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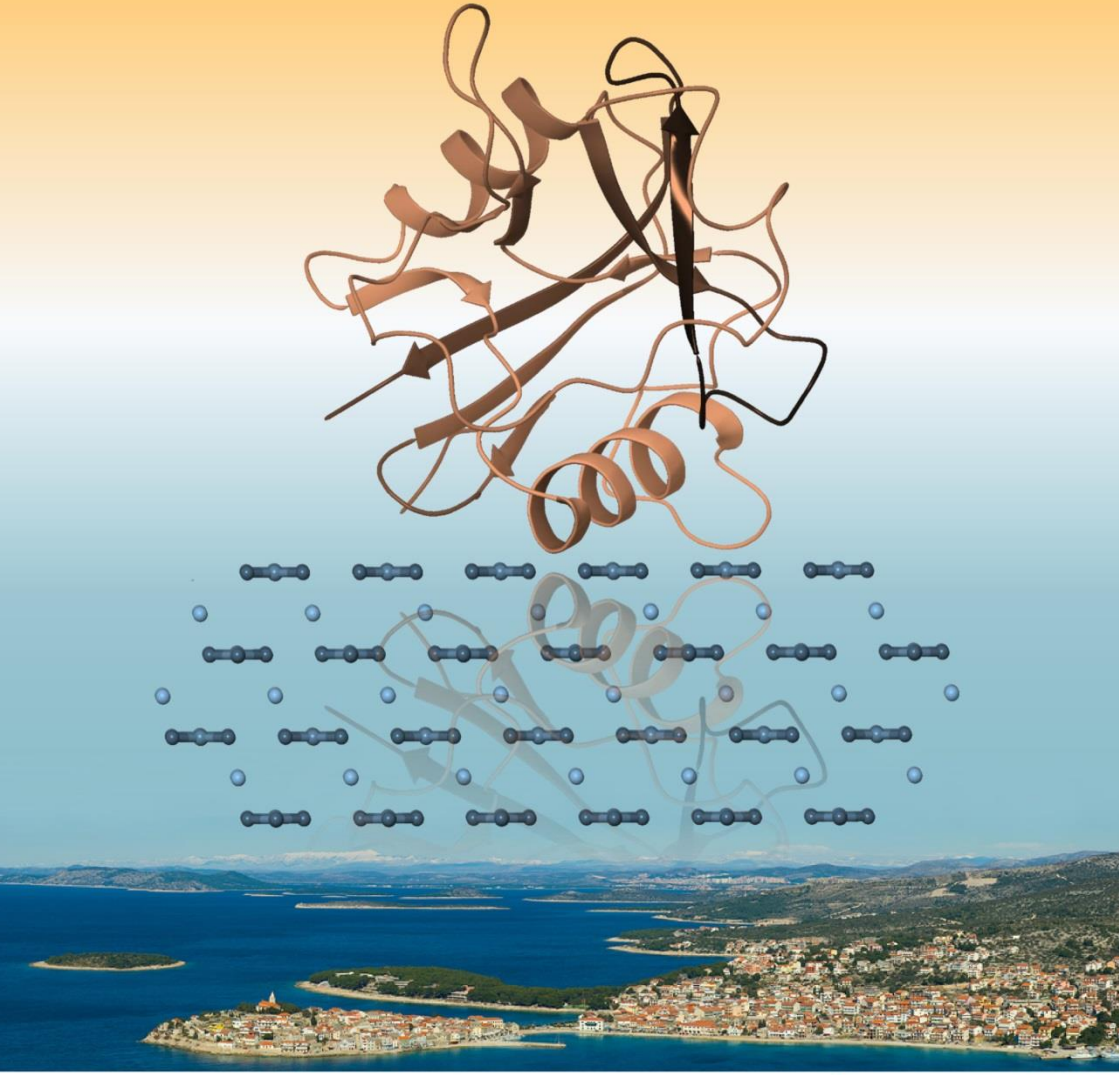
Workshop Innovative Surfaces and Materials

August 28 to 31, 2016, Primošten, Croatia



Ruđer Bošković Institute

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MIPoMat

Workshop Innovative Surfaces and Materials 2016

Sunday, August 28th – Wednesday, August 31st 2016

Welcome to the workshop Innovative Surfaces and Materials organized within the context of the project Networks for professional training of young scientists in interdisciplinary research of innovative surfaces and materials (MIPoMat).

The workshop is organized with objectives to bring together researchers – experimentalists and theorists from various areas of physics and chemistry who share a common interest in the study of the kinetics of heterogeneous processes, structural analysis, characterization of surfaces, organic synthesis, molecular modeling and application of absorption-emission spectra of biomolecules near the surfaces.

Promoting breakthrough of modeling molecular and nanostructures, to complex functional systems, this workshop aims to reach the sphere of applied research. Namely, synthesized targeted materials of advanced properties, fundamentally changed the world of electronics, optics and communications, and medical and pharmaceutical industries. Innovations starting at the atomic level affect the whole process of creating the material.

The properties of advanced materials are not only about the chemical nature of the atoms of which they are composed, but are primarily determined by their three-dimensional arrangement and layout within the microstructure of materials, including defects. Therefore, in this workshop all levels of the research chain are included, from design and synthesis of materials on the nanoscale, to modeling, structural characterization and possible manipulation.

Contents

Workshop Schedule

Sunday, 28.08.

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15:10	Plenary Lecture I: Sabine Maier
	On-Surface Synthesis and Self-Assembly of Molecular Nanostructures: From Metal to Insulator Surfaces
15:55	Tajana Preočanin
	Charging of Solid Surface / Aqueous Interface: Surface Potential Measurements
16:30	Break
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17:00	Milena Petković
	Formation and Oxidation of a P-$C_{carbone}$ Bond
17:35	Aurora Ponzi
	TRPES as a Probe for Ultrafast Excited State Dynamics: an Exploratory Investigation of Furan
18:00	Jurica Novak
	Photodynamics of Retinal Chromophore-Counterion Pairs
18:25	Marin Sapunar
	Nonadiabatic Dynamics and Photoelectron Spectroscopy Simulations of Pyrrole
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Monday, 29.08.

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09:45	Christian R. Wick *Semiempirical MO-Theory for Large Systems*
10:10	Chiara Panosetti *Better (Random) Walking Through Chemistry: How Not to Get Lost in Vast Configurational Spaces*
10:35	Break
11:00	Janez Mavri *How are Biogenic Amines Decomposed by Monoamine Oxidases: Lessons from Multiscale Simulation*
11:35	Jernej Stare *Reaction Pathway Sampling by Empirical Valence Bond Simulation: From Gas Phase to Enzymes*
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16:05	Ines Despotović *Pyridine-Based Macrocyclic Compounds as an Efficient Tool for the Metal Cation Binding*
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17:00	Sonia Coriani *The Molecular Response to Electromagnetic Fields: A Wonderful Playground for a Computational Chemist*
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18:25 Antonio Prlj
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Acetylacetone Femtochemistry at FERMI-LDM

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10:10	Lara Štajner *Interaction between Calcium Carbonate and Selected Amino Acids*
10:35	Robert Stepić *Theoretical Study of Amino Acid-Calcite Interface*
10:55	Break
11:30	Davor Kovačević *Polyelectrolyte Multilayers: Properties and Applications*
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17:10	Yaroslava Lykhach *Model Catalysis with Ionic Liquids*
17:35	Daniel Berger *Multiscale Simulation of SILP Catalysis*
18:00	Christof Jäger *Towards Engineering Radical SAM Enzymes – Insights into Biocatalysis and Biomaterial-Ionic Liquid interactions*
18:25	Nataša Vučemilović-Alagić *Ionic Liquids at Interfaces*
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Chair: Ana-Sunčana Smith

20:15	Plenary Lecture VI: Jens Harting *Soft Particles at Fluid Interfaces: the Interplay of Deformability and Surface Tension*
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09:35	Maryam Aliee *Interaction of Polarity Fields Driving Pattern Formation in Tissues*
10:00	Robert Blackwell *A Biophysical Model for the Formation of Mitotic Spindle Bipolarity*
10:25	Sara Kaliman *Formation of Epithelial Tissues on Inorganic Functional Surfaces: Space Tessellation on Micro and Macro Scale*
10:45	David M. Smith: Closing Remarks
11:00	DS: Ionic Liquids / Free Time
12:30	Lunch

Lectures

On-surface synthesis and self-assembly of molecular nanostructures: From metal to insulator surfaces

Sabine Maier

Department of Physics, Friedrich-Alexander-University Erlangen-Nürnberg

The interest in molecular nanostructures on surfaces emerges from their prospective applications in nanoscale electronics, solar cells, energy storage devices, and other fields. The self-assembly of organic molecules on surfaces relies on non-covalent intermolecular interactions and facilitates the formation of long-range ordered patterns. In recent years, the on-surface synthesis of covalently-linked molecular structures has emerged as a route to prepare more stable and atomically well-defined nanostructures. The ability to control these chemical reactions to grow well-ordered two-dimensional networks is still limited due to the irreversible nature of the newly formed covalent bonds, which prevents an error correction.

Here, I will review recent results on the self-assembly and on-surface synthesis of molecular structures built from carefully designed functionalized triphenylamines on metal and insulator surfaces based on high-resolution scanning probe microscopy experiments complemented by density functional theory. First, hierarchic formation principles of covalently-linked nanoporous networks through surface-assisted Ullmann coupling reactions are shown on Au(111). Design rules to potentially overcome the lack of long-range order in such networks will be discussed together with their electronic properties and host-guest chemistry. In the second part, electronically decoupled molecular self-assemblies on bulk insulators are presented. We show how intermolecular and molecule-substrate interactions can be tuned by functional groups on KBr(001) and MgO(001) in order to achieve one-, two- or three-dimensional assemblies in a controlled way.

