong linkage through carboxylic groups [1-3].

New type of functionalized PEG-polymers was synthesized (PEGMA-AA and PEGA-AA), where the number of anchoring groups and the length of PEO blocks are optionally variable parameters. The functional groups were quantitatively characterized by potentiometric acid-base titrations. Infrared spectroscopy (ATR FT-IR) revealed that these new PEG-polymers bind through carboxylic groups on the nanomagnets surface. Electrophoresis experiments showed that the chemically attached PEG-polymers influence the aggregation of MNPs depending on the amount of added molecules. An increase in hydrodynamic diameters (from ~90 to ~115 nm) was measured for fully coated nanomagnets by DLS, which suggests a steric contribution to the stabilization besides the electrostatic one. The hemocompatibility was checked and the theranostic potential was tested in MRI and magnetic hyperthermia measurements.

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Controlling the Oriented Deposition of LC Polysaccharide at Evaporative Interface in a Confined Geometry

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ABSTRACT

Self-assembly of polymeric liquid crystals (LC) has emerged as a powerful technique to recreate the complex hierarchy found in nature. By tuning the conditions of drying, it is possible to gain control over their mobility in solution and in turn on the orientation during deposition. Recently, our group reported a macrospace-partitioning phenomenon upon drying a polysaccharide aqueous LC solution from a limited evaporative interface. Vertical membranes were deposited, bridging a millimeter-scale gap between the substrates and formed highly oriented structure as a result of a non-equilibrium process between polymer deposition and hydration. Here, in order to generalize this space-partitioning phenomenon and explore structural changes due to temperature variations, we have explored the drying of xanthan gum solution.

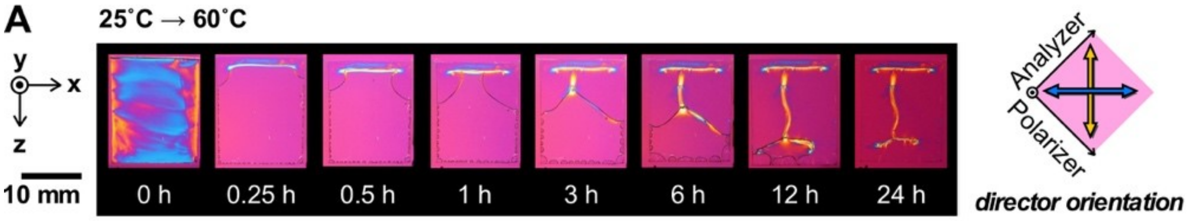

Figure: Side views of xanthan gum aqueous solution during drying from a top-side-open cell as observed under cross-polarizers with a first-order retardation plate, λ = 530 nm.

The xanthan LC state was affected by changes in temperature and demonstrated interface-assisted orientation. By varying the conditions of temperature and initial concentration, the depositions induced in the limited space have been monitored and a comparative phase diagram prepared. We envision that this work of drying-induced condensation will provide a simplified methodology to design self-assembled biomimetic materials with highly-ordered structures.

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Creating electrospun 3D artificial matrices for biomedical purposes

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Huge amount of polymers are used for a wide range of medical or pharmaceutical purposes. The technology, and new materials we have now are always being developed for better or for new purposes. The bases of such materials are coming from polymers which can be found in nature. We expect from these polymers to be biocompatible and biodegradable, so not to cause immune reaction and after degradation build into the living system. Poly(aspartic acid) can be a good choice for medical application, which can be created from Poly(succinimide) by alkaline hydrolyzation.

Nanotechnology is one of the most intensively developed discipline. With its help, we can create artificial matrices which have fibre diameters like in the living organism. Among other technologies, the method of electrospinning is good for creating such fibres. We can modify fibre parameters by adding silver nanoparticles or salts. With different setups and modifications, 3D structures have been experienced but for the causes there is no universal explanation yet. The questions need to be answered to make this process reproducible because there is a lot of potential uses for this 3D structures. Among other things with the change of electric field or the shape of the collector similar effect can be reached.

Our aim was to create artificial 3D fluffy fibre structures from Poly(succinimide) with the help of electrospinning. Therefore, the effect of the presence of different salts were investigated ($CaCl_2$, $MgCl_2$, LiCl, LiBr, NaBr, NaI, KI, KBr) on the process of creating fibres. The scaffolds were analysed with the help of Scanning Electron Microscopy and Raman spectroscopy. We analysed the relation of the solvent (Dimethyl-formamide) and the used salts as well with the help of Fourier-transform infrared spectroscopy and Raman spectroscopy.

Reproducible three dimensional scaffolds were created successfully with the appropriate salt concentrations and setup. The solvent-salt examinations correlate to what we experienced with the electrospinning process therefore, we got closer to the understanding of the phenomena. In the future, our results could contribute to creating designed structures which main and most important area of usage could be biomedical applications.

Acknowledgement: This research was supported by NKFIH FK 124147, János Bolyai Research Scholarship of the Hungarian Academy of Sciences and ÚNKP-18-4-SE-1 New National Excellence Program of the Ministry of Human Capacities.

Poly(aspartic acid) hydrogels: potential scaffold for tissue engineering

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ABSTRACT

Tissue engineering is one of the most research fields in regenerative medicine. In tissue engineering, isolated cells are seeded on/in to a scaffold material which facilitates 3 dimensional proliferation and migration of cells to support the tissue formation. Therefore, development of novel biocompatible and biodegradable scaffold is a crucial part of the process. Ideal artificial scaffolds are more than an inert platform; they possess all the important properties of the extracellular matrix (ECM) such as, cell attachment regulation, appropriate mechanical properties, biocompatibility and degradability [1].

Natural ECM is a three dimensional fibrous system which contains different amino acid based polymers, such as collagen, elastin or fibronectin. Synthetic, poly(amino acid) based hydrogels are good candidate for tissue engineering due to their high physical and chemical similarity to the ECM. Application of poly(aspartic acid) (PASP) hydrogels in the field of tissue engineering was introduced by our research group in 2016 [2]. In this presentation I would like to demonstrate the crucial points of our research which led to the better application of these hydrogels as a scaffold.

PASP hydrogels have been prepared with different mechanical properties and chemical constitution. Stability of the hydrogels has been investigated in different biological relevant environments. For in vitro experiments, MG-63 human osteoblast-like and two different (periodontal ligament and Dental pulp) stem cell lines were chosen. The cell viability was followed by WST-1 measurement. 3D arrangement of the cells was investigated by 2 photon microscopy.

According to our results, poly(aspartic acid) based hydrogels are can support proliferation, differentiation as well as migration of human cells, which implies that our system could be a good candidate for 3D cell culturing of osteoblast cells

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Self-propelled Dipolar Nanocubes

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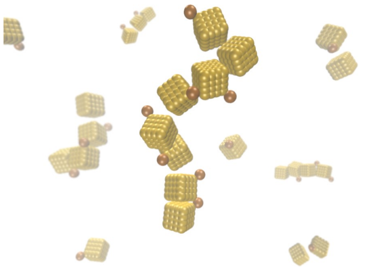
ABSTRACT

Microscopic active particles, including self-propelled cells, microorganisms and artificial swimming colloids, have gained a lot of attention due to their relevance in such important fields as biology, biomedicine, nanoscience and nanotechnology. The term "active" describes the ability of certain particles or units, to convert energy from their environment into motion, hence, kinetic energy [1]. This highly interesting property can arise from various mechanisms, such as localized concentration gradients, where an asymmetric distribution of reaction products (i.e., chemical fuel) on a coated particle propels the particle by self-diffusiophoresis.

In this study, we use active matter to create a new type of nanomotor, which is oriented by an applied magnetic field and propelled by an active particle. One of those units consists of a dipolar cube that can be directed due to its interaction with a magnetic field, whereas a second non- dipolar active particle with a propulsion force directed into the cubes centre of mass, creates a field controlled swimming unit.

This scenario is investigated using molecular-dynamic simulations, setting the above described unit in an obstacle free environment, while applying a constant magnetic field. By computing the mean- square-displacement, we investigate if the diffusion of the self-propelled motor is enhanced in field direction and look at its dependencies on the unit parameters, which are compared with reported literature [2].

In collaboration with Dr. Schmidt from the University of Cologne, those nanomotors are also investigated experimentally. CoFe2O4 cubes use an added platinum cap as a catalyser, to trigger the reaction that creates the propulsion force. As well as in the simulations, the mean square-displacement is measured to describe the units diffusive behavior.



Simulation snapshot of an ensemble of active-dipolar nanocubes forming clusters.

