CPP 15: Poster: Membranes, Biomaterials, Biopolymers

Time: Monday 18:30–21:00 Location: P1C

CPP 15.1 Mon 18:30 P1C

The fluorescence activity of nano-confined dyes — Khalil Alizadeh[2], Seyyed Mahdi Shavakandi[2], Soheil Sharifi[2], Othmar Marti[1], and •Masoud Amirkhani[1] — [1]Universität Ulm Albert-Einstein-Allee 11, 89081 Ulm, Germany — [2]Department of Physics, Faculty of Sciences, Ferdowsi University of Mashhad, Mashhad 91775-1436

Dyes molecules are widely used for imaging, lasing and coloring application thus increasing the photostability and decreasing the quenching rate are very crucial. One way to deal with mentioned problems is embedding dye molecules in the environment, which increase thermal diffusion and also hinder the aggregation. A two-phase medium such as emulsion is an ideal system due to their ability to enhance the solubility and also decrease the dimerization of dye molecules. In this study two Xanthene type dyes (Rhodamine B and Fluorescein sodium salt) are dissolved in a water-in-oil microemulsion. The optical activity of both dyes were examined using their fluorescence and absorption spectrum. Rhodamine B (RhB) florescence activity enhanced in microemulsion solution compare that of in water solution, which can be attributed to a decrease in dimerization. The opposite trend was observed for Fluorescein sodium salt, the difference between the behavior of RhB and FSS is linked to their solubility in water. We additionally, used Lippert-Mataga equation to calculate the change of dipole moments in the ground and exacted states.

CPP 15.2 Mon 18:30 P1C

Surfactant-induced Porous Polymer Film — •Dan Peng[1], Farid Farajollahi[2], Susanne Sihler[3], Ulrich Ziener[3], Othmar Marti[2], and Masoud Amirkhani[2] — [1]Institute of Advanced Materials, Ulm University, Germany — [2]Institute of Experimental Physics, Ulm University, Germany — [3]Institute of Organic Chemistry III, Ulm University, Germany

The basic working mechanism of Breath Figure (BF) method is the condensation of water vapor on the polymer solution during the evaporation of the solvent. Holes structure left on the surface of the polymer film after complete evaporation of solvent and condensed water. BF method is an effective way to prepare ordered-arrangement porous polymer films. The aim of this study is to use a surfactant to produce honeycomb structure of polystyrene films by BF method. Samples cast from polystyrene solution without surfactant in three solvents including chloroform, cyclohexane and toluene show no honeycomb structure. After adding the surfactant into these solutions, the best honeycomb pattern films are achieved from the solution with toluene. The result shows that humidity and evaporation rate effect the structure of pores on the surface.

CPP 15.3 Mon 18:30 P1C

Fabricating Complex Composite Porous Structures — •Yize Shao[1], Susanne Sihler[3], Farid Farajollahi[2], Ulrich Ziener[3], Othmar Marti[2], and Masoud Amirkhani[2] — [1]Institute of Advanced Materials, Ulm University, Germany — [2]Institute of Experimental Physics, Ulm University, Germay — [3]Institute of Organic Chemistry III, Ulm University, Germany

The Breath Figure process is a self-assembly based method for producing honeycomb-structured porous films. In the process, evaporation of the solvent induces cooling of solution surface, which will result in water droplets condensing and arranging into ordered hexagonal structure. In Breath Figure technique,mini-emulsion can be used to help stabilize water droplets condensed on the solution surface. Mini-emulsions are stable systems containing oil, water, and surfactant. It is obtained by a high shear process (ultrasonication technique) resulting in small, homogeneous nanodroplets. In our study, we choose organic solvent such as Chloroform and Toluene as the oil phase to make the mini-emulsion, and we measure the nanodroplets size distribution with the help of dynamic light scattering (DLS). We carry out a series of experiments to explore the different parameters like concentration of polymer, relative humidity and especially the effect of surfactant in the polymer solution on forming ordered hexagonal structures by using the Breath Figure method.

