Wednesday, 28.08.2019, Room G 91

Time	ID	Biophysics, Medical Physics and Soft Matter *Chair: Giovanni Dietler, EPFL*
17:00	901	**Amyloid fibril growth: A multiscale view** *Ioana Ilie [1], Wouter Den Otter [2], Wim Briels [2], Amedeo Caflisch [1]* *[1] University of Zürich, [2] University of Twente* The accumulation of amyloid fibrils is the hallmark of Parkinson's and Alzheimer's disease. We use atomistic and coarse-grain simulations to explore the intricate dynamics and aggregation of α-synuclein and amyloid-β(42), the proteins associated with these disorders. We represent α-synuclein as a chain of deformable particles that can adapt their geometry, binding affinities and rearranges into disordered and ordered structures. Results offer valuable insight into the internal dynamics of α-synuclein and indicate that a protein attaching to a fibril gets trapped in sub-optimal configurations, explaining the experimentally observed stop-and-go-growth of an amyloid fibril. We use atomistic simulations to explore the peptide dissociation from an amyloid-β(42) fibril. Simulations show structural stability of the fibrillar core and high flexibility registered at the tip.
17:15	902	**Effects of gravity on the alpha-synuclein aggregation** *Jiangtao Zhou [1], Francesco Ruggeri [2], Sergey Sekatski [1], Giovanni, Dietler [1]* *[1] EPFL, [2] Cambridge* Amyloid fibrils are the pathological hallmarks of many neurodegenerative diseases, including Alzheimer's and Parkinson's diseases, yet the mechanism of protein aggregation and fibrillization are not fully understood. Studying the protein aggregations in the microgravity/un-gravity condition can play a fundamental importance in discovering the aggregation mechanisms, and the influence of gravity on morphologies and configurations of aggregates as well as their aggregation behavior. In this research, we mainly focus on the low-gravity effect on alpha-synuclein aggregation in vitro, and combined various techniques, including atomic force microscope (AFM), Thioflavin T (ThT) and circular dichroism (CD), to measure the morphological transformation, aggregation kinetics, secondary structural transition during aggregation, and reasonable achievements have been achieved.
17:30	903	**Picture of Wet Electron: A Localized Transient State in Liquid Water** *Michele Pizzochero [1], Francesco Ambrosio [2], Alfredo Pasquarello [2]* *[1] Chaire de Physique Numérique de la Matière Condensée (C3MP), EPFL* *[2] Chaire de Simulation à l'Echelle Atomique (CSEA), EPFL* A transient state of the excess electron in liquid water preceding the development of the solvation shell, the so-called wet electron, has been invoked to explain spectroscopic observations, but its properties have remained elusive. Here, we carry out hybrid functional molecular dynamics to unveil the ultrafast mechanism leading to the hydrated electron. In the pre-hydrated regime, the electron is found to repeatedly switch between a quasi-free electron state and a localized state with a binding energy of 0.26 eV, which we assign to the wet electron. This state self-traps in a region of the liquid which extends up to 4.5 Å and involves a severe disruption of the hydrogen-bond network. Our picture provides an unprecedented view on the wet electron.

17:45	**904**	**Gap plasmon resonance-enhanced high spatial resolution imaging by photothermal induced resonance in visible spectral range** *Sergey Sekatski, Jiangtao Zhou, Anton Smirnov, Giovanni Dietler, EPFL* The method of infrared nanospectroscopy and high spatial resolution imaging by photothermal induced resonance (PTIR) proved its viability and utility for many studies. We discuss our results on development of the method in visible spectral range. Its performance was enhanced by both factors: the coincidence of the resonant frequency of an AFM tip dithering with the laser pulse repetition range, and plasmon gap resonance. In the visible, the latter is very sensitive to the properties, first of all thickness, of the sample studied, and this dependence may create a contrast mechanism for the imaging even in the case of inefficient light absorption. We present a few nm resolution images of chlorophyll a monolayers and amyloid fibrils.
18:00	~~**905**~~	*cancelled*
18:15	**906**	**Combined optical and acoustic trapping for optical tomography** *Mia Kvåle Løvmo, Benedikt Pressl, Gregor Thalhammer, Monika Ritsch-Marte* *Division of Biomedical Physics, Medical University Innsbruck* Exploiting the benefits of the two types of forces from optical and acoustic trapping schemes in a single setup allows us to manipulate biological samples in a contact-free and non-invasive way. With our system we levitate sub-millimeter sized samples in solution on a microfluidic chip compatible with various optical imaging techniques. We have developed a 3D ultrasonic resonator with custom made transducers to optimize the acoustic power transfer and controllability. The combination with optical tweezers allows for force estimations, increased precision in patterning, manipulation and induced rotation of the sample for optical tomography. Long-term monitoring of samples without mechanical confinement would potentially be a valuable tool for studying embryos, cell clusters and organoids for development and drug-screening purposes.
18:30	**907**	**Phase behavior in polydisperse microgel suspensions controlled by spontaneous particle deswelling** *Urs Gasser, Paul Scherrer Institut, Andrea Scotti, RWTH Aachen University,* *Alberto Fernandez-Nieves, GaTech and Univ. Barcelona* Crystallization is often suppressed by point defects due to larger impurity particles. Surprisingly, microgels can overcome this limitation: Large microgels can spontaneously deswell to fit into the crystal lattice of smaller but otherwise identical microgels. We find this unique reduction of polydispersity and particle deswelling to be triggered by a difference in osmotic pressure between the inside and the outside of the microgel particles that is set by counterions. We find the freezing point of polydisperse and bidisperse pNIPAM suspensions to be linked to particle deswelling. In comparison to hard, incompressible colloidal particles, this particle deswelling mechanism fundamentally changes the role of polydispersity in microgel suspensions.
18:45		***END***
19:00		***Transfer to Dinner***
19:30		***Conference Dinner***

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Microfabricated cantilever beams for rapid bacterial sensitivity tests

Anton Malovichko, Sandor Kasas, Giovanni Dietler, EPFL

With the misuse of antibiotics, antimicrobial resistance becomes a very serious public health issue. Proposed technique of antibiotic sensitivity characterization is based on the bacterial nanomotion. The organism of interest is attached onto a cantilever and nanoscale movements induce cantilever oscillations. If the organism is exposed to an antibiotic to which it is sensitive, the oscillations stop.
Alternative approach to conventional AFM, based on the use of light-transmitting polymer as a waveguide and cantilever at the same time, allows to have simple parallel optical readout. Light can be coupled into several waveguides simultaneously, to collect signal from several output lightspots with a CCD camera. Custom design of the cantilevers also gives possibility of micropatterning of cantilever surface with microorganisms.

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Simulation of a microfluidic system of droplets

Johannes J. Schneider, Mathias S. Weyland, Dandolo Flumini, Rudolf M. Füchslin
Institute for Applied Mathematics and Physics, Zurich University of Applied Sciences

We simulate how droplets released from a linear droplet generator arrange themselves in a threedimensional way within a surrounding hull. During this arrangement process, droplets touching each other can form bilayers, which then can be broken up and reformed again. For studying this process, we perform macroscale Monte Carlo movement simulations with a simplified rule set for the slowing down and acceleration of droplets, embedding some extent of randomness in the change of movement and in the probabilities for bilayer formation and destruction. We aim at qualitatively reproducing the three-dimensional structures achieved in experiments performed by our EU project partners in Cardiff. As a next step, we aim at predicting the experimental outcome.