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Investigation of the thermodynamic properties and the liquid-vapor interface in formamide-water systems

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ABSTRACT

Considering five potential models of formamide and three models of water, the thermodynamic properties and miscibility of these potential model combinations was investigated by using Monte Carlo (MC) simulation with an appropriately chosen thermodynamic cycle, which includes performation of thermodynamic integration. The results of the simulations indicate that the mixing of formamide and water is very close to the ideal mixing, since both the energy and entropy of mixing is near to the ideal one in the entire composition range. The OPLS/AA_mod formamide model shows negative mixing energy with the water models, in contrast with the other four models and with the experimental data. The Helmholtz free energy of mixing stays always negative in the case of every model combination. Most of the model combinations either show immiscibility, or approach the miscibility limit very closely in certain compositions. Based on the energy of mixing and the miscibility of the model combinations, we selected the CHARMM formamide and SPC/E water models for further simulations of the formamide-water mixtures. Molecular dynamics (MD) simulations were then performed in the canonical (*N,V,T*) ensemble to study the liquid−vapor interface of formamide-water mixtures. The molecules in the interfacial layer were determined by the method of Identification of the Truly Interfacial Molecules (ITIM). The surface molecules indicate the presence of a strong lateral hydrogen-bonding network, in which the water and formamide molecules mix with each other even on the molecular level. The results show no strong adsorption or lateral self-association of the components on the surface. The preferred orientation of the surface molecules is parallel with the macroscopic plane of the surface. This preference is governed by the requirement of maximizing the hydrogen bonds of the surface molecules. The dynamics of the molecules in the interface layer is also governed by the hydrogen bonds. Thus, the formamide and water molecules stabilize each other in the interfacial layer, slowing down the lateral diffusion of each other, or even preventing each other from lateral diffusion.

VSFG spectrum prediction from classical molecular dynamics simulations

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ABSTRACT

Vibrational Sum Frequency Generation (VSFG) is well-established experimental method that can explore processes on various water/solid interfaces. Hand in hand with development of this experimental technique, theoretical approaches to get SFG spectrum from classical and ab-initio molecular dynamic simulations have arisen. Recently, new approach that uses velocity-velocity correlation functions (VVCF) to calculate VSFG spectra [1] was demonstrated to properly describe VSFG spectrum of a fluorite surface using ab-initio molecular dynamics (AIMD). The advantage of this method is that it only requires the atomic positions and velocities without the cost of calculation of molecular dipoles and polarizabilities in each step.

We have adopted the method based on VVCF and explored possibilities of the phase-resolved VSFG spectra prediction from classical MD simulations (CMD). Performance of various flexible water models based on well-established SPC and TIP3P models was compared to predict VSFG spectra of the alumina (0001) and fluorite (111) surfaces corresponding to a range of pH values. Results show good agreement between CMD computed spectra and AIMD computed or experimental ones. Of course, with much less computational effort in the case of CMD simulations compared to AIMD ones.

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NMR studies upon aggregation behavior of hydrophobically functionalized poly(4-styrenosulfonic-*co*-maleic acid)

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ABSTRACT

Design of hydrophobically functionalized polyelectrolytes is an interesting approach to study their unique properties due to similarity to biological systems as well as their strong tendency toward self organization in aqueous solution caused by combination of electrostatic and hydrophobic forces. An important issue in this context is connected with synthetic routes and comprehensive physico-chemical characterization of adsorption and aggregation properties, of new amphiphilic polyelectrolytes, obtained by chemical conjugation of a hydrophobic chain to the polyelectrolyte backbone via a pH-labile moiety [1]. High resolution NMR techniques constitute powerful techniques for complex investigations of the above mentioned functionalized polyelectrolytes toward their application in the nanomedical field. The main aim of the present research is to synthesize and study aggregation properties in aqueous solution of hydrophobically functionalized poly(4-styrenosulfonic-*co*-maleic acid) with differing percent degree of hydrophobization, side chain lengths and pH-labile moiety type (secondary amide or ester bond). The physicochemical desrciption of pH-responsible hydrophobically functionalized polyelectrolytes includes the following: analysis of their aggregation in aqueous solution, pH and/or ionic strength dependence of aggregate size, charge and zeta potential as well as viscoelastic properties. Dynamic light scattering (DLS) and/or diffusion-ordered nuclear magnetic resonance (DOSY NMR) techniques were utilized to monitor the modified polyelectrolytes self-assembly in the appropriate aqueous media. The performed studies enabled us to obtain crucial information about the hydrophobized polyelectrolytes structure and its influence on aggregation properties toward their application in the fields of pH-sensitive nanosized thin films and nanocarriers.

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Using nanopores as sensors: The effect of the charge pattern from symmetric to asymmetric leading to a dual-response device

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ABSTRACT

Artificial nanopores the basic elements of nanofluidic devices. These devices can be used as parts of nanofluidic circuits, or for filtering and sensing thank to the rapid improvement in experimental techniques. Chemical modifications on the nanopores' wall make it possible to bind certain ions selectively, thus the nanopore can function as a sensor. In this work, a systematic modeling study about the application of a nanosensor is made via optimizing the charge pattern on the nanopore’s wall in order to improve the efficiency of the sensor.

As an effect of an applied electric field, ions move through the pore. Ions of the background electrolyte serve as the main charge carriers. The binding sites (modeled with a square-well potential) selectively bind the analyte ions. This binding, on the other hand, influences the current of the background electrolyte. We analyze various mechanisms of sensing based either on the competition of the background cation with the analyte cation for space in a negatively charged nanopore region [1] or on attraction between the analyte cation and the background anion in a positively charged region [2]. Which mechanism takes action depends on the charge pattern. We show that the latter mechanism makes it possible to detect analyte ions in trace concentrations. We also show that using a nanopore with an asymmetric charge pattern makes it possible to construct a dual response device: both current and rectification serve as signals sensitive to the presence of analyte ions.

In this work, the Nernst-Planck transport equation is used to compute current together with the Local Equilibrium Monte Carlo method that is suitable to simulate ions in trace concentrations due its grand canonical design. Electrolyte is modeled as hard-sphere ions in an implicit-water background.

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Effect of Added Surfactant on the Poly(Ethyleneimine)-Assisted Gold Nanoparticle Formation

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ABSTRACT

In a variety of applications, functionalization of the gold nanoparticles is needed to ensure adequate surface charge and hydrophobicity of the particles for their biodistribution, interparticle interactions or self-organization. In the present paper, we provide an economic way for the synthesis of hydrophobized poly(ethyleneimine)(PEI)-capped gold nanoparticles at room temperature using sodium dodecyl sulfate (SDS). The approach is based on the controlled competition between the Au(III) ion reduction within the PEI molecules and the SDS binding onto their amine groups. This is achieved via utilizing the strongly non-equilibrium association between the oppositely charged polymer and that of the surfactant molecules. Specifically, by varying the order and timing of SDS addition during the process of gold nanoassembly formation, the size distribution, the morphology and the local hydrophobic environment of the PEI-Au/SDS nanohybrids can be easily tuned even at one total composition of the system. The results may be further exploited for the preparation of noble metal nanoassemblies with controlled hydrophobicity and charge.

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Polarisation Corrections and the Hydration Free Energy of Water

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Water remains one of the most fascinating molecules to study at the theoretical level, not least due to its well-documented “anomalies” in terms of dynamic and thermodynamic behaviour. The importance of water means that development of accurate and computationally efficient water models is still an area of intensive research. In this context, fixed-charge (i.e. non-polarisable) models have been the “weapon of choice” for the vast majority of simulation studies to date. Nevertheless, a unique classical non-polarisable model of the water molecule is still to emerge. To better understand why this is the case, one must delve deeper into the intrinsic approximations involved in the development of such models. In this work, we focus on the ability of fixed-charge models to describe the hydration free energy of water. Using thermodynamic integration methods, we have calculated the hydration free energies of over 10 different fixed-charge water models and compared them against experimental data. Our calculations show that none of the most recent models is able to simultaneously predict the hydration free energy and the enthalpy of vaporisation, and that a systematic error is at the origin of this failure. More precisely, we argue for the need to appropriately account for polarisation during this process. Such corrections have been proposed in the past [1], but they fail to account for purely electronic contributions to the polarisation. We show [2] that a recently proposed framework that implicitly accounts for polarisation contributions in non-polarisable models [3] is able, with appropriate adaptations, to reconcile the predictions of free energy and enthalpy for water. This approach relies on an estimate of the dipole and quadrupole moments of liquid water (calculated here from the *ab initio* molecular dynamics data of a recent study [4]), whose dipole is in excellent agreement with experiment [5]. Our work also suggests an explanation for why the rather outdated TIP3P model is still widely used for the prediction of solvation free energies.

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Biocompatible, biodegradable and implantable poly(amino acid) based fibrous networks

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Hydrogels are well-known soft and wet materials for their wide range of applications in the biomedical fields as drug carriers or scaffolds for cell cultivation. However, in many cases, they lack the mechanical strength for suturing, thus limiting their suitability for implantation.