Charging of solid surface / aqueous interface: Surface potential measurements

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Electrostatic potential at the inner surface plane is the consequence of the charge (ion/electron) transfer at the electrical interfacial layer and is therefore one of the main parameters characterizing the interface [1]. Inner surface potential could be measured by Single Crystal Electrodes (SCrE) [2] and provide information on the state of charged groups bound to the surface. In addition, together with adsorption and electrokinetic data, inner surface potential may serve in evaluation of equilibrium parameters. For some metal oxide crystal planes the measured surface potential and electrokinetic potential give unexpected results [3]. While the measured inner surface potential is zero, the electrokinetic measurements for the same particular crystal plane provide a higher (absolute) values of the zeta potential. This finding could be explained by considering the pH dependent charging of the interfacial water layer *via* protonation or deprotonation, resulting in the presence of physically adsorbed hydronium or hydroxide ions. While the pH of the electrolyte solution affects the electrokinetic behavior but not the surface potential, the specific adsorption of strongly bound ions to oxide surfaces affect both the inner surface and zeta-potentials. The SCrE is the framework to study the more complex, environmentally significant, charge transfers occurring at the charged interfaces.

Acknowledgements: This work is supported by Croatian Science Foundation under the project (IP-2014-09-6972).

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Formation and oxidation of a P-$C_{carbone}$ bond

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Due to the presence of two lone pairs on the carbon atom, carbone molecules are highly nucleophilic spiecies, which can act both as reducing agents and ligands in synthesis of electron deficient systems. Carbodiphosphorane $C(PPh_3)_2$ undergoes carbon-for-chloride ligand exchange in a series of reactions with dichlorophosphines, except with $MeN(PCl_2)_2$. Density Functioal Theory was used to explain P-N bond cleavage observed in the later reaction, and it was shown that it proceeds *via* an S_N2'-like mechanism [1].

We have analyzed another system with a P-$C_{carbone}$ bond, oxophosphonium dication $[(Ph_3P)_2C(N\mathit{i}Pr_2)P(O)(O\text{-}py)]^{2+}$ [2], which undergoes oxygen insertation into the P-C bond and represents the first example of a Baeyer-Villiger oxidation that involves O-py. The intermediate in this reaction is identified to be Criegee-like, which is not characteristic for Baeyer-Villiger mechanisms.

Acknowledgements: This work is supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (MP, project 172041) and by the A*STAR-MSHE grant (DV, # 1220703062). Numerical simulations were run on the PARADOX cluster at the Scientific Computing Laboratory of the Institute of Physics, Belgrade (project ON171017).

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TRPES as a probe for ultrafast excited state dynamics: an exploratory investigation of furan

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The present work is focused on the photoionization of furan from the ground state and from the two lowest-lying excited states. This molecule represents a prototypical biomolecular chromophore; together with pyrrole and thiophene, its photochemical and photoionization properties are of great interest due to an extensive collection of available experimental and theoretical results [1].

This work is part of a wider project which concerns a high level theoretical description of Time-resolved photoelectron spectroscopy (TRPES) observables obtained from pump-probe experiments. In particular, we combined photoionization observables calculation, using Dyson orbitals, with trajectory-based nonadiabatic dynamics calculation of prototype chromophores. The final goal will be an accurate and computationally efficient simulation of TRPES experiments.

The use of Dyson orbitals, recently implemented [2], allows the description of ionization from excited states at the single channel level, and a correlated description of the initial and final ionic bound states. The Dyson orbitals were computed at the TDDFT, ADC(2) and CASSCF levels. The high quality calculations of the photoionization dynamical observables are performed via an accurate solution of the continuum one particle wavefunctions in a multicenter B-spline basis at the DFT level [3], which provides an adequate description of the electronic continuum. The approach can be conveniently used to provide results for a series of snapshots along the trajectories generated.

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Photodynamics of retinal chromophore-counterion pairs

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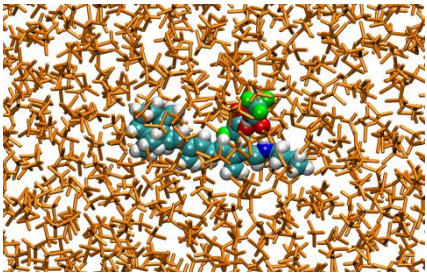
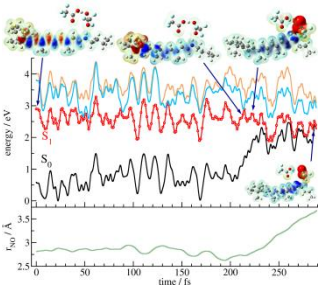
The fundamental understanding of photochemical processes of complex biomolecular systems like retinal is only one piece of puzzle in understanding the Nature and one step closer to the construction of artificial biomimetic light driven photo-switches.

Quantum-mechanical anharmonic frequency calculations confirmed the existence of two types of aggregates between protonated all-*trans n*-butylamine Schiff base of retinal (*n*SBR$^+$) and the hydrogen bonded trifluoroacetic acid counterion [1]. Using nonadiabatic dynamics simulations of the chromophore-counterion pairs in the dichloromethane, it is shown that the relaxation processes that set in after photo-excitation involve as a decisive step a formation of an inter-molecular charge transfer state *via* hole translocation from the retinal backbone to the counterion. In solution, this leads to dissociation of the chromophore-counterion pair and abortion of the photoisomerization, but constraining the distance of a counterion results in increasing biologically active C13=C14 bond length. Simulations of solvated *n*SBR$^+$ reveal rotations around formally single bonds as a non-reactive channel [2].





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Nonadiabatic dynamics and photoelectron spectroscopy simulations of pyrrole

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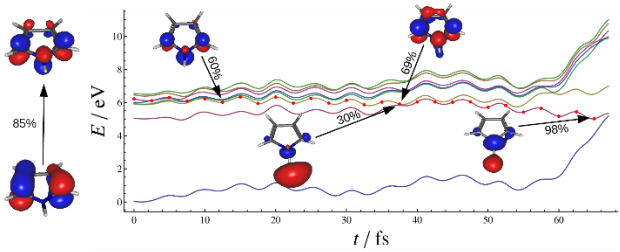
Pyrrole is a prototype example of a molecule displaying $\pi\sigma^\star$ mediated internal conversion. Recent experiments have shown that the time scale of this process is dependent on the wavelength of the initial excitation [1]. To better understand this effect, we have performed nonadiabatic surface-hopping dynamics simulations of the relaxation of pyrrole following excitation in three different energy regions [2].

The primary state populated in the ≈ 200 nm wavelength region is the lowest B_2 state. Historically, this state has been described both as a pure Rydberg $3p_x$ state and as a pure $\pi\pi^\star$ state. We have shown in our simulations that the results of the dynamics simulations are highly dependent on the description of this state in the chosen electronic structure method. We also suggest photoelectron spectroscopy as another experimental observable which is sensitive to the electronic structure of this state and can be used to confirm the validity of the theoretical results.



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Local properties in simulations of charge transport

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It is now possible to treat up to 100,000 atoms with semiempirical molecular orbital (MO) theory.[1,2] This allows us to simulate charge transport through crystals,[3] in self-assembled monolayers (SAMs) [4] or across domain boundaries by using local ionization energy [5] and electron affinity [6,7] as the external potential in specific simulations of the quantum movement of the holes or electrons, respectively.[8] The charge-transport paths obtained with these techniques agree with each other and with calculations based on Landauer theory using the semiempirical wavefunction.[9]

Examples of simulations of crystals and SAMs will be given after a short outline of the theory and practice of MO calculations on very large systems.

Acknowledgement: This work is supported by the *Deutsche Forschungsgemeinschaft* as part of the Excellence Cluster "*Engineering of Advanced Materials*".

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Semiempirical MO-Theory for Large Systems

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We present a comparison of conventional semiempirical wavefunction based MNDO-like methods and approximate linear-scaling methods for large molecules. Until recently, linear-scaling methods such as divide and conquer (D&C)[1] or localized-molecular-orbital (LMO)[2] techniques were essential for the treatment of large systems by means of semiempirical MO theory. However, conventional full SCF calculations based on a massively parallel code (EMPIRE[3]) now allow very large systems to be treated without local approximations. The comparison revealed a very slow SCF convergence for gas-phase calculations on zwitterionic proteins using a full SCF routine, whereas LMO SCF converges rapidly. Further comparative calculations with both techniques showed that the very slow inductive charge-transfer process that made the conventional SCF calculations so slow to converge is prevented in the LMO-SCF scheme. Therefore, the LMO procedure can lead to artificially over-polarized wavefunctions in gas-phase calculations. Example molecules have been constructed to demonstrate this behavior.[4] Further, recent applications of semiempirical MO-theory in the field of Self-Assembled Monolayer Field-Effect Transistors (SAMFETs) are presented.[5]

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Better (random) walking through chemistry: how not to get lost in vast configurational spaces.

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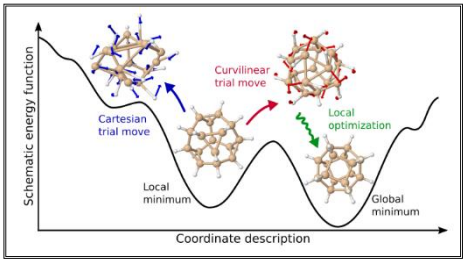
Ab initio structure prediction can systematically aid computational discovery and rational design of new materials, as well as provide interpretative insights when atomistic details are difficult to resolve experimentally. However, global geometry screening–the method of choice for finding relevant (meta-)stable structures–is rarely applied to large-scale systems. The main challenge lies in the necessity of efficient ways to traverse configurational spaces where the number of minima explodes with system size. We recently adapted the Basin Hopping scheme [1] to perform its random trial atomic displacements in collective, automatically generated curvilinear coordinates. The physical correspondence of these coordinates with vibrations naturally facilitates the generation of chemically meaningful trial structures for covalently bound clusters [2]. Concomitantly, we observe a significantly increased efficiency in identifying low-energy structures and a reduction of unphysical geometries when compared to the same number of typical random Cartesian trial moves. Following the *fil rouge* of the exploitation of chemical connectivity, we further extend this to the study of organic molecules on surfaces–by suitably imposing partial constraints–and complex interfacial systems with variable or unknown stoichiometry–by applying strategies to alleviate the strain of newly generated structures upon grand-canonical particle insertion. A selection of prototypical results will be presented to illustrate how all relevant portions of chemical space can be accessed in this approach, whereas "conventional" sampling often even struggles to produce sensible structures besides starting geometries at all.



