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Advanced Computer Simulation Approaches for Soft Matter Sciences II

Volume Editors: Christian Holm, Kurt Kremer

With contributions by

A. Arnold · C. Holm · D. Levesque · P. Linse
M. Müller · F. Schmid · J.-J. Weis

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The series *Advances in Polymer Science* presents critical reviews of the present and future trends in polymer and biopolymer science including chemistry, physical chemistry, physics and material science. It is adressed to all scientists at universities and in industry who wish to keep abreast of advances in the topics covered.
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Preface

Soft matter science is nowadays an acronym for an increasingly important class of materials, which encompasses polymers, liquid crystals, molecular assemblies building hierarchical structures, and the whole area of colloidal sciences. Common to all of them is that fluctuations and thus the thermal energy $k_B T$ and the entropy play an important role. Soft then means that these materials are in a state of matter that are neither simple liquids nor hard solids of the type studied in hard condensed matter, hence sometimes soft matter firms also under the name complex fluids.

Soft matter, either of synthetic or biological origin, is a subject of physical and chemical research since the early findings of Staudinger that long chain molecules exist. From then on synthetic chemistry as well as physical characterization underwent an enormous development. One of the outcomes of this is the abundant presence of polymeric materials in our every day life. Nowadays, methods developed for synthetic polymers are being more and more applied to biological soft matter. The link between modern biophysics and soft matter physics is quite close in many respects. This also means that the focus of research moved from simple homopolymers to more complex structures, such as branched objects, heteropolymers (random copolymers, proteins), polyelectrolytes, amphiphiles and so on. While basic questions concerning morphology, dynamics and rheology are still of interest, additional, more advanced topics, concerning for example the link between structure and function, are being tackled as well.

For many years now there have been attempts to understand these systems thoroughly by theoretical concepts. Beginning with the early work of Flory, simplified models were studied, which were able to explain certain generic/universal aspects but failed to provide a solid theoretical basis for this universal behavior. It was then up to the seminal works of deGennes and Edwards to provide a link between statistical mechanics of phase transitions (critical phenomena) and polymer chain conformations. This link to modern concepts of theoretical physics provided an huge momentum for the field, which shaped many theoretical schools and formed the basis for modern soft matter physics. Despite all these developments, soft matter theory still is an active and growing research field. Due to the high degree of the complexity of the problems it is not surprising that analytical theory can only treat highly ideal-

ized and simplified models. Consequently, with the availability of computers, problems in polymer science were among the first to be tackled by simulations. Already the problem of an isolated self avoiding walk cannot be solved exactly in space dimension 3. As early as 1954 Hammersley and Morton, and Rosenbluth and Rosenbluth, tried to overcome the related attrition problem in growing self avoiding walks by introducing the so called inversely restricted sampling. In addition, basic multi-chain features, such as the noncrossability of chains, are hard to deal with analytically, and can only be included properly with a simulation approach. Thus, with the rising availability of computing power, simulation methods play an increasingly important role in soft matter research. Sole computing power is, however, only one aspect. Even more important has been the development of advanced numerical methods and highly optimized programs. There, very different areas, ranging from quantum chemistry studying molecules on the sub-Ångstrøm level, all the way to macroscopic fluid dynamics come together and offer a unique set of research opportunities. Over the years the role of computer simulations went beyond the traditional aspect of checking approximative solutions of analytical models and bridging the gap between experiments and theory. They are now an independent, in some cases even predictive, tool in materials research, for example for complex molecular assemblies or specific rheological problems.

It is the purpose of this small series of volumes in Advances in Polymer Sciences to provide an overview over the latest developments in the field. For this, internationally renowned experts review recent work in the general area of soft matter simulations. The second volume contains four contributions, and has a very strong topical focus on long range interactions.

In the first contribution M. Müller and F. Schmid show how fluctuations and dynamics can be described in polymer blends using self-consistent field theories. Starting from the Edwards model external potential theory and self-consistent field theory are introduced. Then the authors show how fluctuations can be treated by field-theoretic means in a Langevin and Monte Carlo approach. Finally dynamical questions and applications to polymer blends and the problem of spinodal decomposition are illustrated. The next three contributions deal all with methods or systems where long range interactions such as Coulomb or dipolar interactions play the dominant role. These kinds of systems are difficult to simulate since the dominant computer time is spent in calculating the long range interaction. Even worse, the computer time can rise with the number N of charged particles as $\mathcal{O}(N^2)$, and not linearly as with purely short range interactions. During the last fifteen years a number of efficient techniques have been devised to overcome the scaling problem, and several of these algorithms are described in the following three chapters. In the contribution by A. Arnold and C. Holm a variety of methods to efficiently sum the Coulomb sum in 3D and partially periodic geometries is reviewed, ranging from the particle mesh algorithm P^3M up to a very recent convergence factor approach called MMM. Particularly the error control is stressed

in this contribution. Also other methods such as the fast multipole methods, and a lattice approach termed Maggswellian dynamics, as well as the standard dipolar Ewald sum, are reviewed. In the third contribution P. Linse introduces efficient Monte Carlo methods to deal with charged colloidal systems. Here, practical guidelines for using the standard Ewald sum, and efficient cluster moves, as well as ways to study solutions within spherical and cylindrical cell models are presented. In the last contribution by J.-J. Weis and D. Levesque especially methods for dipolar systems are presented and an extensive review of simple dipolar fluids, which includes ferrofluids and dipolar liquid crystals are given. The review ends with a section of the closely related and industrially interesting electro- and magneto-rheological fluids.

We are confident that this collection of reviews will turn out to be a proper guidance to interested scientist and advanced students, as well as to provide detailed background information to the experienced researcher in the field.

Mainz, August 2005 *C. Holm* and *K. Kremer*

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