In this work, the authors try to give a solution for enhancing suturability of hydrogels by fabricating hydrogel fibrous membranes with electrospinning. Two types of polysuccinimide based fibrous membranes are presented. One with a short biodegradation time, containing disulfide bonds and one, cross-linked with an alkyl-chain cross-linker, that has longer biodegradation time. According to the mechanical tests, the synthesized samples are mechanically suitable for suturing and implantation. The biocompatibility and biodegradability of the membranes were tested *in vivo* in a one weak long experiment. Both membranes undergo hydrolysis in three days and turn into poly(aspartic acid) fibrous membranes. After one week the disulfide cross-linked membranes almost completely degrade, while the alkyl-chain cross-linked ones, mildly lose their strength as the surrounding tissue invades them. Histopathology showed mild acute inflammation, which after seven days decreases to a minimal level. The results indicate that generally higher flexibility and suturability can be achieved in hydrogels by preparing fibrous membranes. In addition, poly(succinimide) based implants have a great *in vivo* potential as they are easy to handle and are able to turn into biodegradable, biocompatible poly(aspartic acid) by *in vivo* hydrolysis.

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The impact of structural inhomogeneities, superparamagnetism and central attraction, on the equilibrium structure of magnetic filaments

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ABSTRACT

Construction of smart materials with sophisticated magnetic response by incorporating magnetic particles (MNP's) within permanently cross-linked structures, opens up the possibility for synthesis of highly magneto-responsive systems.[1] Construction of appropriate magnetic filaments (MF's polymer-like structures in which magnetic colloids are represented as monomers) has recently been made possible using DNA origami technology [2,3].

Structural inhomogeneities alter the equilibrium properties and the magnetic response of MF's. Coiling and persistence length of MF's depend on the magnetic particle distributions, along with temperature and applied magnetic field. Using MD simulations, we compare the structural properties and magnetic response of various configurations of MF's.

We extensively discuss the projection of magnetic moments along the orientating magnetic field direction, on both the filament and colloid level. Furthermore, we contextualize the implications of this within an exhaustive, comparative analysis of the field dependent, structural behavior of MF's, for ferromagnetic and superparamagnetic colloids within different crosslinking scenarios. Finally, we scrutinize the effects of a central attraction potential (i.e. inclusion of Van der Waals forces) on the dynamics of the filaments and their magnetic response.

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Eger, Hungary

Structural characterization of aqueous magnetic fluids stabilized by sodium oleate

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ABSTRACT

Magnetic fluids (MFs) are unique artificial colloidal systems combining magnetic properties and fluidity. They consist of magnetic nanoparticles (MNPs) with a characteristic size of about 10 nm dispersed into a liquid medium. Colloidal stability of the MNPs in the liquid carrier is reached by steric repulsion between the surfactant coatings adsorbed on the MNPs' surfaces. The study of MFs is of great practical and fundamental importance. In recent years, much attention was drawn to the bulk structure of magnetic fluids at various conditions, which is well observed by small-angle neutron scattering (SANS) [1]. In the case of water based MFs, with many applications in biotechnology and biomedicine, MNPs have to be nanosized, monodispersed, nontoxic and have stability to aggregation due to effective-hydrophilic coatings.

It is well known, a creating of steric stabilized water based ferrofluids with biocompatible surfactants usually are technically problematic. Recently successful attempts of aqueous MFs' synthesis were done at the Vernadsky Institute of general and inorganic chemistry (Kiev).

Several kinds of MFs, with respectively narrow size distribution of MNPs and stabilized with sodium oleate, were studied in the given work by means of Small-Angle Neutron and X-Ray (synchrotron) Scattering. The structural investigation was performed under two types of ferrofluids, where magnetite NPs were synthesized by different methods using cryotermal conditions and deposition from diethylene glycol. By comparative analysis it was concluded the effectiveness of the methods of synthesis.

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DNA building block adsorption on SiO_2@ZrO_2 NPs

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ABSTRACT

Identification of cancer associated antigens allows the development of therapeutic vaccines against specific types of tumors. New generation active cancer vaccines, however, require novel delivery systems to transport cancer antigens and adjuvants to target immune cells. A promising class of adjuvants are short, synthetic analogues of microbial single stranded DNA, which are able to trigger an immune response required for fighting cancer by recognition on innate immune receptors. Nanoparticle based carriers also have adjuvant activities, because they can boost the response of immune cells due to their size similar to viruses (20-200 nm). Moreover, they can ensure targeted delivery of the adjuvant and the antigen immobilized on their surface as a result of their elimination by the immune cells.

In this study, we designed and built up an inorganic nanoparticle based vaccine delivery system. We prepared silica@zirconia core-shell nanoparticles of different sizes but identical surface chemistry. In the current report, we investigated the adsorption conditions of deoxynucleoside monophosphates, the building blocks of DNA.

The nanoparticle synthesis have been performed using the methods of Stöber[1] and Kim[2], the latter optimized in our research group[3]. We characterized the obtained samples by DLS, FTIR, TEM, NMR, XRD, TGA, zeta potential and UV-Vis measurements. We carried out a time-dependent study of the particles' structure. In view of the biological application, we performed adsorption tests in different buffers: phosphate, HEPES, PIPES, MES, MOPS and MOPSO. Finally, we built up hypotheses about the adsorption of dNMPs on a molecular level.

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Use of microorganisms in environmental bioremediation

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ABSTRACT

Nowadays biotechnological processes involving biosorption, bioaccumulation and biodegradation have attracted the attention for environmental decontamination. Study of biosorption and bioaccumulation using a variety of biomasses (bacteria, algae, yeast, and fungi cells) has already given some promising results for removal of inorganic and organic pollutants from aqueous medium, however, information on interaction of biomass cells and pollutant compounds for technological application under dynamic condition is still limited.

Uptake of heavy metal ions by living and dead microorganisms may offer an alternative method for bioremediation of aqueous environment compared with the conventional methods. Microorganisms accumulate metals by a number of different processes such as uptake by transport, biosorption to cell walls and entrapment in extracellular capsules, precipitation, and oxidation-reduction reactions. Biosorption may be primarily a function of binding of heavy metal cations to chemical functional groups on the cell wall via ionic and coordinate bonds.

The relation between specific cell surface charge, cell size distribution, cell surface and total protein profile characterization, viability and adsorption processes by various microorganism cells even in lyophilized forms for removal of metal ions and phenols from aqueous suspensions have been studied. Simultaneous adsorption in binary systems containing metal ions or metal ions and phenol molecules have also been examined.

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Simulations of ions and oxalic acid on rutile and quartz surfaces

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ABSTRACT

This talk summarizes our simulation work on adsorption of atomic (Li^+, Na^+, K^+, Rb^+, Ca^{2+}, Mg^{2+}, Sr^{2+}) and molecular (oxalate, hydrogenoxalate) ions on rutile (110] and quartz (101) surfaces. While our previous studies [1] with selected ions modeled with their full nominal charges were in good agreement with experiments, our attempts to model ions of oxalic acid with nominal charges of the molecular ions, even in bulk water, were not successful. As a result, we developed Electronic continuum correction (ECC) models of oxalate and hydrogenoxalate with charges scaled to 75% of nominal values [2]. Our extension of ECC to modeling solid-liquid interfaces and electrokinetic properties will be also illustrated [3]. ECC has been proved before to bring significant improvement in the modeling of interactions of ions (especially multivalent) in aqueous solutions [4].

Results of analysis of adsorption of oxalic acid will be detailed, as well as comparison of results for adsorption of atomic ions using full vs. scaled charges. Inner-sphere vs. outer-sphere binding motifs will be discussed and compared with information inferred from published ATR-FTIR spectra. Advanced sampling techniques, namely potential of mean force determination and metadynamics, were applied.

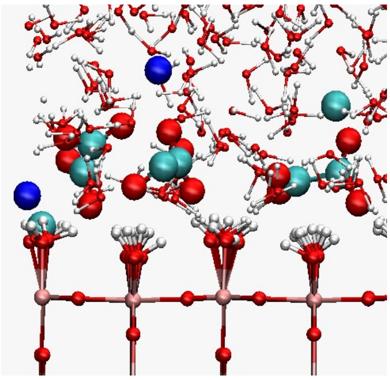

Figure 1: Snapshot of oxalate ions interacting with the positively charged (110) rutile surface (+0.2 C/m^2).

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Self-assembly of hollow colloidal silica cubes

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ABSTRACT

Among the multitude of recently synthesized non-spherical colloids, hollow silica cubes distinguish themselves by their charged surface and the strong influence of van der Waals forces on their behavior. While their self-assembly has been observed in experiment, its origins have not yet been fully understood. Gaining control of the underlying self-assembly mechanisms of charged cubes is the basis for designing new soft materials with desired rheological and optical properties.

Using MD simulations that take the superball model of cubes, developed in [1] for the study of hematite cubes [2], and expand it to consider the electrostatic aspects of the system, we investigate the electric double layer surrounding the cubes. The anisometric cubical shape of the colloids leads to an overall anisometry of the counterion distribution near the surface, studied on the level of a single cube. Based on the acquired knowledge, we are able to compute the interaction potential of two weakly charged cubes as a function of their mutual orientation, allowing for the effects of Van der Waals forces[3]. Doing so, we also investigate the influence of the intercube distance and their mutual orientation on the distribution of counterions. Obtained quantities show the preference of two cubes to approach each-other corner to corner, slide along the edges and only then assume a final face to face configuration.

