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Polymers - Soft Matter

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Synthetic polymeric materials, most biological, colloidal and many other systems are nowadays termed soft matter. They are soft because they are dominated by a typically nanometer (and larger) length scale and the corresponding energy density for the non-bonded interactions is many orders of magnitude smaller than for conventional solids. This energy density to a very first approximation is a good guess of the elastic constants, thus they are "very soft". In particular for the above mentioned materials the thermal energy k_BT is the characteristic energy scale and consequently entropy plays an important role. Soft matter means strongly fluctuating matter. When the fluctuations are mostly frozen one usually is left with a disordered, glassy system. Only in exceptional cases one can obtain (then very important) crystalline structures. For simulation studies and a quantitative understanding in general, this means that it is not sufficient to study just local interactions but one must link this to larger scales. Depending on the problem this can reach from the Å-level up into the μm scale and some times beyond. Each length scale under consideration has its own characteristic methods of investigation. Sometimes they are treated individually in order to study specific effects; in other cases they are combined in order to derive a more quantitative overall understanding. In this respect the four contributions on macromolecules in this report to some extent represent the width and the typical questions of the field. They range from basic studies towards a better design of specific fuel cell components to highly idealized protein models where generic aspects of how a large molecule can fold/unfold in the presence of a (selective) surface are studied. Similarly they range from aspects close to application to fundamental first principle tests.

First Bachmann and Janke study a lattice model of HP proteins. This is a most basic model, where the protein is reduced to hydrophilic (polar) and hydrophobic units and is frequently employed to study fundamental aspects of protein folding. Each unit models a residue. By the use of an improved growth algorithm for the condensed phase they were able to study different heteropolymers (statistical proteins) of up to 103 units. Their emphasis was not so much on the folded configuration itself but rather on the behavior close to an adsorbing surface, where this surface attracts the P, the H or both units. With the help of their improved algorithm and massive CPU time support from NIC they were able to map out a characteristic structure diagram as function of the surface coupling. Questions like this occur in fields like protein crystallization as well as many technical applications where protein coatings are wanted or are encountered as contamination. Surfaces and interfaces in general play an important role in polymer physics, chemistry and technology. Seidel and Kumar study polyelectrolyte chains bound by one end to the surface, so called polyelectrolyte brushes. Most synthetic polymers are strongly hydrophobic, thus they are not at all water soluble. One way to change that is to add side groups, which dissociate ions in water. Then the chains are charged and become water soluble due to the high

osmotic pressure of the released ions. Attached to the surface of e.g. a colloid, the colloid can not coagulate any more; they are electrostatically and sterically stabilized. Seidel and Kumar now treat such a polyelectrolyte brush as a function of salt added to the solution. The addition of salt reduces the osmotic pressure of the counter ions and consequently the brushes shrink. It is this shrinking which they study in comparison to analytic theory and also in relation to experiment.

So far simple chains or rather dilute systems have been discussed. Dense polymeric melts and solutions, however, represent a continuing challenge to scientists. For simulations the extremely long relaxation times often limit the studies. Thus there is a continued effort to overcome this by new methods. Müller, Paul and Binder shortly review extensive work on phase transitions employing so called single chain mean field (SCMF) simulations. The trick is to couple a Monte Carlo simulation of a single polymer with a density field of the surrounding polymers and then in a self consistent way evolve the surrounding field due to the simulation of the chain. The power of this approach is demonstrated for several examples and compared to more conventional Monte Carlo simulations. For the cases applicable it reduces the computational effort dramatically. They start out with the benchmark problem of spinodal decomposition in binary polymer blends, a very well studied problem which allows best to test the power of the method. Then this is applied to two cases, which are important to nanotechnology, namely the drying of thin polymer films and the microphase separation of block copolymers on patterned substrates, which selectively bind one of the two components with a pattern which is commensurable or incommensurable with the ordered block copolymer melt.

Finally Kulikovsky and Spohr look at low temperature fuel cells as a whole as well as at specific components. They follow an integrated ansatz in order to support the technology developed at the FZ Jülich. These calculations are very involved and link quantum chemical studies, all atoms force field simulations as well as systems engineering methods. In each case specific problems which are crucial for a better technical design are investigated. On the quantum chemical side they study the oxidation of methanol on noble metal catalysis as it occurs in DMFCs (Direct Methanol Fuel Cell). Currently the technological setup requires a high, thus costly load of noble metals, which also turns out to participate in performance limitations. Therefore the authors study such processes under realistic conditions. In a second part the mobility of protons in typical fuel cell membrane such Nafion is studied by careful all atom force field molecular dynamics simulation of type, which allows the formation of strong hydrogen bonds and proton transfer. Finally the whole system is studied with a continuum approach on an engineering level in order to better understand fluxes of charges, heat but also gases and water in the PEFLs (Polymer Electrolyte Fuel Cell) which use hydrogen instead of methanol as fuel. These are just three problems of recent fuel cell research, which require significant support from computer simulations.

These examples give a short overview of the soft matter activities at NIC. Current scientific and technological developments which more and more incorporate knowledge and capabilities from very different areas, such as physics, chemistry, biology and materials engineering to name just the most important ones, demand a comprehensive understanding of complicated systems. Such an understanding is not possible without the use of well focussed massive computer simulations.