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How are Biogenic Amines Decomposed by Monoamine Oxidases: Lessons from Multiscale Simulation

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Monoamine oxidase (MAO), which exists in two isozymic forms, MAO A and MAO B, is an important flavoenzyme responsible for the metabolism of biogenic amines such as dopamine, serotonin and norepinephrine. In this work, we present atomic details of the rate-limiting step of dopamine degradation by MAO B, which consists of the hydride transfer from the methylene group of the substrate to the flavin moiety of the enzyme. This contribution builds on our previous quantum chemical study of the same reaction using a cluster model [1], but now considering the full dimensionality of the hydrated enzyme. Well converged activation free energies were calculated by employing the empirical valence bond (EVB) approach of Warshel and coworkers [2]. We show that the MAO B enzyme is specifically tuned to catalyze the hydride transfer step from the substrate to the FAD prosthetic group and that it lowers the activation barrier by 12.1 kcal/mol compared to the same reaction in aqueous solution, a rate enhancement of more than 8 orders of magnitude [3]. The calculated barrier in the enzyme of 16.1 kcal/mol is in excellent agreement with the experimental value of 16.5 kcal/mol. Path integral calculation of H/D kinetic isotope effect for MAO B will be discussed [4]. Preliminary results for simulation of MAO A catalyzed decomposition od noradrenaline will be given [5] and the effects of MAO A point mutations on decomposition of phenylethylamine will be presented [6]. Relevance of MAO inhibition for prevention of neurodegeneration will be discussed [7].

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Reaction Pathway Sampling by Empirical Valence Bond Simulation: From Gas Phase to Enzymes

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When chemical reactions are treated by theoretical approaches, the issue of reaction phase space sampling commonly emerges. While substantial evidence suggests that for enzymatic reactions the complete sampling is beyond the reach of simulations (requiring millisecond timescale of for fully converged free energy profiles), little is known about the criteria for the completeness of sampling. Simulation in the free space allows for considerably longer timescales, possibly providing clues for the acquisition of converged reaction profiles and revealing the factors that govern the sampling quality.

We presently studied a biomolecular reaction in the gas phase, namely phenylethylamine oxidation by lumiflavin (see above), which plays an important role in the pharmacology of the central nervous system. We performed reaction simulation using the free energy perturbation sampling technique coupled with the Empirical Valence Bond method for the calculation of free energy profiles. Factors governing the convergence of the profiles were analyzed in detail, revealing that convergence can be attained only when reversibility of the slowest processes accompanying the reaction is achieved, thereby improving the sampling quality in the transition state region. For the present reaction the required simulation time reaches about 20 microseconds. Geometry restraints commonly used in simulations somewhat improve the convergence, but at the expense of greatly reduced phase space. A comparison was made between unrestrained and restrained simulation in the gas phase, confronting the results with the simulation of the same reaction within the active center of monoamine oxidaze, an enzyme catalyzing oxidative degradation of neurotransmitters. We conclude that the use of restraints is essential to obtain reasonable free energy profiles of enzymatic reactions, but one needs to be aware of the phase space sampling limitations currently preventing from reaching completeness. Geometric features of the reaction in the gas phase provide valuable guidelines for the design of simulations within the enzyme.

Reduction of Ribonucleotide in Prebiotic Conditions

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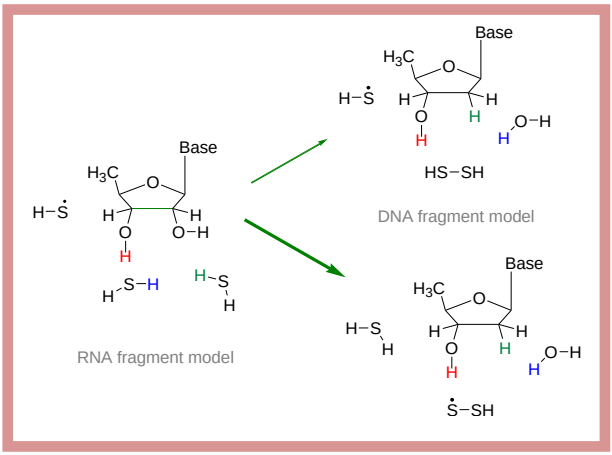
The prerequisite for creation of the first living organisms on Earth was the existence of a "molecules of life" such as nucleic acids, amino acids and sugars. Model studies of prebiotic chemistry have revealed persuasive routes for the formation of the building blocks of proteins and RNA, but not DNA. Nowadays, the deoxyribonucleotides required for the construction of DNA are formed in reduction of ribonucleotides catalyzed by radical enzymes ribonucleotide reductases.

This work considers potential non-enzymatic routes *via* intermediate radicals for the ancient formation of deoxynucleotides. We will present several computationally modeled mechanisms of ribonucleotide reduction without the presence of enzymes.



Perspectives in studying free radical-surface interaction by synchrotron radiation

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Short-lived radicals are often key reaction intermediates in processes occurring in the gas phase as well as at the gas-surface interface, which are important in various fields of chemistry, physics, and material sciences, such as heterogeneous catalysis, surface and nanostructure functionalization, environmental chemistry etc. The characterization of the inner-shell electronic structure of these intermediates can allow identification of transient surface species in complex processes, thus contributing to shed light into the reaction mechanisms [1,2]. Methods for generating hyperthermal reactive free radicals (e.g. allyl [3], ethyl, methyl [4], etc.), their experimental and theoretical study by soft x-rays synchrotron radiation [3,4], and recent developments achieved in our group aiming at studying in future experiments fundamental aspects of the interaction between hyperthermal radicals and surfaces (e.g. fullerenes, graphene, SWCNT) in ultra-high vacuum, will be described. Recent theoretical studies on simple radical-surface model systems pertaining to the subject will also be reviewed.

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Pyridine-Based Macrocyclic Compounds as an Efficient Tool for the Metal Cation Binding

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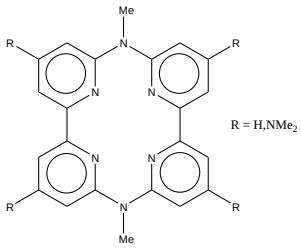
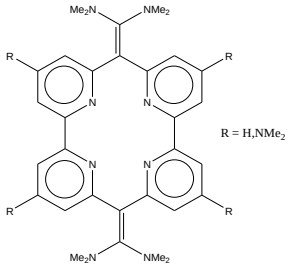
Macrocyclic ligands have ability to bind metal ions selectively, which has proved to be very useful in ion transport, chemosensing, metalloenzyme mimics, catalysis, and nuclear west treatment [1]. Among a large variety of macrocycles synthesized as scavengers of metal ions those containing pyridine building fragments have attracted considerable attention. Introduction of the pyridine moiety strongly influences the thermodynamic properties by increasing conformational rigidity and changing their basicity.

Here, we discuss the complexation of conformationally rigid, pyridine-based, four-fragment macrocycles [2] with the some alkali (Li^+, Na^+ and K^+) and doubly-charged alkaline earth (Be^{2+}, Mg^{2+} and Ca^{2+}) metal cations in the gas phase and in acetonitrile solution.





Gas phase molecular structures and complexation energies were calculated by the B3LYP/6-311+G(3df,2p)//B3LYP/6-31G(d) method. The solvent effects were assessed using the polarized continuum method (PCM). It has been shown that investigated macrocyclic compounds are good complexing and very selective ligands exhibiting gas phase cation affinities laying in the range between 58.5 kcal mol^{-1} and 553.8 kcal mol^{-1}.

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The Molecular Response to Electromagnetic Fields: A Wonderful Playground for a Computational Chemist

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The interaction of matter with light is at the heart of spectroscopy and a fundamental way of probing, characterizing and manipulating molecules in complex environments. The molecular response to electromagnetic fields in a variety of macroscopic media is also an important property per se, as exploited, for instance, in multi-photonic imaging, photonics, electronics, light harvesting.

This has prompted the development of computational methodologies that can model the response of molecules in complex environments and in a broad frequency range. Further development of such methodologies is granted by the continuous development, over the last few decades, of increasingly sophisticated experimental techniques, as exemplified by the advances in synchrotron, laser and detection technology, which will allow probing the properties of matter in ways and/or regions hitherto unexplored.

In my talk, I will present an overview of my past, present and perspective research dedicated to the development and application of reliable computational methods to rationalize the interaction of electromagnetic radiation with matter, and hereby investigate the electronic structure and microscopic properties of materials, as well as rationalize and validate novel experiments.

Structure-related fluorescence and proton delocalization in amyloid proteins

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Peculiar optical properties, including absorption of low-energy photons (3.5 eV) and fluorescence in the visible range in the absence of aromatic amino acids, has been recently found in amyloid fibrils - protein aggregates rich in beta-sheet structures interconnected by a network of hydrogen bonds [1]. Fluorescence spectroscopy experiments indicate strong sensitivity of the fluorescence to both pH and to the change of isotope. Using state-of- the-art ab initio molecular dynamics simulations of large model systems of the fibrils, we find evidence for proton hopping between the N and C termini of the beta strands. The proton transfer events appear to be coupled to subtle changes in the optical properties as gauged by TD-DFT calculations used to characterize the excited states [2]. Results suggest fluorescence is controlled by subtle changes in the vibrational degrees of freedom involving proton transfer processes, potentially shutting off non-radiative decay mechanisms. Our results thus point to an unconventional, structure-related chromophore, where extended conjugation is not anymore a prerequisite for the observation of fluorescence in the visible range. Besides, we found nuclear quantum effects are likely to play an important role at room temperature. Further computational investigations on smaller model systems are now in progress to specifically address the excited state dynamics.