In combination with experimental observations and calculated trajectories, we then examine the microstructures formed by small clusters of cubes, which differ significantly from those exhibited by comparable spheres. These investigations give us a multifaceted understanding of the behavior observed in these systems and pave the way for future applications.

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Semiconductor nanoparticle/graphene oxide composites for environmental applications

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ABSTRACT

The size-tunable optical properties of semiconductor nanoparticles have long been discovered and their use in catalytic processes was extensively investigated. Particularly, titanium dioxide has been demonstrated to exhibit excellent photocatalytic activity, which can be exploited in the degradation of environmentally relevant pollutants. The TiO_2 products obtained by flame pyrolysis such as P25 from Degussa AG have become standard materials in the broad field of photocatalysis and have been successfully commercialized. While many efforts failed to produce photocatalytic solids that overcome P25 TiO_2 in terms of catalytic activity, at least regarding UV irradiation, there is a lot of potential in the improvement of the overall catalyst performance involving the processability of the catalyst suspended in the treated wastewater. To realize that aim, the synthesis and application of semiconductor nanocomposites is a very promising way because some of their physicochemical (e.g. sedimentation) properties may be enhanced as compared to their single-component counterparts. This presentation will feature the synthesis and environmental application of several nanocomposites comprised of nanoparticles (TiO_2 and ZrO_2) and graphene oxide (GO) nanosheets. We demonstrate that the nanoscale dispersion of these semiconductor particles in an open, porous fractal aggregate structure is beneficial for the following environmental applications: (i) processability of suspensions after photocatalytic [1] or adsorption based removal of pollutants and (ii) enhanced photocatalytic hydrogen production [2].

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On the analogies and peculiarities of charging and colloidal stability of humic acids and graphene oxides

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ABSTRACT

In biogeochemical cycle, successive transformation of organic material (OM) from biopolymers results in several intermediate products such as humic acids (HAs) with significant oxygen-content, and end products like pure graphite having layered, planar structure [1]. HAs are operationally defined as base-soluble, but acid-insoluble OM. Their chemical structure is ill-defined, having a polycondensed aromatic ring system, several cross linkages, and polyionic structures emerge with, e.g., phenolic hydroxyl, carbonyl and carboxyl groups. Similar O-containing groups form on graphene sheets during chemical exfoliation of graphite as graphene oxide (GO) is prepared. Oxidation of graphite generates oxidative debris (humic/fulvic-like substances) that should be removed through washing. During purification of GO from fulvic acids residual, we experienced almost the same pH-dependent behavior as used in separation of HA from fulvic acids, occurring both in the natural mixture of humic substances.

In the present work, the pH- and ionic strength dependent charge formation of some HA and GO samples, and their colloidal stability in aqueous solution are compared. Preparation, fractionation of samples and the need of their exhausted purification are explained in detail. Potentiometric acid-base titration was used to quantify the dissociation of O-containing functional groups and to check the reversibility of deprotonation/protonation processes [2]. The pH-dependent charge state of HA and GO samples as characterized by electrophoretic mobility (zeta-potential) measurements in parallel with the colloidal stability characterization are elucidated.

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Wetting and evaporation properties of carbon nanotube buckypapers doped by hydrophilic nanowires

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ABSTRACT

Recent developments in nanotechnology have highlighted the importance of the classical topics of wetting, droplet spreading and evaporation due to their pronounced effect in technological applications. Carbon nanotubes (CNTs) can be transformed by filtration into a self-supporting, porous, paper-like film (buckypaper (BP)). Besides offering a convenient alternative to handle CNTs macroscopically, buckypaper is an interesting porous material on its own right. The main goal of this work was to obtain a more detailed picture of the surface properties (namely, wetting and vaporization) of the buckypapers prepared from non-functionalized multiwall CNTs doped by hydrophilic nanowires (i.e., titanate nanowire – TiONW and goethite nanowire – FeONW).

The evaporation of sessile droplets (e.g. water, methanol, iso-propanol, 1,4-dioxane) was studied by simultaneous weight monitoring, electric resistance measurement (Fig. 1.) and infrared imaging at 50 °C [1]. There are several parameters characteristic for the evaporation process, the most important ones being the total evaporation time, time of evaporation only from the surface, evaporation rate, initial area of the droplet, etc. The results allow us to presume that this experimental setup and theoretical approach are suitable for future analytical applications.

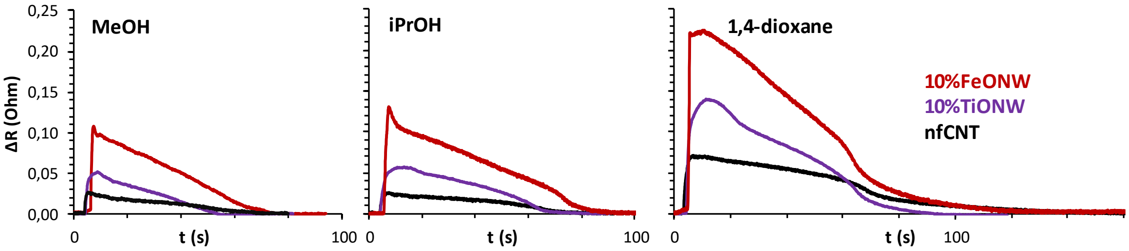

Fig. 1. Solvent specific change of resistance during the evaporation of sessile droplets from *nf*CNT buckypapers (black) doped by TiONW (purple) and FeONW (red) samples.

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Characterization of dopamine containing fibrous polymer-drug conjugates

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ABSTRACT

Since biopolymers are chemically similar to natural polymers, they are suitable materials for preparing biocompatible drug-delivery systems[1]. Poly(succinimide) is an anhydrous form of poly(aspartic acid), hence it has outstanding degradation property at physiological conditions[2]. Prolonged drug release can be obtained with nanofibrous polymer meshes produced by the electrospinning technique. These systems have large specific surface and porosity[3], therefore the dissolution kinetics and drug absorption can be increased.

The aim of this work was to prepare biocompatible, biodegradable drug conjugates using poly(aspartamide) based nanofibers, to characterize the dissolution kinetics and drug release kinetics of these samples and to investigate the incidental cytotoxicity.

The dopamine-polymer fibrous conjugates were characterized by FT-infrared spectrometry, scanning electron microscopy, atomic force microscopy and two-photon microscopy. The kinetics of dissolution and dopamine release were monitored by UV-Vis spectrophotometry. The biocompatibility of the conjugates was examined by culturing of human periodontal ligament stem cells. The cell viability was assessed by WST-1 cell proliferation reagent. The morphology of the cells was observed by phase-contrast and two-photon microscopic techniques.

Dopamine containing nanofibrous poly(aspartamide) based conjugates were prepared with prolonged dopamine release. The cell viability tests show the biocompatibility of the conjugates. Applying these conjugates, the non-toxic concentration of the dopamine can be higher than in case of treatment with free dopamine.

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A novel method for surfactant binding isotherm measurements of polyelectrolyte/surfactant mixtures validated by neutron reflectivity data

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ABSTRACT

The interactions of oppositely charged polyelectrolyte/surfactant (PE/S) mixtures have attracted significant interest in the last decades due to their widespread applications. While the bulk interactions are traditionally described by surfactant binding isotherms (the amount of surfactant bound to the polyelectrolyte), interactions at the air/water interface are usually discussed in terms of surface tension isotherms. Due to the enormous difficulties associated with the surfactant binding measurements, unfortunately experimental surfactant binding isotherms are available only for a limited number of PE/S mixtures. Further, despite the significant efforts, a general understanding of how the bulk binding isotherm and the surface tension are related to each other is still missing. A further complication to the behavior of PE/S mixtures is the associative phase separation region where complexes lack colloidal stability, and over time they aggregate, precipitate and sediment. These non-equilibrium effects have resulted in a lot of confusion in the literature over the years about how to interpret the interfacial properties.[1]

Recently, we have shown that in the associative phase separation region, the surface tension of equilibrated (precipitated) PE/S mixtures can be described by the surface tension isotherm of the pure surfactant following removal from the aqueous phase of all of the polyelectrolyte and a certain amount of the surfactant in the form of PE/S aggregates.[2] In this contribution, we go full circle to show that when the experimental conditions are chosen carefully, the surfactant binding isotherm can in fact be determined easily and quickly in the associated phase separation region by straightforward surface tension measurements. Our new approach is validated on various PE/S mixtures including DNA/C16TAB, Pdadmac/SDS and NaPSS/DTAB, and crucial neutron reflectivity measurements are used to provide the validation. Our results provide an important and simple tool for the characterization of PE/S mixtures in the associative phase separation region that was missing until now.

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Poly(aspartic acid) based nano gel fibers for tissue engineering

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Tissue engineering is one of the most intensively studied fields of medicine. A new direction in medicine is the regeneration of damaged tissue by culturing cells on a host artificial matrix and implanting it back to the damaged area to induce generation of new, healthy tissue, trying to restore its original structure and function. For this, there is a constant need for new materials, to which cells can adhere and proliferate on.