CPP 15.4 Mon 18:30 P1C

Optical studies of thermal properties of materials — •David Schönebeck[1], Jonas Pfeil[1], Anna Sailer[2], Martin Müller[1], Kay-E. Gottschalk[1], and Masoud Amirkhani[1] — [1]Institut für experimentelle Physik, Universität Ulm, D-89069 Ulm — [2]Wissenschaftliche Werkstatt Feinwerktechnik, Universität Ulm, D-89069 Ulm

Polymeric materials adsorb on suspended gold nano particle (GNP) surfaces depending on their solubility behavior in the surrounding medium. GNP have an optical absorption maximum in the visible range. This is where they heat up and can act as point heat sources to their environment. Exploiting this, one can control the solubility of UCST and LCST materials in the vicinity of GNP in the suspension. This has an influence on the hydrodynamic radius of the gold-polymer aggregates. These effects shall be studied by standard DLS investigations, thermal diffusion experiments, and later also fluorescence and fluorescence-correlation spectroscopy. The main goal of this work is to realize an experimental setup that is capable of exciting the GNP and measuring their response at the same time. We use one excitation laser near the absorption maximum and one measurement laser with lower energy pointing at the same or slightly offset position. The centerpiece of the setup is a temperature controlled glass cylinder to house the sample containers at biologically relevant temperatures. Two photon counting detectors, of which one can be rotated around the cylinder by a desired angle, detect the excitation (straight line) and the measurement (rotated) signal from the two light sources separately.

CPP 15.5 Mon 18:30 P1C

A theoretical model of the frame-guided assembly process — •Simon Raschke and Andreas Heuer — Inst. für Phys. Chem., Corrensstr. 28/30, D-48149 Münster

The formation of self assembled structures such as micelles and vesicles has been intensively studied and is well understood. Recent studies [1] use a new approach of vesicle formation by starting with a molecular frame (based, e.g., on DNA) which serves as the basis of new micelles/vesicles. In this way (i) shape and size of the desired micelle/vesicle can be predefined, e.g., by using ellipsoidal rather than spherical molecular frames, and (ii) the ability to generate regularly shaped vesicles can be enhanced.

While the self assembly of micelles/vesicles is relatively well understood, the frame-guided assembly process has not yet been explored in depth from a theoretical perspective. We developed a theoretical model of the frame and the amphiphilic molecules which via Monte Carlo simulations can be analysed to obtain information about the driving forces and the kinetic properties of micelle/vesicle formation. Via optimized simulation routines very large systems can be handled in order to be close to the typical sizes, relevant for the experimental situation.

[1] Dong, Y., Yang, Z. & Liu, D. Small 11, 3768*3771 (2015).

CPP 15.6 Mon 18:30 P1C

Investigating structure and water permeability of bilayers containing beta-cyclodextrin using MD simulations — •Alexander Kötter, Djurre Hendrik de Jong, and Andreas Heuer — Institut für Physikalische Chemie, Corrensstraße 28/30, 48149 Münster

Vesicles, based on amphiphilic cyclodextrin derivatives and phospholipids, display an interesting host guest chemistry. We study permeability and structural properties of corresponding bilayers on coarse grained and atomistic level using molecular dynamics simulations. Comparison of atomistic and coarse grained simulation for exemplary systems suggests that the structural properties are essentially preserved in the coarse grained model. Coarse grained simulations indicate, that variations of the cyclodextrin molecules, such as the length of the alkyl chain, or the length of the ethylglycole group have no significant impact on the the structural or dynamic properties of the bilayers. In particular, free energy calculations as well as the analysis of trajectories suggest that the experimentally observed dependence of the water permeability on the alkyl chain length only results from the presence of different phases in this experiment. In contrast, the introduction of phospholipids to the cyclodextrin bilayers seems to impact the microscopic structural properties of these bilayers severly. This might explain the experimentally observed differences in the shape of the pure cyclodextrin vesicles compared to the mixed phospholipid

vesicles.

CPP 15.7 Mon 18:30 P1C

Adhesion of deformable fluctuating interfaces by multiple types of functional complexes — •Josip Vlajčević[1] and Ana-Sunčana Smith[1,2] — [1]Rudjer Bošković Institute, Division of Physical Chemistry, Zagreb — [2]PULS Group, Institut für Theoretische Physik, Univesität Erlangen-Nürnberg

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, the phase behavior and the dynamics of adhesion mediated by multiple functional pairs is poorly understood.

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.

CPP 15.8 Mon 18:30 P1C

Effects of microwaves on graphene quantum dots in solution — •Alexandra Steina, Stefan Fasbender, and Thomas Heinzel — Heinrich-Heine-Universität Düsseldorf, IPkM

Fluorescent graphene quantum dots (GQDs) are prepared by the method of Wu et. al [1] via hydrothermal treatment of citric acid and dicyandiamide with subsequent dialysis to obtain a pure GQD solution. The obtained aqueous solution is treated with microwaves for various times and the effect on the chemical composition of the GQDs is studied with XPS. Fluorescence spectroscopy and UV-vis spectroscopy are used to determine the optical properties of the GQDs.