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Coherence and ionic state produced after multiphoton molecular ionization

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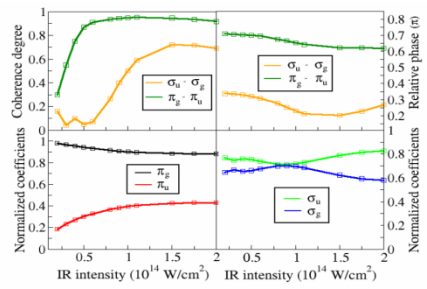
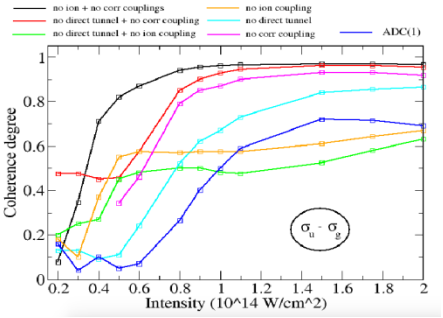
The groundbreaking development of the attosecond laser pulse [1] in the extreme ultraviolet (XUV) spectrum where atoms and molecules can be ionized has enabled the experimental study of attosecond physics [1]. After photoionization the molecular ion can undergo an internal non-trivial dynamical evolution, which may take the form of hole-migration [2] where a localized hole charge density oscillates between different sites of the molecule with a period of a few femtoseconds. The coherence of the resulting ionic system and the knowledge of the nature of the initial ionic wavepacket produced after ionization is crucial to the theoretical interpretation of the hole migration dynamical information that can be obtained in time-resolved (pump-probe) experiments. In this work we introduce a novel fully ab-initio tool for solving the 3-D many-body time-dependent Schrödinger equation (TDSE), i.e. TD B-spline ADC [3] and we use it to answer these questions in the example case strong field ionization of CO2 molecules by high-intensity ultra-short IR laser pulses [4]





In the cases where the final produced ionic states show an appreciable level of coherence, we have been able to give a quantitative prediction on the resulting

ionic wave-function coefficients. Moreover, we have been able to study the importance and the effect of the various mechanisms responsible for the establishment of the coherence, which are the direct tunneling ionization in the same electronic continuum state, the electron rearrangement within the ionic system caused by the dipole transitions driven by the IR electric field and the coulomb driven interchannel coupling [4].

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Challenges in description of optical and electronic properties of heteroaromatic molecules

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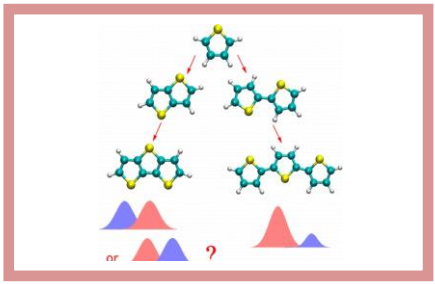
The growing interest in low-cost materials for organic electronic devices has coincided with an increasing number of electronic stucture computations performed on small conjugated molecules. Owing to the favorable compromise between accuracy and computational efficiency, TDDFT is often the method of choice for investigating the molecular excited states. However, our recent letter [1] highlighted qualitative discrepancies between the low-lying $\pi\pi^*$ states of thiophene and thienoacenes computed at the TDDFT and post-Hartee-Fock levels. We extended our analysis to a larger class of small and middle-sized conjugated systems and compared various functionals to the state-of-the-art wavefunction-based methods.[2,3] Furthermore, we reported ab initio excited state molecular dynamics of thiophene and its short oligomers realized via surface hopping scheme.[4]



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Acetylacetone Femtochemistry at FERMI-LDM

M.N.Piancastelli

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The unique performances of the newly built Low-Density Matter (LDM) beam line at the FERMI free-electron laser (FEL) facility in Trieste, Italy, have been exploited to follow the excitation-deexcitation and fragmentation dynamics of a complex molecule, acetylacetone, by pump-probe experiments on the femtosecond (fs) time scale. Electron and ion spectra have been measured with a newly developed high-efficiency magnetic bottle spectrometer after pumping with a UV-vis laser frequency (266 nm) and probing with the FERMI monochromatic beam at 19.23 eV. The measurements have been performed in 100-fs steps up to a total pump-probe delay of 200 picoseconds (ps). By exploiting the available photon energy and time reproducibility, it has been possible to measure good-resolution valence photoelectron spectra and ion yield spectra with the same pump-probe delay, therefore obtaining a picture of unprecedented clarity on the time evolution of the system.

The ultrafast photochemistry of acetylacetone has been enlightened in great detail. In particular, following pumping at 266 nm, which is known to induce the π-π^* electronic transition, the valence photoelectron spectra of the excited species have been measured at 19.23 eV photon energy with energy and time resolution sufficient to reveal the evolution pathway of the system in the delay range 0-2 ps. The 266 nm-pump photoexcitation leads to the S_2 ($\pi\pi^*$) singlet state, followed by decay to the S_1 (πn^*) state, and then to the E-T_1 ($\pi\pi^*$) triplet state. In the ion spectra, the main fragmentation pathway of the UV-vis excited species in the 0-2 ps delay range yields the methyl group, while on a longer time scale (hundreds of ps) the main reported product was the OH radical. The experimental data are fully supported by molecular dynamics calculations.

Biomaterials Inspired from Biomineralization

Giuseppe Falini

Department of Chemistry "Giacomo Ciamician"
Alma Mater Studiorum – University of Bologna

Along the evolutionary process organisms have constantly been exploring different pathways to use crystals for building sophisticated structures with different purposes. While that search occurs by trial and error, the efficient hierarchical crystalline architectures found by life are made by the strict control of the nucleation and growth steps during their formation, with different patterns depending on the scale [1]. This presentation will give a brief overview on the current knowledge on the nucleation, growth and organization of crystals within living organisms, either inorganic or organic crystalline structures. Three examples will be presented as representative cases of study. First the structure of the shell from Abalone rufescens will be illustrated pinpointing the role of the diverse organic component present in proximity of the green layer, a unique part of the Abalone r. shell [2]. The biomineralization in coral will be focused on the role of the intra-skeletal organic molecules on the crystallization of calcium carbonate [3]. The crystalline lipidic layer in reptilian molts will be presented as an example of organic crystalline structure [4]. Finally, current trends and future perspectives of biological crystallization linked to its potential applications in fields such as biomedicine and materials science.

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Biomineralization and Biomineralization-Inspired Drug Design: Calcite - Peptide Interactions

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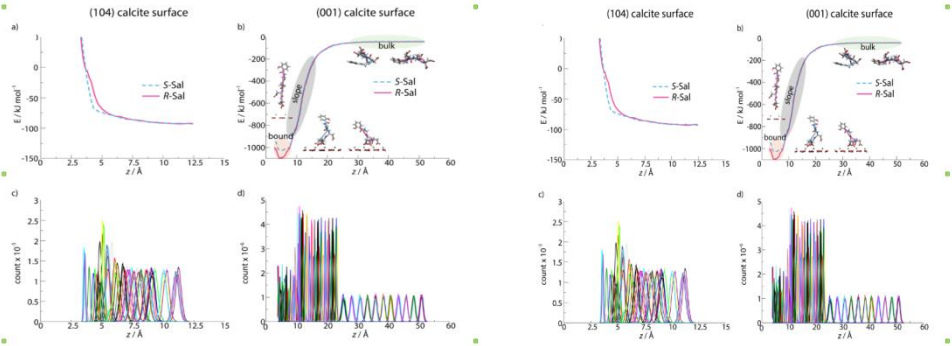
The field of interface chemistry has been heavily focused in recent years on the development of systems that could be used for the controlled introduction and release of active pharmaceutical compounds in the living organisms and tissues. Some of the most interesting systems in this respect, attracting interest from both the pharmaceutical and food industry, are the bioinorganic composites of calcite (calcium carbonate, CaCO3) functionalized by small, biologically active molecules, with the aim of controlled drug delivery. [1] In this respect, we decided to investigate the interactions of calcite with two highly active biomolecules, which are experimentally found to strongly interact with the biomineral, [2] in an attempt to uncover the roles of flexibility and chirality in biomineralization and biomineralization-inspired drug design.



More precisely, using advanced simulation techniques we characterized the adsorption behavior of two epimeric peptides, namely R- and S-Sal (N-Sal-Gly-S-Asp-R-Asp-S-Asp and N-Sal-Gly-S-Asp- S-Asp-S-Asp respectively, where N-Sal denotes the N-terminal residue which is a salicylic acid derivative), on both the stabile (104) and growing (001) surfaces of calcite.

This, on one hand, allowed us to analyze the conformational behavior of the adsorbed peptides in detail, while, on the other hand, permitted us to investigate the underlying thermodynamics of the process by calculating free energy profiles of adsorption. We thereby found that even small differences, such as the change in the chirality of only one constituent amino acid, can change the conformational behavior/flexibility of the peptide to an extent significant enough to induce different binding patterns and interactions on mineral surfaces, leading to an overall different adsorption of active biomolecules/peptides. Finally, by applying our developed methodology [3] we have calculated CD spectra of both investigated epimeric peptides (growing (001) calcite surface), both in the bulk and at the interface. We have thereby found that CD spectroscopy allows us not only to discern between the two epimers, but also represents a certain "device" which can be used to monitor the process of biomineralization, as we find significant differences between the calculated CD spectra of the peptides in the bulk and at the interface, for both epimers respectively.