Fibrous hydrogel membranes prepared by electrospinning would be ideal materials mimicking the native soft tissue with their high water content and fibrous structure. Poly(amino acid) based hydrogels are emerging materials aiming for bio-medical applications. Their peptide like structure can be easily degraded by enzymes thus their biodegradability is ensured.

Hence our aim was to synthesize poly(aspartic acid) fibers by electrospinning for cell culturing.

In our research we prepared cross-linked poly(aspartic acid) polymers with hydrolysis, which contain disulphide bonds and 1,4-diaminobutane as cross-linkers [1]. FTIR was used to confirm the chemical structure. We tested the biocompatibility of the meshes using MG63 human osteoblast-like cell line. Cell viability was assessed 24 and 72 hours after cell seeding with WST1 reagent.

Crosslinked poly(aspartic acid) nanofibers were prepared, the hydrogel form prevented the dissolving in water via cross-linkers. During the test of cell viability we found that cells can adhere and proliferate on these membranes. Hence we have observed, that the artificial tissues are non-toxic for the cells, but we need more experiments to prove, that they are really suitable as scaffolds for tissue engineering.

The use of this type of biodegradable implant can be a huge step forward towards tissue regeneration, because the poly(aspartic acid) mesh has desirable chemical, mechanical and biological properties.

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Investigation of different human serum albumin-based composites for kynurenic acid drug delivery

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ABSTRACT

Kynurenic acid (KYNA) and its more hydrophilic modified version (SR72) was encapsulated in different human serum albumin (HSA)-polyelectrolyte systems both in static and flow synthesis methods. Prior to drug encapsulation the pH-dependent properties of HSA like hydrodynamic diameter, fluorescence emission intensity, surface charge and α-helix content were examined. The effect of drug presence on these properties were also studied in both physiological conditions and in distilled water. The drug-macromolecule interaction was investigated by isothermal microcalorimetric (ITC) and fluorescence emission quenching experiments. The composites were composed of polyelectrolytes such as PAH (poly-allylamine hydrochloride), PEI (polyethylene imine) or PSS (polystyrene sulfonate). By applying different flow rate, the HSA/PAH particle size decreased from 109.9 nm to 66.2 nm with increasing HSA amount. For the other method the charge compensation was calculated and 10 % excess amount of macromolecule was applied to obtain composite nanoparticles. The average particle diameter for the HSA/KYNA/PAH system proved to be 219 nm for 3 mg/mL HSA-containing composite based on dynamic light scattering measurements (DLS). The α-helix content increased from 54 % (determined for the pure HSA) to 61 % for the composite. The particle size if SR72 was the drug was about 72 nm with 49 % of α-helix content. Practically the same hydrodynamic diameter, 7 nm, was measured for HSA/KYNA or SR72/PEI colloids while significant difference in protein structure was observed with 25 % and 74 %, respectively. In the Blood brain barrier (BBB) model experiments the PAH-containing system proved to be the most promising with the highest permeability in the endothelial cells.

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Poly(vinyl alcohol) as a potential material for new surgical meshes

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ABSTRACT

Abdominal hernias are defined as the protrusion of abdominal structures due to a defect in the abdominal wall. Currently used surgical meshes for the repair of such hernias are still far from perfect and post-operative complications are observed more frequently than expected. Consequently, research of materials with better properties is still competitively conducted with the aim being the synthesis and production of better surgical meshes.

In this regard poly(vinyl alcohol), a material known for its favorable biocompatible properties was chosen by our research group as a candidate to fabricate surgical meshes. Electrospun PVA (Mw~72 000, Merck), scaffolds were implanted into Wistar rats (N:30) to repair artificially created abdominal wall defects. Following a six-month period, animals were terminated. Neither the macroscopical (autopsy) or microscopical (histopathology) examination reviled complications.

With such positive in vivo results, the current objective was to investigate if the same methodology can be applied and surgical meshes can be manufactured from a lower molecular weight (Mw~ 61000, Aldrich), FDA approved PVA.

The new meshes were fabricated (at 15kV, 15cm target distance and 0.8 ml/h flow rate). After successful fabrication, samples were mechanically assessed by an Instron 4952 System (uniaxial pulling measurements at 1mm/sec) while Scanning Electron Microscopy was utilized to investigate the mesh morphonology.

Mechanically the meshes performed competently retaining their structure through the measurements with minimal deformation even after being torn. Samples proved strong enough meeting the prerequisites for in vivo animal experiments to start. In addition, scanning electron microscopy confirmed the expected nanofibrous microstructure.

Due to the positive results received thus far, PVA investigation will continue with optimizing the current meshes followed by in vivo animal experiments.

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Poster presentations

Oppositely charged polyelectrolyte/surfactant assemblies as emulsion stabilizing agents

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ABSTRACT

Oppositely charged polyelectrolyte(PE)/surfactant(S) nanoassemblies have attracted special interest in the recent decades because of their several application possibilities. Due to their accumulation at the interfaces they could act as emulsion stabilizing agent [1]. When PE/S nanophases adsorb at the liquid/liquid interface then they may provide a Pickering type stabilization, where the accumulated particles at the interface provide high resistance to coalescence [2,3]. The combination of solid particles and more elastic PE/S nanoparticles as stabilizing agents could improve further the emulsions properties.

In our present study different nanoparticle/polyelectrolyte/surfactant assemblies have been utilized for the preparation of stable water/dodecane based emulsions. Specifically, we systematically applied oppositely charged oil and water soluble polyelectrolytes and surfactants in the presence of solid particles of different polarity. The as-prepared nano and macroemulsions were characterized by light microscope or dynamic light scattering (DLS) measurements. We have shown that the ratio of the immiscible phases, the PE/S nanoassembly and particle concentrations and the applied preparation methods can be successfully manipulated in order to optimize emulsion stability. Depending on the applied particle and solvent type special emulsion structures could be evolved. The application of interfacial polyelectrolyte/surfactant nanoassemblies as stabilizers could provide a powerful way to tune the size distribution and properties of the emulsions as well as to synthetize novel hierarchical nanosystems.

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Interactions of peptides with poly(ethylene oxide) grafted onto carbon nanotubes

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ABSTRACT

Due to the exceptional electronic, thermal, and mechanical properties carbon nanotubes (CNTs) are important constituents in nanotechnological devices. However, recently CNTs have found utilization also in biomedicine as biosensors, biomolecular recognition devices, molecular transporters especially in cancer therapy and diagnoses [1]. The disadvantage of using CNTs in biological systems is their insolubility in water. This is avoided by coating CNTs with hydrophilic polymer chains, which in addition, prevent undesired protein adsorption. Poly(ethylene oxide) (PEO) belongs to the most frequently used polymers for forming protective layers [2].

With the help of molecular dynamics simulations, the present study deals with interactions between PEO coated CNTs and peptides of different affinity for water. Peptides built of 24 monomers of valine, glycine, serine, aspartate, and lysine have been chosen as the representatives of hydrophobic, slightly hydrophilic, hydrophilic, hydrophilic negatively charged, and hydrophilic positively charged protein moieties, respectively. The effect of water, presence of NaCl in the physiological concentration, and the coverage density of PEO on the interactions of PEO and the peptides is scrutinized. The hydration and steric theory worked out for planar surfaces is also checked for the curved CNTs surface. This study is supposed to help to understand the controversial experimental results concerning the protection of surfaces against protein adsorption by PEO chains.

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A General Tool for Zeta Potential Predictions from Molecular Simulations

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ABSTRACT

Zeta potential (ZP) is among key properties characterizing colloidal solutions, and this macroscopic measure has been commonly reported in many experimental studies. However, molecular interpretation of ZP, which relies on complex interplay of solid surface properties and ion sorption abilities, has been a challenging task over many years.

Recent work of Předota et al. [1] has presented both simple and effective method to predict ZP from nonequilibrium molecular dynamics (NEMD) simulations, and consequently investigate its microscopic origin. Linking streaming mobilities, which could be directly extracted from simulations, to ZP values through the Helmholtz-Smoluchowski equation, Předota et al. concluded that the ZP arises from spatially varying structure, dynamics, and electrostatics of a solution in a narrow solid/liquid interfacial region.

The limitation of the original work was that the results were obtained using a self-written simulation code, which cannot be used to investigate complex systems. Hence, we generalize the application of the method [1] to popular freely available simulation packages like Gromacs and LAMMPS, allowing investigation of solutions with even molecular ions. We will detail the preparation of a setup for NEMD, correct settings for running simulations, and required data analysis.

The obtained simulation results include not only data for TiO_2 surfaces interacting with aqueous solutions of atomic ions (reproduction of the original work [1]), but also data for other systems containing SiO_2 surfaces and molecular ions. Good agreement between our computational results and available experimental data confirms the validity of the method and promotes its further application. In the case of molecular ions, the additional attention will be devoted to Electronic continuum model [2] that serves for accounting solvent polarization effects, which are vital in interactions between ionic species and charged solid surfaces [3].