[1] Wu et al., Nanoscale, 2014, 6, 3868

CPP 15.9 Mon 18:30 P1C

Tight-Binding Simulation of Graphene Quantum Dots — •Christian Wimmenauer and Thomas Heinzel — Solid State Physics Laboratory (IPkM), Heinrich-Heine-Universität Düsseldorf

Graphene quantum dots (GQD) are simulated with an tight binding approach to obtain a better understanding of recent experimental findings regarding the electronic and optical properties of these nanoparticles. The emphasis lies on studying the influence of different edge structures, functional groups and defects on the fluorescence spectra. Using the KWANT software package, hexagonal zigzag edge type, as well as armchair edge type, GQDs have already been modeled. The results are supposed to be used to prepare GQDs with improved optical properties for biological applications.

CPP 15.10 Mon 18:30 P1C

Analysis of orange graphene quantum dots for biological applications — •Lisa Zimmermann[1], Stefan Fasbender[1], Ron-Patrick Cadeddu[2], Rainer Haas[2], and Thomas Heinzel[1] — [1]Heinrich Heine Universität Düsseldorf, IPkM — [2]Universitätsklinikum Düsseldorf, Klinik für Hämatologie

Orange fluorescent graphene quantum dots (GQDs) with an excitation optimum around 500 nm are prepared by thermal decomposition of citric acid and diethylenetriamine slightly modifying the method of Qu et al. [1]. In order to analyse the properties of the particles X-ray photoelectron spectroscopy spectra as well as fluorescence and UV-vis spectra are taken. The latter ones provide the photoluminescence quantum yield of the GQDs. The uptake of GQDs into primary human blood cells is investigated using flow cytometry and visualised via confocal microscopy.

[1] Qu et al., Light: Science & Applications, 2015, 4, e364

CPP 15.11 Mon 18:30 P1C

Polymer chains: how they influence the red blood cell motion — •Carina Bezold, Christian Bächer, and Stephan Gekle — Univesität Bayreuth

A system called glycocalyx covers the luminal surface of blood vessels. The interaction between glycocalyx, represented by polymer chains, and red blood cells and between glycocalyx and the blood flow are examined with the simulation package ESPResSo. Our simulation results show that the velocity of the red blood cell and the effective viscosity of the fluid are altered significantly by the presence of polymer chains.

CPP 15.12 Mon 18:30 P1C

Controlled Assembly of Plasmonic Core/Satellite Nanostructures for Efficient SERS Enhancement — •Roland Höller[1], Izabella Jahn[2], Martin Dulle[3], Dana Cialla-May[2], Martin Mayer[1,5], Stephan Förster[3], Jürgen Popp[2], Munish Chanana[4], Christian Kuttner[1,5], and Andreas Fery[1,5] — [1]Leibniz Institute of Polymer Research, 01069 Dresden, Germany — [2]Leibniz Institute of Photonic Technology, 07745 Jena, Germany — [3]Physical Chemistry I, University of Bayreuth, 95440 Bayreuth, Germany — [4]Institute of Building Materials, ETH Zürich, 8093 Zürich, Switzerland — [5]Cluster of Excellence Centre for Advancing Electronics Dresden (cfaed) and Technische Universität Dresden, 01062 Dresden, Germany

We present a novel protein-assisted self-assembly route of small spherical gold or silver NPs (as satellites) with a hydrophilic protein corona onto larger gold NPs (as cores) into three-dimensional nanoassemblies with core/satellite architecture in dispersion. Their interparticular gaps represent hot spots for surface-enhanced Raman scattering (SERS) detection. The highly modular bottom-up fabrication of homo- and heterometallic core/satellite combinations allows for tailored plasmonics. A precise characterization of the morphology in dispersion was achieved using small-angle X-ray scattering (SAXS). By combining the results from SAXS, UV/Vis spectroscopy, and electromagnetic simulations we were able to correlate the structural parameters with the plasmonic coupling within the core/satellite nanoclusters.

[1] Höller, R.P.M. et al., ACS Nano 2016, 10, 5740-5750.

CPP 15.13 Mon 18:30 P1C

The Dielectric Permittivity of Protein Solutions — •Susanne Liese and Roland R. Netz — Department of Physics, Free University Berlin, Arnimallee 14, 14195 Berlin, Germany

Electrostatic interactions are essential to understand the conformation and function of proteins. For a quantitative understanding of electrostatics of biological systems, for instance to describe the internal electric field of transmembrane proteins, the dielectric permittivity of proteins has to be known. We here present molecular dynamic simulations of protein solutions, which especially allow us to take the interaction of the protein and the hydration water into account. By studying the dielectric permittivity in dependence of the protein concentration, we can extrapolate our results to the limit of a pure protein and disentangle water and protein contributions to the electrostatic interaction.