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Interactions between calcium carbonate and selected amino acids

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A need for novel and advanced materials, as well as for their environmentally friendly synthesis is constantly growing. Biomaterials and processes of their formation in organisms (biomineralization) are good pattern for production of such materials [1]. Calcium carbonate ($CaCO_3$), main inorganic component of invertebrate's hard tissues, is considered to be a relevant biomineralization model. $CaCO_3$ can precipitate (crystallize), either as a polymorph (calcite, vaterite and aragonite), or hydrated and amorphous phase. The calcite skeletal elements regularly contain small amounts of macromolecules (glycoproteins) which are either, incorporated or adsorbed on the single crystals of calcite. It has been shown previously that the isolated fragments of proteins extracted from mineralised tissue, or their synthetic macromolecular analogues, exert a significant influence on the morphology and crystal structure of calcium carbonate when precipitated in the appropriate model systems [2].

The aim of this research is to investigate a role of the selected amino acids as simple models of macromolecules supposed to be responsible for precipitation of specific calcium carbonate polymorph or different crystal morphology, during the biomineralization processes. Thus, the aspartic acid (Asp), asparagine (Asn) and lysine (Lys) are selected because of different charge of their side chains, while tyrosine (Tyr) and phenylalanine (Phe), as well as serine (Ser) and alanine (Ala), are chosen because of different polarity. The hypothesis is that not only the acidic, but also the hydrogen bonding amino acid can specifically interact with selected $CaCO_3$ surfaces. Therefore, the Langmuir adsorption constants are calculated from growth kinetic data [3,4] and used as an indication of extent of organic/inorganic interaction.

Acknowledgements: This work is supported by Croatian Science Foundation under the project Bio-Mat-Form (IP-2013-11-5055).

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Theoretical study of amino acid-calcite interface

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[c]*CLS Group, Ruđer Bošković Institute, Zagreb, Croatia*

Calcite is one of the most widespread minerals on earth which interacts favourably with a variety of biomolecules. This interaction can mediate the growth of calcite resulting in formation of biominerals with remarkable mechanical properties useful in a number of applications [1]. In this work we study the interaction of amino acids, which polymerize to give peptides and proteins, with the neutral (104) surface and the polar (001) surface of calcite. Amino acids are studied in their native zwitterionic and protected forms. Our method of choice for this study encompasses fully atomistic molecular dynamics simulations using two different state of the art force fields for these types of systems [2, 3]. We employ enhanced sampling techniques with biasing potentials to obtain free energy profiles for binding of amino acids to the surfaces. This enables us to estimate the free energies of binding of amino acids to calcite as well as the molecular details of the interaction. Importance of polar groups for binding to the neutral (104) surface and significance of charged side chain groups for binding to the polar (001) surface is illustrated. These results provide a force field benchmark and reference data on binding energies and conformations of specific amino acids which could help interpret the experimental data on peptide and protein mediated calcite functionalization and growth.

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Polyelectrolyte multilayers: properties and applications

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Polyelectrolyte multilayers (PEMs) are surface coatings obtained by alternated deposition of positively and negatively charged polyelectrolytes (polycations and polyanions) on a solid surface. It was shown earlier [1] that the PEM build-up strongly depends on various experimental conditions (*e.g.* ionic strength, type of supporting electrolyte, pH and polyelectrolyte concentration). Answers to some fundamental questions dealing with PEM build-up could be obtained by relating the PEM properties with the properties of corresponding polyelectrolyte complexes (PECs) in solution. Therefore, we compared the results we obtained earlier [2,3] for the complexation of poly(allylammonium) chloride (PAH) and sodium poly(styrenesulfonate) (PSS) with the results obtained for PAH/PSS multilayer build-up. In order to do so, we studied the formation of PAH/PSS multilayers in aqueous solutions of various electrolytes by means of QCM-D and AFM. The QCM-D measurements indicated the largest deposition was noticed in the case of nitrate and perchlorate anions. This is in accordance with the results obtained for PECs by means of DLS and spectrophotometric experiments which showed anion specific aggregation of positive complexes and the formation of precipitates containing larger amount of PAH with respect to PSS. The thickness of deposited films could be correlated with the complexation enthalpies of used supporting electrolyte ions which provides a path for the modification of multilayer properties simply be changing the type of salt during their preparation. The ions counterbalancing the charge at the surface of PEMs also enable the modification of surface wettability. Since PEMs are promising coatings onto which biomolecules (e.g. proteins, bacteria) could be adsorbed, such studies can enable additional progress in the field of biosensing surfaces and drug delivery.

Acknowledgements: This work is supported by the Croatian Science Foundation under the project IP-2014-09-6972.

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Holes in Liquid Water and Other Hydrophobic Effects

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Density fluctuations in liquid water are at the heart of numerous phenomena associated with hydrophobic effects. One of the most fundamental processes in this regard, is the solvation of hydrophobic solutes in water. The vast majority of theoretical and numerical studies examine density fluctuations at the short length-scale focusing exclusively on spherical cavities. In this work, we use both first principles and classical molecular dynamics simulations to demonstrate that density fluctuations in liquid water can deviate significantly from the canonical spherical shapes. We show that regions of empty space are frequently characterized by exotic, highly asymmetric shapes that can extend far beyond the first solvation shell. Interestingly, density fluctuations of these shapes are characterized by Gaussian statistics with larger fluctuations. An important consequence of this is that the work required to create non spherical cavities can be substantially smaller than that of spheres despite having a much larger surface area. This feature is also qualitatively captured by the Lum-Chandler-Weeks theory. The scaling behavior of the free energy as a function of the volume at short length scales is also qualitatively different for the non-spherical entities. We also demonstrate that non spherical density fluctuations are important for accommodating a hydrophobic amino acid and are thus likely to have significant implications when it comes to solvating highly asymmetrical species such as branched alkanes, polymers or biomolecules.

The role of water in the electrophoretic mobility of hydrophobic objects

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It is well established that hydrophobicity of an interface, droplet or a particle can be modulated by an external electric field. However, the provided explanations why these essentially uncharged objects like oil droplets exhibit a directional specific movement in the presence of electric fields remain controversial and continuously challenged. Here we study the static and the dynamic behaviour of a model hydrophobic object (Lennard-Jones particle) in water (SPC/E model), by performing extensive molecular dynamics simulations in the absence and the presence of electric fields using the GROMACS software package. We first combine simulations with the linear response theory to show that shear viscosity of water increases with the strength of the electric field. Furthermore, we identify a novel relaxation process in the water network that originates in the collective reorientations of hydrogen-bonded water molecules occurring locally on a picosecond time scale. After establishing a sound simulation protocol, we show that the electric field evokes on an average asymmetric distribution of the water molecules around the Lennard-Jones particle. This acts as a steady state density gradient, inducing a phoretic motion of the hydrophobic object towards the region of higher concentration of water. We interpret our data on a basis of Derjaguin theory for diffusiophoresis which predicts the steady state velocity of a colloidal particle as a function of the first moment of the concentration gradient, the effective hydrodynamic radius of the particle, and the shear viscosity of the solvent. This theoretically predicted driving velocity agrees exceptionally well with the results of the simulations.

Surface influences on catalytic performance of supported ionic liquid phase (SILP) materials

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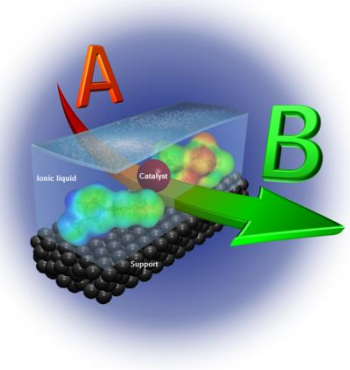
The supported ionic liquid phase (SILP) technology is a fundamental, new approach to achieve the goal of long-term stable, immobilized homogeneous catalysis, involving surface modification of a porous solid by a thin film of an ionic liquid catalyst solution.[1] Due to the extremely low vapor pressure of ionic liquids, the surface of SILP materials remains coated permanently even in contact with a continuous gas stream or at elevated temperature.



By variation of anions and cations, solubility, reactivity and coordination properties of the ionic liquids can be modified according to the special requirements of the given process. By an appropriate choice of the IL ions, it is possible to transfer specific properties of the fluid onto the surface of a solid material by simply confining the fluid onto the surface. Thus, the SILP concept allows tailor making of solid surfaces resulting in uniform and well-defined surface topologies with defined and uniform properties and controlled chemical reactivity. Importantly, the SILP concept thereby constitutes an attractive methodology to circumvent the lack of uniformity of solid surfaces in traditional heterogeneous catalysis at least for continuous gas phase reactions.

In this presentation the latest results from SILP material design are presented. By appropriate modification of the surface it is possible to improve the catalytic performance of the SILP material significantly.

References:

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Model catalysis with ionic liquids

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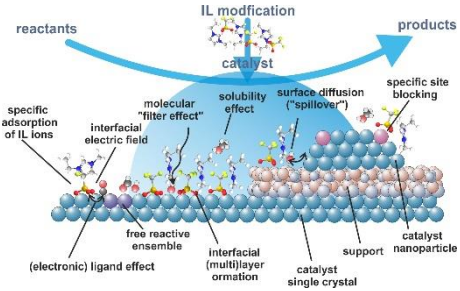
IL films can be used to modify the physical and chemical properties of functional interfaces in an outstandingly flexible fashion. Various concepts including the 'Supported IL Phase' to immobilize molecularly-defined reactive species and the 'Supported Catalysts with Ionic Liquid Layer' to enhance catalytic selectivity can be realized at nanoscale.



Whereas the impressive potential of IL-modified materials has been proven in many experimental studies, our current understanding of the molecular interactions that drive these effects is still rather poor. The present report reviews our recent progress towards an understanding of IL-solid interfaces using a surface science and model catalysis type of approach [1-4]. Here, thin IL films are prepared in-situ under ultrahigh vacuum conditions on atomically clean and well-defined surfaces by means of physical vapor deposition. Due to their low vapor pressure, these systems can be studied using a broad spectrum of surface science techniques. We explore the interaction of imidazolium-based ILs with prototypic model surfaces – metals, oxides, and supported nanoparticles. A detailed picture of the molecular interactions at the interfaces and of the influence of the IL the interaction with reactants is obtained.

