CPP 76: Focus: Polymers in Multi-Compartment and Aqueous Solutions II - organized by Jens-Uwe Sommer and Debasish Mukheri

Time: Friday 9:30–11:30 Location: C 130

Topical Talk CPP 76.1 Fri 9:30 C 130

Optimal inhibition and spatial organization of irreversible protein aggregation using liquid compartments — •Christoph A. Weber[1,2], Thomas Michaels[1], and L. Mahadevan[1] — [1]Harvard John A. Paulson School of Engineering and Applied Science, Cambridge — [2]Max Planck Institute for the Physics of Complex Systems, Dresden

Protein aggregation in cells is an ubiquitous phenomenon and linked to a large variety of diseases, such as Alzheimer's and Parkinson's disease, amyloidosis or type II diabetes. So far, there is no effective strategy to suppress or inhibit protein aggregation in these systems. Typically, it has been suggested to design drugs which stabilize monomers against aggregation, or block the surface or the ends of aggregates. We show that this treatment strategy can be optimized increasing dramatically the life time of the cell. In addition, we suggest a novel strategy, namely to spatially segregate protein aggregation in distinct liquid-like cellular compartments in a controllable fashion. Many cells actually use droplet-like compartments to spatially organize the cellular cytoplasm but only little is known about their biological function. Here, we show that liquid compartments are ideally suited to spatially organize protein aggregation. Aggregation only occurring in these compartments keeps the toxic aggregates away from the sensible intracellular surrounding and allows subsequent localized and specific degradation by the cellular machinery or drugs. Since the compartment assembly creates costs we employ optimal control theory to determine the optimal physical parameter for spatial segregation of protein aggregation.

CPP 76.2 Fri 10:00 C 130

Molecular insights into the temperature-induced transition of Poly(N-n-propylacrylamide) (PNnPAm) in aqueous solution. — •Tiago Espinosa de Oliveira[1], Carlos Marques[1], and Paulo Netz[2] — [1]Institut Charles Sadron, CNRS, Strasbourg, France — [2]Universidade Federal do Rio Grande do Sul, Proto Alegre, Brazil

The possibility of tuning the molecular structure of smart polymers increases the potential of technological applications of these materials. In this context, N-substituted acrylamide-based polymers exhibit a drastic phase transition by slight changes in temperature. Moreover, Poly(N-n-propylacrylamide) (PNnPAm) and Poly(N-isopropylacrylamide) (PNIPAm) are polymers which exhibit a lower critical solution temperature (LCST) at 297 and 305 K, respectively. Furthermore, PNnPAm exhibits a sharp and discontinuous phase transition in aqueous solution, in contrast to PNIPAm. In this work, we carried out all-atom molecular dynamics simulations to understand, from a microscopic point-of-view, the influence of chain size and concentration on the LCST of PNnPAm compared to PNIPAm. Our analysis not only shows that the chain length has a strong influence on the LCST but allows also to discriminate the role of the hydration and intramolecular interactions in the collapsing transition.

CPP 76.3 Fri 10:15 C 130

Implicit-solvent coarse-grained models of thermoresponsive polymers — •Richard Chudoba[1,2], Jan Heyda[3], and Joachim Dzubiella[1,2] — [1]Inst. für Physik, Humboldt-Universität zu Berlin, Germany — [2]Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin, Germany — [3]Dept. of Physical Chemistry, University of Chemistry and Technology, Prague, Czechia

Thermoresponsive polymers have become an integral building block for the development of 'smart', environment-sensitive materials with tunable properties. In particular close to their lower-critical solution temperature (LCST), those polymers show dramatic changes in their physicochemical properties, in response to only tiny changes in the solvent environment, e.g., salt concentration.

Here, we develop and employ a coarse-graining strategy for explicitly temperature-dependent implicit-solvent models of thermosensitive polymers in aqueous solution that are applicable in a wide temperature range, including the crossing of the LCST. We combine both bottom-up and top-down approaches, i.e., atomistic simulations coupled with the iterative Boltzmann inversion method and adjustment of the force field parameters based on the experimental data, to faithfully capture structural and thermodynamic properties of the thermoresponsive polymers. Our primary target is polyethylene glycol (PEG), a versatile polymer in soft material development.