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A scaling behavior of the transport of multivalent ions through rectifying nanopores

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ABSTRACT

Rectification is an important property of nanopores that have asymmetric geometry. We study ionic transport through bipolar nanopores, where the pore's surface is asymmetrically charged and rectification is present due to the appearance of deeper depletion zones in the reversed biased state of the diode. Our research group previously showed that nano-transistors show similar switching behavior for a given value of $R_{\text{pore}}/\lambda_{\text{D}}$, where R_{pore} is the radius of the nanopore and λ_{D} is the Debye-length of the electrolyte [1]. The Debye-length is the screening length characterizing the thickness of the double layer at a charged wall. The device function (switching) scales with the parameter $R_{\text{pore}}/\lambda_{\text{D}}$, namely, all the points are located along a single curve for a 1:1 electrolyte. The scaling behavior practically means that we get a device that behaves similarly in a narrow nanopore containing a more concentrated electrolyte (smaller λ_{D}) and in a wide nanopore containing a less concentrated electrolyte (larger λ_{D}). The deepness of the depletion zones depends on the degree of double layer overlapping, which, in turn, depends on the $R_{\text{pore}}/\lambda_{\text{D}}$ ratio. Scaling is a useful feature in nanopore design, because it makes prediction of device behavior as a function of tunable device parameters possible. In this work, we extend our study to electrolytes containing multivalent ions (2:1, 3:1, 2:2). Ionic correlations are important in such systems and charge inversion also occurs. We found that scaling is present for given z_{+}:z_{-} values, but the curves as functions of $R_{\text{pore}}/\lambda_{\text{D}}$ are shifted with respect to each other. We show that plotting rectifications as functions of a new rescaled parameter, $R_{\text{pore}}/\lambda_{\text{D}}/(z_{+}z_{-})^{1/2}$, we obtain the same scaling law for the different electrolytes. We use both the mean-field Poisson-Nernst-Planck (PNP) theory, and the Local Equilibrium Monte Carlo (LEMC) method [2] that computes ionic correlations. The differences between the two models are larger for multivalent electrolytes. A better scaling behavior is obtained if we use the screening length as given by the Mean Spherical Approximation (MSA) in LEMC method instead of λ_{D}.

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Ionic liquids with natural terpene derivative as an effective fungicidal and protective preparation for the preservation of historical paper

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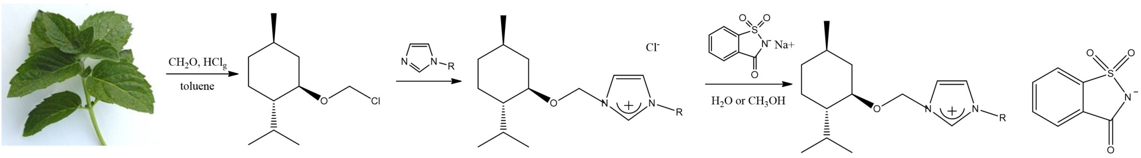
Natural monocyclic terpen alcohol: (1*R*,2*S*,5*R*)-(–)-menthol is obtained from various varieties of mint (*Menthae L.*). Saccharinate sodium is well known sweetener, 300 times sweeter than saccharose. Those two popular commercial compounds have been used to prepare new fascinating ionic liquids. A series of 3-alkyl-1-[(1*R*,2*S*,5*R*)-(–)-menthoxymethyl]imidazolium saccharinates have been obtained by metathesis reaction of proper imidazolium chlorides:



(1*R*,2*S*,5*R*)-(–)-menthol quaternization agent quaternary imidazolium chlorides ionic liquids with sweet saccharinate anion

Obtained salts from methyl to propyl substituent are crystal with low melting points, whereas consecutive saccharinates in homologues series are liquids. Discussed saccharinate salts belong to chiral ionic liquids (CILs) where the chirality resided in the cation and is associated with the presence of optical active (1*R*,2*S*,5*R*)-(–)-menthol.

The physicochemical characteristics of sweet salts was prepared in order to support their future applications. Their surface tension decreases with elongation of hydrocarbon chain attached to imidazolium cation; however at lower T this quantity for higher homologues (from C_9H_{19}) is practically the same. Despite of high viscosities, they reveal a good wetting behaviour of paper, which is more pronounced again for longer chain saccharinates. Antifungal properties of these CILs were tested *in vitro* on mycelium samples isolated from the tested library material from a private collection. The microorganisms included in the study were classified as *Aspergillus Niger van Tieghem, Chaecetomium globus, Penicillium chrysogenum*. Among CILs homologues those with C_6H_{13} and C_9H_{19} chains have fungicidal activity against all strains that were tested. Moreover their protecting properties on Whatman filter and historical paper samples have been investigated. Good penetration, apparent non-staining properties and flexibility improvement along with antimicrobial activity are promising results guarantying further research.

Optical properties of hydrogel fiber membranes

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The application of micro- and nanofibrous artificial tissues and implants is amongst the most heavily researched fields in biomedical science. Such fibrous networks can be synthesized using electrospinning [1]. A special type of fibrous membranes are hydrogel membranes in which the polymer chains inside the fibers are cross-linked. These upon submerging into a solution would not dissolve, but rather swell while taking up the surrounding fluid. Fibrous hydrogel membranes would be perfect candidates for see-through wound dressing where they would enable the monitoring of the healing process. In such applications it is important to investigate the optical properties of these membranes.

Thereby the aim of this study is the synthesis of implants consisting of gelfibers suitable for biomedical and optometrical implementations and the investigation of optical and other physical and chemical properties of said membranes.

The main constituent of the work is poly(succinimide) (PSI), which is an anhydride of poly(aspartic acid) (PASP). The PASP subunits are connected by peptide bonds similar to proteins, thus the polymer is presumably biocompatible. Initially meshes of varying thickness were synthetized by electrospinning PSI/dimethylformamide. The polymer-chains making up the fibers were cross-linked by soaking the meshes in ethanol solution of 1,4-diamino-buthane (DAB). Subsequently the samples were hydrolyzed in an imidazole based buffer of pH 8 whilst creating PASP matrices. The success of the synthesis process was proven using Fourier Transform Infrared Spectroscopy. The fibrous structure of the membranes and the diameter of their constituent fibers were assessed using Scanning Electron Microscopy (SEM). The optical properties of the membranes were determined through light absorption measurements (UV visible light spectroscopy).

We have synthetized fibrous gel membranes with success which had fiber-diameters of about 500-600 nm. During the light absorption measurements we have observed a reduction in light intensity which is not connected to chemical structure but is rather due to light scattering.

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Chemistry and water dynamics at the surface of hydrated magnetite

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ABSTRACT

The application of magnetic nanoparticles as drug carrier in cancer therapy was already proposed decades ago. For such applications, high stability, increased salt tolerance as well as full biocompatibility of nanoparticles have to be ensured. It is thus vital to understand how coating organic ligands as well as drug molecules are bound to the surface to design efficient drug delivery systems. Molecular simulations lend themselves well to acquiring such insight otherwise hardly accessible by experimental techniques. The necessary reliable molecular models for such simulation studies are, however, still missing. In this study, we develop a molecular model through studying the chemical and physical behavior of water, omnipresent in all biologically relevant conditions, at the surface of magnetite.

To this end, first, we carried out detailed first principles calculations to determine how water molecules chemisorb at the surface of the bare (001) 0.5 ML FeA surface of magnetite. We found that the chemisorption of multiple water molecules at both the tetrahedral FeA and the octahedral FeB atoms is favorable. However, not all potential adsorption sites are covered with chemisorbed water molecules.

We then extended our already existing classical magnetite model for the non-hydrated surface by including the chemisorbed water molecules as well as the corresponding bonded and nonbonded interaction parameters derived from our DFT calculations. We assessed the structure and the dynamics of several layers of water molecules in contact with the previously established hydrated (001) surface. In particular, we characterized the structure and the dynamics of water molecules by computing normal and lateral density profiles, orientation preferences of water as well as the typical residence times. Among others, we also found a hydrogen bonded network of water molecules commensurate with both the mineral surface and the bulk hydrogen bonded network of water.

Preparation of Poly(N-isopropylacrylamide-co-4-vinylimidazole) microgel particles

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ABSTRACT

The synthesis of soft, responsive microgel particles has attracted a considerable interest in the last decades [1]. However, to meet the challenges of nanotechnology, there is compelling need to develop synthetic methods for the preparation of microgel particles with novel composition and structure. In this contribution we report a new approach to synthetize poly(*N*-isopropylacrylamide) based microgel particles with imidazole functionalities. Recently, the application of polyvinylimidazole has been considered in various catalytitic reactions, separation methods and diagnostic techniques. In this contribution we present a simple approach for the preparation of both poly(*N*-isopropylacrylamide-co-4-vinylimidazole) (p(NIPAM-co-4VI) copolymer microgels and core/shell microgels of pNIPAm core and 4-vinylimidazole shell to combine the unique properties of smart microgel particles with the functionalities offered by polyvinylimidazole.