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Multiscale Simulation of SILP Catalysis

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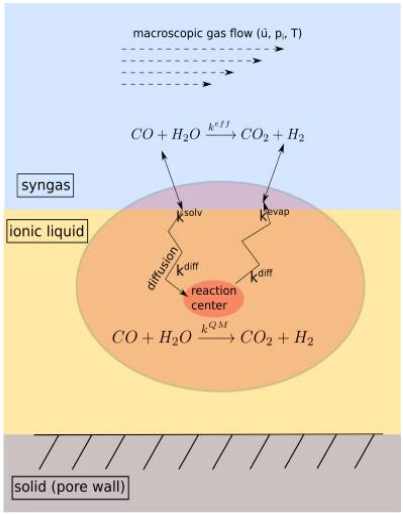
The society is in urgent need for novel energy solutions to manage the transition towards a clean and sustainable energy future. Catalysis plays a key role for clean energy storage and fuel production. The novel class of supported ionic liquid phase (SILP) catalysts is a high potential candidate for many applications in the energy context. Here the catalytic agent, a transition-metal complex, is solvated in an ionic liquid (IL). The surface/volume, i.e. turnover rate, is maximized by coating the inner pores of a porous host material. The rate and life-time limiting mechanisms happening on a wide range of length and time scales are however only vaguely understood. In specific, it is not clear how the IL or the porosity and tortuosity of the porous material affect the overall turnover rate. At this point detailed information is required to overcome the technological barriers.

In this talk I will present our multiscale simulation approach which covers all involved length and time scales: the chemical reaction kinetics is predicted through *ab-initio* quantum chemical calculations; local diffusion and the local electrostatics are determined at an atomistic level through molecular dynamics. The macroscopic heat and mass transport through the porous material is simulated with a thermal multicomponent Lattice-Boltzmann approach. I will discuss simulation technique at every scale and explain our way of accurate and efficient coupling between the scales, which is essential for the predictive power of such an approach.



Acknowledgements: Jens Harting, Ana Smith, David Smith

Towards Engineering Radical SAM Enzymes – Insights into Biocatalysis and Biomaterial-Ionic Liquid interactions

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During the process of developing enzymes for biotechnological applications it is necessary to account for a multitude of requirements. Understanding the principles of naturally-occurring biocatalysis is only one first step towards designing enzymes with a broader substrate range or that catalyse non-naturally occurring reactions. It is also important to account for variables like enzyme stability, potential product inhibition and toxicity and the process of extracting the products from the reaction system, e.g. through using ionic liquids.

Using the example of radical SAM enzymes, [1] which are capable of controlling radicals during their catalytic action, we present recent results illustrating how computational approaches can be used to shed light on enzymatic radical control mechanisms, particularly with a view to understanding how these enzymes might both prevent unwanted transformations and facilitate desired conversions.

Based on the need for affordable computational strategies for rational enzyme design, we show methods combining 'snapshot' (e.g. electronic structure methods) and classical simulation methods for radical reaction profiling through calculating radical stabilisation energies (RSEs). [2]

Further, we present our latest results in understanding the organisation of ionic liquids around amino acid and peptide-based substrates, with a view to developing a predictive understanding of ionic liquid-peptide interactions. These results have future implications for optimising both solubility and reactivity of proteinacious materials in ionic liquids.

Acknowledgements: This work is supported by STFC, IDB and by the EU FP7 Marie Curie Actions - People, Co-funding of Regional, National and International Programmes (COFUND) under Grant Agreement no PCOFUND-GA-2012-600181.

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Ionic Liquids at Interface

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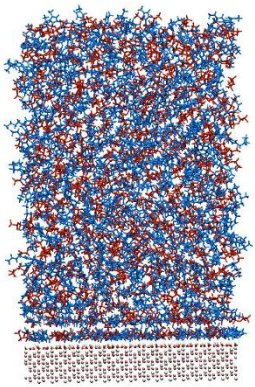

Understanding the molecular-level behavior of ionic liquids (ILs) at the boundary between the solid and liquid phases is of fundamental importance with respect to their application in, for example, electrochemical systems and electronic devices.

We have studied the interfacial organization of an IL using a complementary combination of high-resolution X-ray reflectivity measurements and atomistic molecular dynamics (MD) simulations [1]. We used a model system consisting of a imidazolium-based cation with increasing alkyl chain length ($[C_nMim]^+$, n = 2, 4, 6) and a prototypical anion species ($[NTf_2]^-$), in contact with a sapphire substrate.

Our strategy enables us to compare experimental and theoretically calculated reflectivities in a direct manner, thereby critically assessing the applicability of several force-field variants. On the other hand, using the best-matching MD description, we are able to describe the nature of the model IL−solid interface and physico-chemical characteristics in appreciable detail.

More specifically, we characterized the three-dimensional layering profile of the ILs. We calculated interface-normal number density and charge density, total in-plane correlation functions and 2D histograms of the in plane position of ions in the first double layer. Changing the length of cation alkyl chain, we calculated the distribution and orientations of cations and anions in the first and the second layer. For each system we found the diffusivity constant in the bulk liquid and near the sapphire surface and compared how the changes in the force-fields affect the results.

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Soft particles at fluid interfaces: the interplay of deformability and surface tension

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Particles adsorbed to a fluid interface are common stabilizers in the food, oil and cosmetic industries. As an alternative to rigid colloidal particles, it has turned out beneficial to consider soft deformable particles that can adapt their conformation at the interface. In this study we compute the shapes of two different kinds of such elastic particles and combine atomistic and coarsegrained simulations with continuum theory. Cross-linked polymer gels are simulated using molecular dynamics simulations and capsules defined by a discretized spherical elastic membrane are simulated using a coarse-grained constitutive description. The numerical results are compared to calculations based on linear elasticity. It is shown that the molecular or coarse-grained simulations are perfectly described by the continuum models, provided that deformations are small. For the cross-linked polymer particles, we discuss the implications of our findings for microgel particles, which are typically in the regime of large deformation, and discuss the adsorption/desorption energies as obtained in the simulations.

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Physical determinants of pathological protein aggregation

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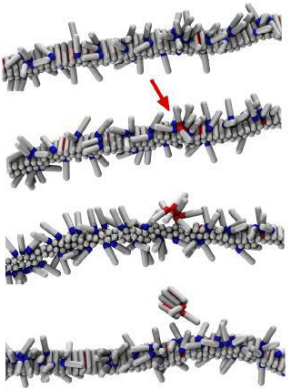
The assembly of normally soluble proteins into large fibrils, known as amyloid aggregation, is associated with a range of pathologies, including Alzheimer's and Parkinson's diseases. It has proven to be challenging to experimentally characterise the mechanisms of amyloid formation. Computer simulations, in combination with quantitative experiments, can provide valuable insight in this case, helping to bridge experimental scales with microscopic mechanisms.

Substantial evidence shows that disordered pre-amyloid oligomers − not the fully grown amyloid fibrils − are cytotoxic and involved in pathological processes. Yet, their relationship to fibrils is not well understood. Using computer simulations, we showed that at physiological conditions, disordered oligomers serve as nucleation centres for fibrils, and are crucial on-pathway species to amyloid formation [1].

Furthermore, recent experiments have revealed that amyloid fibrils are able to catalyse formation of their copies from soluble peptides. By combining simulations with biosensing and kinetic measurements of the aggregation of Alzheimer's Aβ peptide, we proposed a mechanistic explanation for the self-replication of protein fibrils. We find that this intricate process is dominated by a single physical determinant − the adsorption of monomeric proteins onto the surface of fibrils [2]. Such mechanistic understanding not only has implications for future efforts to control pathological protein aggregation, but is also of interest for the rational assembly of nanomaterials, where achieving self-replication is one of the unfulfilled goals.



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Interaction of polarity fields driving pattern formation in tissues

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Biological tissues can be considered as active polar matters. Polarity fields reveal long range patterns which are critical in tissue development. Non-uniform concentration of different molecules, anisotropic stress, cell elongation, and average orientation of cytoskeleton can define polarities for each cell. It has been shown that distinct polarities can interact and tend to coordinate within a cell. There can also be interaction between polarities of adjacent cells. We present a basic mathematical description of polarities and their possible interactions to coordinate their orientations. Our approach is rather general and represents a coarse-grained picture of polarity fields in a tissue. We write an effective energy function to describe this system. This energy function can be minimized to find steady state solutions. With the help of this model, we analyze some interesting cases, for instance in a tissue with singularities or specific geometries and boundary conditions. We compare these cases with some biological examples, particularly in the plant tissues like the shoot apical meristem.

Apart from equilibrium condition, we look at the time-evolution of polar tissues. A striking example is the dynamics of the coupling between a fast rotating main polarity and a polarity responding slowly to the main one. We also implement this model to perform growth simulations of a polar tissue to study consequences of field interactions in developing tissues. In particular, we compare how long-range patterns are influenced when division axis is coordinated by distinct polarities.

A biophysical model for the formation of mitotic spindle bipolarity

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[b]*Department of MCDB, University of Colorado at Boulder*
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When cells divide, a molecular machine called the mitotic spindle ensures that a cell's duplicated genetic material is faithfully passed to the daughter cell. This process depends on the spindle assuming a characteristic bipolar structure. While the dynamics of mitotic spindle formation have been characterized biologically, a complete physical picture of the process has not been achieved. In particular, the physical processes that drive self-assembly of a bipolar assembly from a monopolar initial condition are not well understood. We have developed a physical model of fission yeast mitotic spindle formation using a basic parts list that includes rigid, dynamic microtubules, a spherical nuclear envelope, spindle pole bodies anchored in the nuclear envelope, and crosslinkers and crosslinking motor proteins. The model parameters are set using available data from experimental literature and our own data, leaving relatively few unconstrained parameters. Using this data, the model robustly reproduces spindle structures. In order to refine the model and bound the unknown parameters, we use available electron tomography and light microscopy data with good agreement for both spindle structure and dynamics. With our best mimic of a "wild type" cell, we can then study perturbations to the model, such as protein deletions, to probe the principles governing spindle formation, set bounds on measurable component parameters, and predict testable novel behaviors.

