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Multiscale modeling of soft matter and its Integration to Experiment

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The systematic multiscale of heterogeneous soft matter systems is an area of current research. Soft matter materials involve complex multiscale problems. Several techniques to systematically and directly link different length scales are presented where the focus will be on the Iterative Boltzmann Inversion (IBI) as well as on reactive modeling. After introducing the techniques I will show three examples of current problems we can address with our techniques which include Organic Electronics, Carbon nanotubes and protein glycosylation. In all examples connections between connections between experiment and simulation will be pointed out.

We apply our multiscale modeling technique to a system for polymer-based solar cells which show promise as a cheap alternative to current silicon-based photovoltaics. Typical systems use a mixture of a light-absorbing conducting polymer as the electron donor and a fullerene derivative as the electron acceptor in the solar cell's photo-active layer. Prediction of the active-layer microstructure based on the constituent materials remains challenging. Atomistic computer simulations are only feasible to study very small systems. We overcome this hurdle by developing a coarse-grained (CG) simulation model of mixtures of the widely used conducting polymer poly(3-hexylthiophene) (P3HT) and various fullerenes. We then use the CG model to characterize the structure and dynamic evolution of the BHJ microstructure as a function of polymer:fullerene mole fraction and polymer chain length for systems approaching the scale of photovoltaic devices. Recently we were able to turn to the very small length scale and explain neutron scattering data.
Carbon nanotubes (CNTs) of finite length assembled in small bundles were modeled with molecular dynamics simulations. An interesting tilt angle is observed in small hexagonal bundles, in which the outer CNTs spirally tilt to one direction with respect to the center. This effect was characterized with CNTs of different lengths. Narrower CNTs are more parallel, while thicker ones show larger tilt angles and stronger vibrations. This tilt effect was confirmed for both armchair and zigzag type CNTs. The present work for the first time unveils the tilt effect of small CNT bundles in finite length. Also such materials can be used to separate gases which are otherwise hard to separate (e.g. noble gases) and we discuss this application.

Glycosylation is an important posttranslational modification of proteins and plays a crucial role in protein efficacy. It also needs to be understood for optimization of recombinant protein expression. Here, glycoprotein 3D structures are studied using highly detailed and coarse-grained models starting from known crystal structures to examine the effect of oligosaccharides on glycoprotein structure to evaluate the accessibility of the oligosaccharide chains to glycan modifying enzymes. Computational methods for modeling glycoprotein structures are employed to understand how changes in site-specific oligosaccharide composition and structure influence 3D glycoprotein structure, protein oligomerization, and product quality attributes such as activity/efficacy, stability, and immunogenicity. We also use mainly Coarse-Grained (CG) molecular dynamics (MD) to study the impact of oligosaccharides on glycoprotein structure and oligomerization, exposure of the oligosaccharides at different sites and match between specific target enzyme active sites and exposed oligosaccharides.

Hörsaal 3, Campus Rheinbach

Donnerstag, 27. Juni 2019, 17.00 Uhr, Meet the Prof. und Diskussion mit Studierenden nach der Vorlesung