The 4-vinylimidazole was generated by the facile decarboxylation of urocanic acid at its vaporization temperature of 220 °C. The copolymer microgel particles were prepared by precipitation polymerization in aqueous solution at 80 °C using *N,N'*-methylenebis(acrylamide) (BIS) as a crosslinker. Both a cationic (V50) and an anionic (ammonium persulfate) initiators were tested for the preparation of the microgels. The temperature and pH dependent swelling of the copolymer and the core-shell microgel particles were determined by dynamic light scattering and correlated with their electrophoretic mobility changes.

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Molecular simulation of kaolinite layer curling

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ABSTRACT

Advanced sorption, catalytic and composite materials can be obtained by delamination/exfoliation of layered clay minerals. The free-standing 1:1 aluminosilicate layers of kaolinite tend to form curled layers or nanoscrolls, in order to minimize the misfit of their tetrahedral and octahedral sheets [1]. According to theory [2], a single kaolinite layer rolls up with the octahedral sheet inside; however, there is as yet no ample experimental evidence to support this curling process. Classical molecular simulations using atomistic force fields (ClayFF [3], INTERFACE [4]) were employed to investigate the behavior of a life-sized model [5] of free-standing kaolinite layers. The simulation results for the curling direction were found to be sensitive to the choice of the force field, cut-off length and long range correction (reaction field or Ewald treatment). The results obtained with the most reliable conditions are consistent with recent TEM imaging [6]. Also, the model layer displayed some tendency to form the experimentally observed twin-tube structure [7].

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Heterocoagulation assisted synthesis of zirconia/graphite oxide nanocomposites

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ABSTRACT

Nano-composites have gained much interest over the past few years. The properties of nano-composite materials depend not only on the properties of their individual parents but also on their morphology and interfacial characteristics.[1] Nanostructured zirconia (ZrO_2) is a less extensively studied semiconductor nanophase material but, because the bulk counterpart is one of the most industrially important materials, it has recently aroused interest owing to its thermal stability, chemical inertness, and concomitant lack of toxicity.[2] Graphite oxide (GO) is one of the most studied material because of a combination of advantageous properties such as tuneable surface charge, hydrophilicity and enormous specific surface area.

Our goal was to combine zirconia nanoparticles (ZNPs) with graphite oxide via preparation of composites by heterocoagulation method. Heterocoagulation is the process in which dissimilar colloidal particles coagulate irreversibly in a suspension that leads to stable coherent structure. An important advantage of this method is that it does not require any harsh conditions. ZNPs were synthesized using three different precursors and the products were treated at 500 and 800 °C. The experiments were carried out with a Hummers-Offeman type graphite-oxide. To prepare the ZNP/GO nanocomposites by heterocoagulation, we had to investigate the optimal pH range. This was accomplished by using potentiometric acid-base titration and zeta potential measurements. The stability of the formed composite samples was followed by DLS measurements and visual observation.

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Selective adsorption of basic compounds from aprotic solvents onto acidic polymers

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ABSTRACT

Synthetic macroporous polymers with pendant carboxylic groups have been investigated. Some of the polymers were prepared by admixing non-polymerizing basic (amine) additives to the pre-polymerization mixture, i.e., these polymers were imprinted with the respective base. The polymers have been used to study the adsorption of different amines from aprotic solvents like acetonitrile and toluene. The selectivity of adsorption was compared between the imprinted polymers and their non-imprinted, but identically composed analogs. The formation of imprinted binding sites was modeled by DFT calculations. These have revealed unusual acid-base interactions in the prepolymerization solvent. A single amine molecule has been found to bind two or more acid molecules by hydrogen bonding. The so formed acid clusters of the acidic monomer (methacrylic acid) become fixed during polymerization and form imprinted binding sites. These binding sites are more acidic than lone carboxylic groups, and this explains the increased binding of amines on the imprinted polymer when compared to the non-imprinted one. The selectivity in the binding of different amines by the same polymer is also influenced by imprinting, but this influence can only slightly modify the inherent selectivity pattern which is also observed with the non-imprinted control polymer [1].

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Tuneable magnetic hyperthermia properties of pristine and mildly reduced GO/MNP nanocomposites

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ABSTRACT

Superparamagnetic iron oxide, i.e. magnetite nanoparticles (MNPs) seem to have great potential for biomedical use (MRI contrast enhancement, targeted drug delivery, magnetic hyperthermia, etc.). Although the MNPs have inherent unique magnetic properties, they should be biocompatibilized, e.g. with carboxylate-type compounds [1] for their application in living systems. Graphite oxide (GO) is a hydrophilic, carbonaceous material, with high surface area and tuneable pH-dependent surface charge properties. Here, we present a study on the magnetic hyperthermia properties of GO/MNP nanocomposites to test the possible enhancement of heat production by tuning the oxidation degree of the carbonaceous host.

Magnetic nanoparticles and the GO nanosheets were combined by heterocoagulation process, which is a mild way to synthesize coherent nanostructures without applying harsh chemical conditions. Nanocomposites were prepared at several GO/MNP mass ratios (1/5, 1/10 and 1/50) and partially reduced by addition of ascorbic and gallic acid at various pHs.

We have found that pristine nanocomposites generated larger heat effects than the suspension containing only MNPs as it was measured 6.8°C and 7.3°C temperature increase for 1/5 and 1/50 GO/MNP, respectively, after 5 minutes of AC magnetic field exposure (109.4 kHz, 24.7 mT) [2] The nanocomposites reduced with ascorbic acid showed slightly enhanced heat production compared to bare MNPs. The temperature increased by 15-25% depending on the GO/MNP mass ratio. However, the gallic acid proved to be more efficient reduction agent, the heat production arose by 140-150 % for 1/5 and 1/10 composites after exposed to magnetic field.

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Synthesis of chemically modifiable p(HEMA)-b-PEG block copolymer

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ABSTRACT

With the emergence of Atom Transfer Radical Polymerization (ATRP) in 1994, the preparation of copolymers with well-defined topologies and composition became possible. [1] In the last two decades numerous possible applications of the prepared polymers could be seen in the field of automotive, medical or military applications. [2] One of the biggest advantages of ATRP is the possibility to control the composition of block copolymers from monomer to monomer. However, the use of monomers with reactive functional groups can lead to uncontrolled reactions, which results in low quality polymers. [3] Furthermore, to synthetize high quality polymers with low polydispersity, it is always necessary to optimize the reaction procedure which might take enormous efforts both in time and costs.

The aim of our work was to develop a di-block copolymer with a hydrophilic and a reactive block, which can be easily modified to prepare a wide range of functionalities. To reach our goals a monomer with a moderately reactive functional group was chosen (2-hydroxymethacrylate; HEMA) and the ATRP procedure of this monomer on a PEG macromonomer was optimized. Since the HEMA monomers contain chemically accessible hydroxide groups, we used an acid chloride reagent to introduce pending alkyne groups along the backbone in controlled amount. The prepared diblock copolymers were suitable for further modification through a straightforward alkyne-azide click reaction and allowed the preparation of a wide range of functional block-copolymers.

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Synthesis and biological properties of new mild amidebetaine and amidesulfohydroxybetaine-type amphoteric surfactants

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ABSTRACT

Amphoteric surfactants, an important group of fine chemicals, are known to exhibit surface activity in a wide range of pH, compatibility with all other classes of surfactants and mildness [1,2]. The combination of both amphoteric polar part and labile linking groups between hydrophobic and hydrophilic parts is the most significant structural feature of amidobetaine and amidosulfobetaine-type surfactants and enables them to possess unique properties and applications as detergents, mild antimicrobial agents as well as rheology modifiers in many application fields. In our study, we report on the synthesis, *in vitro* antimicrobial activity and hemolytic action of novel amidebetaine and amidesulfohydroxybetaine type surfactants with different hydrophilic head groups, i.e., [(3-alkanoyilomethyoamine)propyl] dimethylammonium acetates and [(3-alkanoyilomethyoamine)propyl] dimethylammonium 2-hydroxypropanesulfonates. The mentioned surfactants were synthesized in the multistep processes, comprising condensation of appropriate fatty acid derivative with N,N,N'-trimethyl-1,3-propanediamine, followed by quaternization with sodium chloroacetate or sodium 3-chloro-2-hydroxy-1-propanesulfonate, respectively. The performed experiments showed mild antimicrobial activity of the newly synthesized surfactants against selected Gram-positive and Gram-negative bacteria as well as yeast strains. Their hemolytic ability was negligible as well.

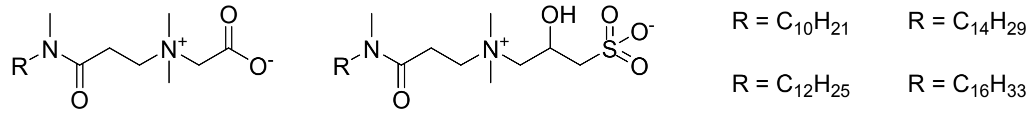

Fig. 1 Chemical structures of the studied betaine and sulfohydroxybetaine type surfactants.