Acknowledgements: We thank Iaian Hagan and Jonathan Millar for providing fission yeast strains. This work was funded by NSF grants DMR-0847685 (MB), DMR-1551095 (MB), and DMR-0820579 (MG); NIH grants GM110486 (MB) and GM033787 (JRM); and the use of the Janus supercomputer supported by NSF grant CNS-0821794.

Formation of epithelial tissues on inorganic functional surfaces: space tessellation on micro and macro scale

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[d]*Institute Ruđer Bošković, Zagrab*

While it is well established that the mechanosensitivity determines the structure of the cytoskeleton, and the protein expression in single cells, the coupling between mechanical and biochemical signals in tissues remains a challenging issue. We address this problem using system model of organic-inorganic interfaces. We study the formation of the MDCK II monolayer as a function of the different elastic stiffness of the polyacrylamide substrates. At physiologically relevant, soft substrates (0.6 ± 0.2 kPa), a monolayer with a very high, steady cell density, surrounded by a three-dimensional unstructured compartment of diving cells, is found already in clusters of 0.005 mm2 [1]. The density in this novel regime of growth was found to be independent of time and cluster size. On hard substrates (elasticity>3 kPa), where the commonly reported growth was found, the tissue compartmentalizes over several days, after reaching millimeter sizes. Thereby a contact inhibited bulk region, followed by a proliferating compartment and a low density moving edge could be distinguished. We use computational methods to model formation of the bulk and edge region, based on Voronoi tessellation, within which we are able to simulate the growth and the associated compartmentalization, thereby providing deeper understanding of the observed phenomena. Furthermore, we develop a new tessellation method based on the shape of the cells' nuclei and prove that our method is systematically better than the existing Voronoi tessellation for all morphological measures. Success of this method implies membrane-nucleus coupling that was widely debated in single-cell mechano-transduction.

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Posters

Crystallization of $CaCO_3$ in alginate hydrogel with the addition of charged amino acids

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$CaCO_3$ is one of the most abundant minerals which occur in a form of three different polymorphs (vaterite, aragonite and calcite) or hydrated modifications. Besides geological forms, calcium carbonate occurs as an important biomineral - hybrid material made from organic and inorganic components. Morphology of such crystals is predominantly controlled by present organic macromolecules, mostly glycoproteins, responsible for gel-like properties of matrix. Crystals formed in such environment meet various structural and functional needs of respective organisms [1]. Fallini et al. [2] studied crystallization of the three $CaCO_3$ polymorphs in chitin gels and concluded that supersaturation within the closed micro space determines the polymorphic structure and morphology of crystals.

In this research the crystallization of calcium carbonate in alginate hydrogel matrix, containing the amino acids (Tyr, Asp) which are found at significant amount in proteins supposed to be relevant for biomineralization, is investigated. The precipitation model system comprised alginate hydrogel beads, made by ionotropic gelation and mineralized by the controlled carbonate ions diffusion. Depending of cross-linking of alginates, supersaturation and addition of amino acids, different calcium carbonate polymorphs, of various morphologies occurred. The samples of gel and precipitated calcium carbonates are lyophilized and characterized by FTIR/ATR and Raman spectroscopy and scanning electron microscopy.

Acknowledgements: This work has been supported by Croatian Science Foundation under the project (IP-2013-11-5055).

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Diffusion in a crowded membrane surface with traps

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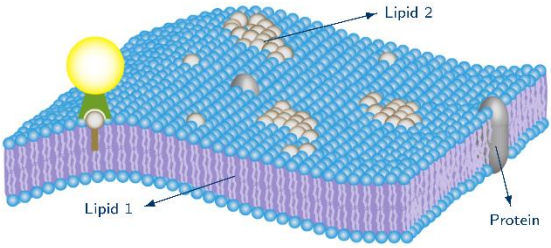
The transport of lipids and proteins in biological membranes is one of the most fundamental processes in living cells. Despite a wealth of phenomenological models that have been developed to address related experiments, no microscopic model has emerged that explains the general biophysical principles underlying the complex diffusion in a membrane. Here we model lateral diffusion in the crowded and multicomponent membrane environment as a random walk on a dynamic lattice in which tracers representing proteins bind and unbind from immobilized counter-partners (traps). The crowding, trapping and cooperative effects on such a scaffold define the nature of diffusion but are themselves dependent on the diffusion.



The model system scheme

To study this problem, we developed a Monte-Carlo simulation scheme that accounts for length scales from 1 nm to 1 mm and in the time domain from 1 μs to 10 s, with which we explored the full parameter space spanned by the densities of the diffusing molecules and the traps, as well as the binding and unbinding rates. We find several regimes of diffusion and types of anomalous transport. We derive an exact expression for an effective diffusion coefficient in the long-time limit that accounts for trapping, avoidance and cooperative effects. We find that the results of the model are in perfect agreement with all the simulation data.

Acknowledgements: This work is supported by ERC MembranesAct Project 337283.

Anomalous Properties in Network Materials

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Thermodynamic and kinetic anomalies are often encountered in tetrahedral liquids, most famously in water (for example, the density anomaly), but also in SiO_2 and BeF_2. The origin of the anomalies is often linked to behavior of quantities associated to phase transition phenomena which occur in the metastable supercooled regime that is largely inaccessible by conventional experiments. As a result simulations are often used to explore this problem. Several theories and scenarios have been proposed that link behavior of anomalous properties to the existence of a liquid-liquid critical point [1]. Stillinger-Weber (SW) potentials are often employed to model tetrahedral liquids. These potentials are composed of a standard pairwise term with exponential decay and a triplet term which penalizes deviations from ideal tetrahedral angles [2]. In recent years the critical point for SW silicon has been uncovered [3] and loci of anomalous properties calculated for constant pressure for different strengths of triplet term in SW potential [4]. However, no systematic study of the SW potential that involves the calculation of critical points and spinodal lines and links them to anomalous properties as a function of the strength of triplet term has yet been reported. In this study we take a systematic approach to explore the parameter space of the triplet term in the SW potential at various temperatures, pressures and densities. This enables us to more thoroughly understand the appearance of thermodynamic and kinetic anomalies in tetrahedral liquids and their connection to the underlying tetrahedrality of the system. Key trends may map onto a range of systems including H_2O and the MX_2 salts for which models which incorporate many-body interactions can be applied.

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Stress-strain relation in tissues grown on functional flexible surfaces

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Epithelial cells form active two-dimensional sheets that are involved in variety of functions like morphogenesis, embryogenesis, wound healing and organ development. Mechanical stress stimulates processes like growth, proliferation and remodeling of the surfaces.

To study the stress-strain relation in model tissues Madin-Darby canine kidney II cells were seeded on fibronectin coated polydimethylsiloxane elastomer chambers in a droplet wise manner. The resulting surface was uniaxially stretched with amplitudes of 10, 20 and 30%. Subsequently the reaction and growth of clusters was imaged in phase contrast on timescales from minutes to days.

We present a comprehensive study of tissue growth after stretching. The change in cell size, elongation and orientation as well as connectivity and relaxation was investigated.

Activin Receptor Type IIA Protein Kinase Inhibitors: Free Energy Calculations and Ligand Binding

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In the present research, we reviewed the use of Molecular Mechanics combined with Poisson-Boltzmann and Generalized Born Surface Area (MM-PB(GB)/SA), as well as the Linear Interaction Energy (LIE) method, for calculating ligand binding free energies. With an aim towards better understanding a variety of biological functions, including muscle growth and bone formation as well as viability and adhesion of prostatic epithelial cells, Dorsomorphin (K_D = 58 nM), LDN-193189 (K_D = 14 nM), and seven other ligands [1] were investigated as Activin Receptor Type IIA Protein Kinase (ActRIIA) [2] ATP-binding site inhibitors. Due to the lack of experimental structural information for the binding of these ligands, 10 ns Molecular Dynamics (MD) simulations in explicit water using Amber 14 software package were performed for each receptor-inhibitor complex.

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Simulating Examples of Cooperating Molecular Motor Interactions

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Molecular motors of different shapes are crucial at every stage of development in animal life forms – from a flagellum propelling a sperm cell over material transport during cell growth to the contraction of muscle fibers. We are using rate equations fulfilling detailed balance to simulate systems of variable numbers of identical or distinct motors dragging an elastically coupled cargo along one dimension in order to categorize the different modes of transport in typical biological systems and quantify the effect of experimentally unknown variables. Applying the model to intraflagellar transport in *C. elegans* we also found some unusual motor interaction effects taking parameters directly from experiment as far as possible.

Morphological properties of the epithelial tissue

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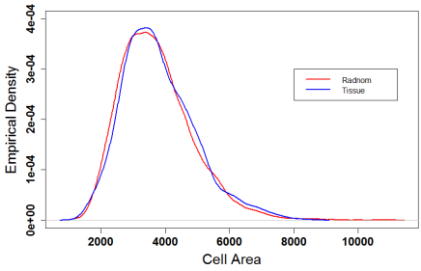
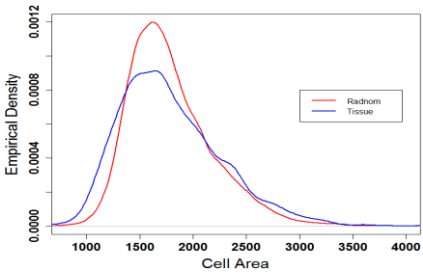
Knowing the morphology of an epithelial tissue is important due to understanding processes like growth and development of the tissue, wound healing and progression of the cancer. We study the structure of the MDCK II epithelial cells in circular colonies. Cell nuclei can be approximated with ellipses and the Voronoi tessellation generated by those ellipses coincides well with the cell membranes. We compare the tissue cells to the Voronoi cells generated by randomly packed ellipses obtained from the cell nuclei. The comparison is done by studying the probability distributions of chosen morphological measures calculated from the cells. We find that randomly packed ellipses reproduce the morphology of the tissue well at the low cell density. At high cell density we observe more regular structure of the tissue and we see the deviations of the random model from the cell tissue.