• Chudoba, R.; Heyda, J.; Dzubiella, J. Temperature-Dependent Implicit-Solvent Model of Polyethylene Glycol in Aqueous Solution. J. Chem. Theory Comput. 2017, doi: 10.1021/acs.jctc.7b00560.

CPP 76.4 Fri 10:30 C 130

Upper Critical Solution Temperature (UCST)-type Thermoresponsive Polymers from Hydrogen-Bonding Monomers — Asad Asadujjaman[1], Vahid Ahmadi[1], and •Annabelle Bertin[1,2] — [1]German Federal Institute for Materials Research and Testing (BAM), Dpt. 6 Materials Protection and Surface Technologies, Unter den Eichen 87, 12205 Berlin, Germany — [2]Freie Universität Berlin, Institute of Chemistry and Biochemistry, Takustr. 3, 14195 Berlin, Germany

UCST-type thermoresponsive polymers (i.e. that phase separate from solution upon cooling) present a tremendous potential not only in aqueous media where they can be used in drug delivery, diagnostic and microfluidic applications, but also in water/alcohol mixtures, where they can be used for instance in sensing systems for alcohol-soluble drugs. However, only a few thermoresponsive polymers have been reported that present an UCST in a relevant temperature range and "green" solvents such as water or ethanol. In this context, acrylamide-based monomers can be very useful building blocks for designing novel non-ionic UCST-type polymers because of their hydrophilic nature (with the appropriate side chain) and propensity to form hydrogen bonds. We will present our latest results on the UCST-type thermoresponsive behaviour of acrylamide- and 2,6-diaminopyridine-based homopolymers and copolymers in water or water/alcohol mixtures, and give some insights about the rational design of UCST polymers relying on H-bonding.

CPP 76.5 Fri 10:45 C 130

Molecular Dynamics simulations of strain-induced phase transition of poly(ethylene oxide) in water — •Sergii Donets[1], Olga Guskova[1], and Jens-Uwe Sommer[1,2] — [1]Institute Theory of Polymers, Leibniz-Institute of Polymer Research, D-01069 Dresden, Germany — [2]Technische Universität Dresden, Institute for Theoretical Physics, D-01069 Dresden, Germany

An aqueous solution of poly(ethylene oxide) (PEO) oligomers is considered as a potential candidate capable of undergoing a phase transition as a result of loss of the hydrated structure. Our simulations using an atomistic model for PEO and water clearly indicate that an elongating force dipole acting on both chain ends of oligomer chains initiates interchain aggregation with the formation of highly oriented fibrillar nanostructures. The strain-induced demixing transition occurs primarily due to the favorable van der Waals interactions between the PEO chains. A tensile stress introduced into the aqueous solution of PEO changes the solvent quality from good to poor as a function of conformational state of the chains and, if there are other oligomer chains present in the simulations box, leads to a phase separation of PEO from water. The strain-induced demixing of the extended PEO chains provides the possibility to obtain polymer fibers with low energy costs.

Topical Talk CPP 76.6 Fri 11:00 C 130

Diffusion of proteins in bicontinuous microemulsions: controlled soft nano-confinement — •Thomas Hellweg, Oliver Wrede, and Ralph Neubauer — Physikalische und Biophysikalische Chemie, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany

The interior of cells is crowded with different objects and the diffusive behaviour of proteins often does not follow the normal Fick type diffusion, where the mean square displacement grows linearly in time $\langle x^2 \rangle \propto t$. The diffusion is considered to be sub-diffusive if $\langle x^2 \rangle \propto t^\alpha$ (with $\alpha < 1$) [1]. However, due to the complexity of the cellular matrix it is very difficult to control the crowding conditions or the confinement and to make systematic studies inside living cells. Hence, to better understand the dependence of protein diffusion on a confining environment, we study the movement of a fluorescent protein (GFP+) through bicontinuous microemulsions via FCS. The sponge like microemulsion structure, which is characterized via small angle scattering, not only slows down the translational movement of the tracer particle with de-

creasing domain size but also changes the characteristics of the diffusion from "Fick like" to "anomalous"[1]. Additional relevance for such works arises due to the use of microemulsions as reaction media for enzymatically catalyzed reactions [2].

[1]R. Neubauer, S. Höhn, M. Dulle, A. Lapp, C. Schulreich, and T. Hellweg, Soft Matter 13 (2017), 1998
[2]S. Wellert et al., Euro. Biophysics J., 40 (2011) 761