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Dynamic properties of aqueous solutions of atomic and molecular ions – effect of scaled charges

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ABSTRACT

Dynamic properties of liquids have been of principle interest in a wide range of applications. Thus water, as the most important solvent in our environment, represents a principle subject for molecular dynamics simulations. Dynamic properties of aqueous solutions include diffusivity of water and ions as well as viscosity of the solution.[1]

It is now well known that full charge models significantly overestimate electrostatic interatomic interactions of multivalent ions due to lack of electron polarization. Thus, electronic continuum correction (ECC) method has recently been developed improving the structural characteristic. In this case, atomic charges are scaled down e.g. to 0.75 of their usual (commonly RESP) charges.[2,3]

In this study, we focus on the diffusion coefficients determination for atomic and molecular ions (e.g. Na^+, Cl^-, Ca^{2+}, Sr^{2+}, SO_4^{2-}, oxalate). We study dynamic properties of aqueous solutions containing ions modelled with both full charges and scaled charges. We also investigate the viscosity of aqueous solutions employing the non-equilibrium molecular dynamics simulation.

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Preparation of multilayer “smart” nanocapsules

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ABSTRACT

At the beginning of the 1990s, Decher prepared polyelectrolyte multilayers on flat surfaces by utilizing the alternating adsorption of oppositely charged polyelectrolytes using a simple dip-coating method [1]. Later this approach was extended to the preparation of polyelectrolyte multilayers on a wide range of nanoparticles. In this case the solution of a charged polyelectrolyte was added to an oppositely charged nanoparticle dispersion in access then the polyelectrolyte coated nanoparticles were separated from the surplus of the polyelectrolyte with centrifugation. Then another oppositely charged polyelectrolyte was added to the nanoparticle dispersion to form the next polyelectrolyte layer. This procedure was repeated until the desired number of polyelectrolyte layers was formed.

The goal of our work was to prepare polyelectrolyte multilayer coated “smart” nanocapsules, which consist of a temperature responsive core and a polyelectrolyte multilayer shell. As a first step we synthetized core/shell microgel beads that poses a crosslinked temperature responsive poly(*N*-isopropylacrylamide) (pNIPAm) core and a shell of poly(sodium 4-vinylbenzenesulfonate) (NaPSS). To achieve this goal we used a single-pot polymerization method developed recently in our laboratory. This method allows the formation of hydrophilic polymer shells with unrestricted composition on a pNIPAm-based core. To monitor the formation of the core/shell microgels we measured the monomer conversion during the particle synthesis and the evolution of the temperature dependent swelling and electrophoretic mobility in various stages of the formation of the core/shell particles.

The high charge density polyelectrolyte shell facilitated the efficient creation of polyelectrolyte multilayers on the neutral temperature responsive core. Since the polyelectrolytes do not bind in the core of the microgels we hypothesized that the temperature dependent swelling of the multilayer coated gel particles remains unaffected by the multilayer formation. Swelling data for the multilayer coated gel particles will be presented as a function of the number of the coating polyelectrolyte layers.

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Damage formation in weak planar fiber texture

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ABSTRACT

Electrospun nano- and micro-fiber networks have attracted an intensive research area over the past decades, due to their high mechanical performances and low weight. Although the electrospinning technology is well developed, little is known on the deformation mechanism of electrospun fiber networks. For biomedical applications damage accumulation, fraction and nonlinear mechanical behavior are important characteristics of the fibrous materials.

The fundamental mechanical properties were studied by unidirectional strain-controlled stretching on fibrous electrospun networks prepared from polysuccinimide. Polysuccinimide is the anhydrous form of poly(aspartic acid), so the networks are biocompatible and biodegradable, ideal for several biomedical applications like scaffold for cell proliferation and artificial extracellular matrix. 2D randomly oriented fibre mats were prepared from the polymer solution, made with dimethylformamide, using a home-made electrospinning instrument.

The experimental loading curve shows a symmetrical parabolic type dependence at large scale and saw tooth-like force–extension behaviour at small scale. The damage formation was quantified by determining the number and the magnitude of abrupt force drops. The experiments evidenced that damage evolution is a consequence of strain induced random events, which are may caused by failer and rupture of fibers. The frequency distribution of the number of damages as well as the magnitude of rupture force were represented by histograms. [1]

The results of the present study provide a better insight into damage tolerance and complex nonlinear tensile properties of electrospun networks. In addition, it could suggest a possible probabilistic approach to the fiber bundle model which has mainly motivated this study.

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Wettability characterization of carbon cloth type gas diffusion layer via infrared thermography and contact angle analysis

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ABSTRACT

Fuel cells are possible alternatives to replace the fossil fuels. The wetting properties of the Gas Diffusion Layers (GDL) are important to know because these can influence the performance of the fuel cells. GDLs have to possess appropriate hydrophilic-hydrophobic features, in order to sufficiently wet but to avoid of “flooding”. During our research the wetting properties of carbon cloth type GDL (against alcohol-water mixtures) were studied by infrared (IR) thermography simultaneously with mass measurement at 60 °C [1]. Static and time-varying contact angles can give further information about the wetting or non-wetting features and about the wetting transition. Some morphology characterizations were carried out on the sample with Scanning Electron Microscopy, X-Ray Micro Tomography and Profilometry measurements. The surface roughness and Teflon® content cause the hydrophobic nature of the carbon cloth.

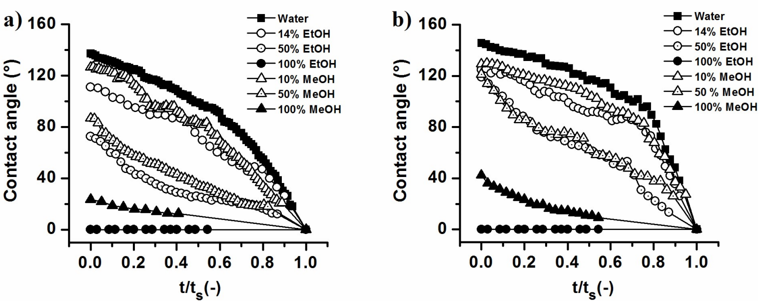

Figure 1. Time-varying contact angles of various solvents on the microporous layer side (a) and uncoated bottom side (b) of the carbon cloth type GDL sample

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Modeling of pH tunable nanodevices

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ABSTRACT

The pH of an electrolyte is an experimentally controllable parameter: pH affects the ratio of the protonated/deprotonated forms of the functional groups anchored to the inner surface of the nanopore. Change in the surface charge, in turn, changes the conductance properties of the pore that makes it possible to use nanopores as sensors [1], diodes, or transistors [2,3]. We relate the surface charge to pH and perform particle simulations (Local Equilibrium Monte Carlo [4]) to compute the ionic flux. Here we present results for two model nanodevices: transistors and sensor. In the case of a *transistor* the current is considerable in the "acidic" and "basic" regions, because the pore contains *either* positive *or* negative surface charges, so *either* anions *or* cations carry current. Current is very small in the "neutral" region, because the pore contains *both* negative *and* positive surface charges, so *both* cations *and* anions have depletion zones. This switch like behavior is controlled by the pH-dependent surface charge pattern. The behavior of our pH-responsive models is characteristically different in the different pH regions. *Nanosensors* selectively bind the analyte ions with which the ionic current flowing through the pore is changed because the local concentrations of the ions of the background electrolyte changes. The analyte concentration can be determined from calibration curves. Inspired by experimental works in the field of nanosensing we constructed asymmetric nanopores with various charge patterns to mimic the pH tunable behavior. The geometrical asymmetry produces an additional device function, rectification, resulting in a dual responsive device. The mechanism behind pH-control of ionic current can be explained by formation of depletion and accumulation zones.

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Electrospun magnetic scaffold for theranostics

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ABSTRACT

Various polymers are used in medicine for a great variety of applications. With the help of electrospinning technology artificial matrices can be created with a fibre diameter like in the living organism. Superparamagnetic nanoparticles can heat the surrounding environment if an alternating magnetic field is applied. Since cancer cells are more sensitive to the temperature increase than healthy cell lines, magnetic hyperthermia is a promising therapeutic method in cancer healing. However, the Magnetic Resonance Imaging (MRI) is also using magnetic nanoparticle to increase the contrast effect between the different tissues. The resulting fibrous mesh merges the unique properties of magnetism and elasticity.

Thus our research is focusing on creating and investigating artificial matrices from biocompatible and biodegradable polymers which contain magnetic nanoparticles as a therapeutic and diagnostic agent.

Poly(aspartic acid) could be a good candidate for medical application. With the help of electrospinning, we created artificial matrixes with a fibre diameter in the nanometer range, loaded with magnetite particles. The artificial matrices were examined with SEM, FTIR, SQUID and the iron content was determined by UV-VIS spectrometer. The magnetic hyperthermic and the magnetic resonance contrast enhancing effect was determined with Magnetherm 1.5 and nanoScan PET/MRI (1T) instruments, respectively.

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List of Presenters