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Synthesis of calcium carbonate crystals with well developed {001} faces

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Calcium carbonate crystals with different morphologies are interesting model for studying the additive-controlled processes which are important for pharmaceutical industry and for understanding the crystallization in biological systems [1]. Calcite is the most stable calcium carbonate polymorph that crystallizes with notable variety of habits under different environmental conditions. The addition of inorganic ions such as Mg^{2+} and Li^{+} can exert profound effect on the calcite morphology [2]. It has been shown that increasing amounts of lithium enhance the formation of {001} calcite form [3]. Atomistic simulation of predicted calcite morphology shows that the crystals, with incorporated lithium ions are tabular, comprising basal {001} and {104} side faces [4]. The aim of this study was to define the factors that favor the formation of plate-like calcite in a number of model systems. For this purpose the hydrodynamic parameters (a mode of mixing) and the concentration of the lithium ions were extensively studied. Calcite samples were studied by FTIR/ATR spectroscopy, thermogravimetry and PXRD method. The SEM and AFM microscopy were used for surface analysis of {001} face. In addition, the chemical composition of the precipitate has been determined by the ion chromatography. The results indicated that the plate-like calcite is preferably precipitated when the ultrasound was applied, as well as after the addition of lithium ions at concentrations higher than $c = 0.3$ mol dm^{-3}. Precipitation of the plate-like calcite is also observed with the higher concentrations of lithium in the systems in which the magnetic and mechanical stirring was applied.

Acknowledgements: This work is supported by MIPOMaT and MEMBRANESACT projects.

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Micro-scale transport of cargo using bead-spring carriers

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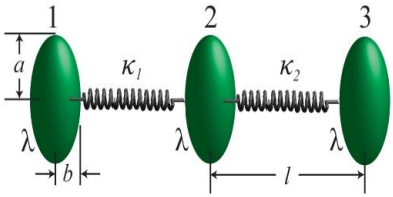
Cargo transport at the micro-scales is an important technological task of the future, with many foreseen applications such as in drug delivery, medical probing, etc. We present here our results on one possible system of micro-cargo transporters, the bead-spring carrier. The model we use consists of three rigid or flexible beads connected with harmonic springs in a series [1] (see the figure). One or more of the beads act(s) as sites for carrying the desired cargo, and the actuation of the assembly is done by deforming the springs in a non-reciprocal manner, which leads to directed motion at the micro-scale.



We show that in spite of the simplicity of design of this assembly, it can move in a controlled yet autonomous manner, given only a source of deformation of the springs. By modulating the various parameters in the problem, we explain how the motion efficiency of the device may be optimised [2]. We also explain how the additional cargo mass can change the fundamental motile properties of the device, causing the flow around it to be potentially non-Stokesian (where the inertial effects dominate the viscous effects). We modify our theoretical approach to include such inertia-dominance, and show that even in this regime good agreement with lattice Boltzmann simulations is achieved.

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[1] K. Pickl, J. Götz, K. Iglberger, J. Pande, K. Mecke, A.-S. Smith and U. Rüde, *J. Comput. Sci.*, **2012**, *3*, 374-387.

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Effective diffusion of bonds interconnecting functional surfaces

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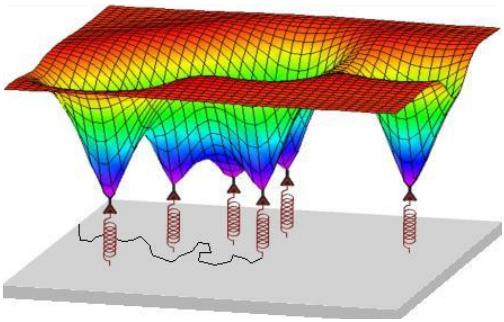
The equilibrium of molecular reactions at the interface between two fluctuating functional surfaces depend strongly on the surface properties. The bonds between those surfaces, realized for example by ligand-receptor constructs, exhibit a specific mobility that is affected by other bonds. The mobility of the diffusing bonds changes because of energetic and entropic contributions arising from surface mediated correlations between bonds.

We address these effects by numerical methods and with simulations. We calculate the time it takes for one bond to escape the influence of a second pinned one. We also determine the effective diffusion constant in a periodic arrangement of affixed bonds. This can be used to control molecular reactions at the interface by choosing specific surface properties.



Reaction kinetics between functional fluctuating surfaces

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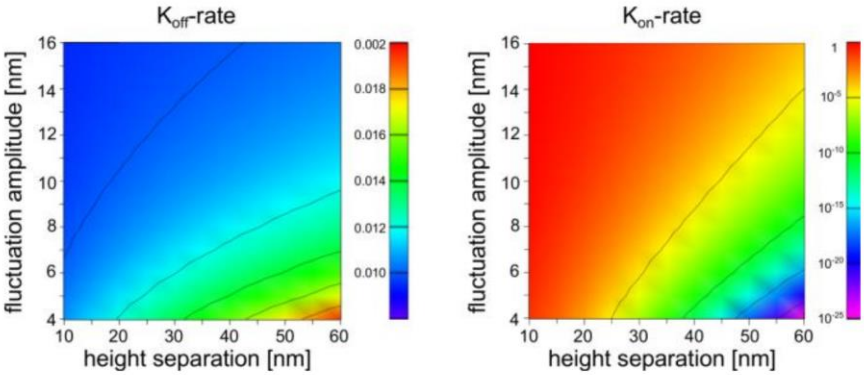
Molecular reactions bridging two fluctuating surfaces depend strongly on the instantaneous distance between the surfaces and their elastic dynamic properties. We not only determine effective reaction kinetics, i.e. rates that integrate the stochastic displacements of the interfaces, but also the effect of the permanently or stochastically bound molecule on the static and dynamics properties of the surfaces themselves. Our theoretical and numerical results will be confirmed by detailed Langevin simulations.



Micro-swimming with inertia

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Increased theoretical study in the past few decades has enabled scientists to gain a good understanding of the motion of micro-swimmers, yet this has focused on the world of inertia-free swimming. While this is a good approximation for many micro-swimmers as the Reynolds numbers of their flow are typically negligible, for some micro-swimmers inertia can have observable effects on the motion, such as affecting the swimming gait and the velocity. In this talk we present a theoretical study of a micro-swimmer where inertial effects are taken into account to the lowest non-zero order. For this we employ the popular Golestanian [1] model of the swimmer, with three beads attached in series in a fluid and the motion along the axis of the swimmer. By combining the Oseen-Stokes equations for the coupled motion of distant spheres in a fluid with Newton's force-mass relations, we obtain a coupled system of first-order differential equations for the sphere velocities.

By solving these equation we derive a closed-from expression for the velocity of the swimmer. We then draw a comparison between the cycle-averaged velocity for different masses, Golestanian's cycle averaged velocity as well as lattice Boltzmann simulated results for the propagation of a three sphere swimmer, which results in a noticeably better agreement of our calculation to the simulations than the existing Golestanian's approach calculation. Moreover we analyze the influence of parameters which characterize the final analytical expression of swimmers velocity.

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[1] Golestanian, R., & Ajdari, A. (2008). Analytic results for the three-sphere swimmer at low Reynolds number. *Physical Review E - Statistical, Nonlinear, and Soft Matter Physics*, *77*(3), 1–6. http://doi.org/10.1103/PhysRevE.77.036308

Adhesion of deformable fluctuating interfaces by multiple types of functional complexes

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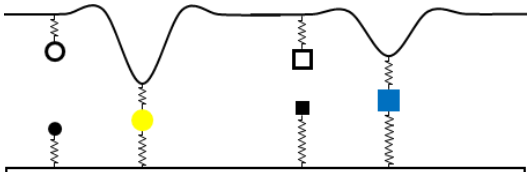
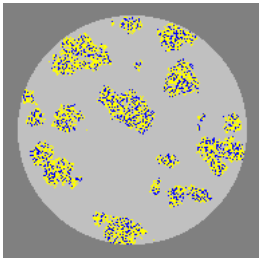
We present a model for the adhesion of flexible fluid membranes to a flat substrate by functional molecules (ligand-receptor pairs) which are freely diffusing on the adherent interfaces. In the absence of molecular complexation, the membrane resides close to a flat surface in a nonspecific potential that originates from van der Waals interactions and the steric repulsion associated with thermal fluctuations. Upon molecular complexation, the interface is deformed introducing cooperative effects for further specific molecular binding. While the system containing only one type functional pairs has been intensively studied in the past [1], the phase behavior and the dynamics of adhesion mediated by multiple functional pairs is poorly understood [2].





To rectify this issue we construct a Monte Carlo scheme that appropriately accounts for the described adhesion process. We study the organization of functional pairs into domains as a function of the molecular flexibility, length, binding energies and other properties of the system, and find a very rich phase diagram as a function of these parameters. Furthermore, we apply this model to the adhesion of T-lymphocyte cells, by binding of TCR to pMHC and LFA-1 to ICAM-1 proteins, to explain the fundamental processes in the formation of the immune synapse.

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Correlating density fluctuations and directed multicellular motion

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Morphogenesis and wound healing both require migration of a large number of constituent cells. This still unresolved problem of collective cell migration is addressed by using MDCK II model epithelium grown on collagen I coated glass substrates. We look at the global development of an initially droplet seeded system of cells which is allowed to expand freely over time. Large scale experiments spanning days and multiple connected fields of view are analyzed with particle image velocimetry of live fluorescent samples. This approach allows for both microscopic and macroscopic (millimeter) scales as the clusters are investigated from the colony border up to the contact inhibited centre. We analyze the correlations between these scales and the perpetually increasing velocity of the colony border. Our recent findings push the limit of cooperative cell motion numbers further than expected to the regime where thousands of cells act simultaneously in a coordinated fashion.

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