From stochastic thermodynamics to the cost of precision

Udo Seifert

Institut fuer Theoretische Physik Universitaet Stuttgart

All processes in cell and molecular biology and those in (wet) micro- and nano-robotics are subject to thermal noise. Still, life relies on the fact that the result of such a process comes with a small enough uncertainty, i.e., large enough precision. While absolute precision is impossible in an environment of finite temperature, an obvious question is whether or not there is a fundamental trade-off between precision and the (free energy) cost of generating the process.

In the talk, after recalling the principles of stochastic thermodynamics, I will introduce the recently discovered thermodynamic uncertainty relation that provides the minimal cost for a given precision of any process running under non-equilibrium steady-state conditions. As another facet, this relation yields a model-free lower bound on the efficiency of any molecular motor just using experimental data as I will show for kinesin. I will close with recent insights into the minimal cost for generating coherent oscillations in (biochemical) networks

Phase behavior and regulation in cell membranes

Martin Girard

Max Planck Institute for Polymer Research

Biological membranes tune their composition when environmental conditions are changed. There are hundreds of different chemical components in membranes. Experimental evidence suggest composition is kept close to a critical point, which requires an astounding precision. A tight regulation of these components would require a sophisticated machinery that still eludes our understanding. Beyond the regulation of biological systems lies the question of why the need of so many different components. Given that cells incur a cost for complexity and that a handful of components in membranes would be sufficient for control of macroscopic properties, e.g. viscosity, this appears counterproductive.

Here, I discuss an alternative basis, where composition is driven by a constrained free energy minimization, which alleviates the need of complex sensing mechanisms. It also allows us to probe phase behavior of mixtures of N components. I will show that such systems can behave as-if critical for all temperatures below an onset temperature Tfs. This is a general phenomenon arising from unusual finite-size effects provided that interactions between components derive from distance along an order parameter, for instance lipid saturation or hydrophobicity. I will discuss the robustness of the model and the consequences on protein ordering. Beyond alleviating the need for active regulation, this highlights that there is some order hidden within the chaotic looks of biological systems.

Understanding experiments in liquid crystals

Helen Gleeson

School of Physics and Astronomy, University of Leeds

Experimental studies of soft matter are an important part of the jigsaw that adds up to a detailed understanding of complex materials. However, working together with experts in simulations allows experimentalists to present a much fuller picture of our understanding. This talk begins with an introduction that exemplifies how simulation and experiment led to a deep understanding of elasticity in the nematic phases formed from bent-core liquid crystals. It then goes on to describe some new experimental results in liquid crystals where we have aimed to use defect transitions to produce a biosensor - which could be used to detect Covid. I will describe our observations and challenges in understanding some fundamental transitions that rely on defects.

Characterizing the Disordered Microphases of SALR Models

Patrick Charbonneau

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The disordered microphases that develop in the high-temperature phase of systems with competing short-range attractive and long-range repulsive (SALR) interactions exhibit a rich array of distinct morphologies, such as cluster, void cluster and percolated (gel-like) fluids. These various structural regimes, however, also give rise to a sluggish and heterogeneous relaxation dynamics, which can be challenging to surmount in numerical simulations as well as in colloidal experiments. In this talk, I present a thorough characterization of the disordered microphases of two families of schematic SALR models. The Bethe lattice solution of a SALR model is obtained using a cavity calculation, and the equilibrium behavior of a real-space SALR model is obtained using advanced Monte Carlo sampling schemes. These results help identify universal features of disordered microphases and contextualize the challenge of colloidal microphase assembly.

Defects and elasticity in liquid crystalline systems

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Breaking of the continuous rotational symmetry, in anisotropic fluids, is associated with a tensorial orientational order parameter (the *director*) field; distortions of the director are controlled by curvature elastic moduli, whereas singularities and discontinuities in the ordering represent topological defects [1]. The latter are responsible for the colored patterns that are usually shown in images of liquid crystals and the name *nematic* was in fact inspired by the thread-like defect textures observed under the microscope. Topological defects have a high energy cost, which can be divided into a contribution of the core, the region in which nematic order breaks down, and an elastic contribution, accounting for the distortion of the director field. Defects can be generated and stabilized by inclusions, boundaries, chirality, microfluidic flows or electric fields. They experience long range interaction mediated by the elastic background and under proper conditions can be organized into ordered structures, such as blue phases and regular arrays obtained by geometric frustration or applied fields [2,3]. Moreover, defects are involved in the organization and dynamics of active nematics [4]. On one side defects are unwanted for most display applications, which rely on perfect alignment of liquid crystals. On the other side, however, defect engineering can be exploited e.g., for polymer templating and colloidal self-assembly [5,6] or for the design of optically functional materials [7].

Deformation free energy is a key element for the control of topological defects. Findings of the last decades have revealed unexplored aspects of liquid crystal elasticity, which have stimulated theoretical and computational research [8-12]. Here, after a brief overview, I will focus on three examples, which are useful to illustrate some emerging concepts and open questions, i.e., modulated nematic phases [13,14] chromonic liquid crystals [15-17] and chiral inclusions in membranes [18,19].

[1] M. Kleman and O. D. Lavrentovich. Soft matter physics: An introduction. Springer, New York, 2003.
[2] T. Araki, F. Serra, and H. Tanaka, Soft Matter 9, 8107 (2013).
[3] P. J. Ackerman, Z. Qi, Y. Lin, C. W. Twombly, M. J. Laviada, Y. Lansac and Ivan I. Smalyukh, Sci. Rep. 2, 414 (2012).
[4] A. Doostmohammadi, J. Ignes-Mullol, J. M. Yeomans and F. Sagues, Nat. Commun. 9, 3246 (2018).
[5] P. Poulin, H. Stark, T. C. Lubensky and D. A. Weitz, Science 275, 1770 (1997).
[6] I. Musevic, M. Skarabot, U. Tkalec, M. Ravnik and S. Zumer, Science 313, 954 (2006).
[7] M. S. Kim and F. Serra, Adv. Optical Mater. 8, 1900991 (2020).
[8] M. Cestari, E. Frezza, A. Ferrarini, and G. R. Luckhurst. J. Mater. Chem. 21, 12303 (2011).
[9] A. A. Joshi, J. K. Whitmer, O. Guzman, N. L. Abbott, and J. J. de Pablo. Soft Matter 10, 882 (2014).
[10] J. V. Selinger. Liq. Cryst. Rev. 87, 129 (2018).
[11] E. G. Virga. Phys. Rev. E 100, 052701 (2019).
[12] D. Revignas and A. Ferrarini. Phys. Rev. Lett. 125, 267802 (2020).
[13] A. Jakli, O. D. Lavrentovich, and J. V. Selinger. Rev. Mod. Phys. 90, 045004 (2018).
[14] J. V. Selinger. ArXiv, page arXiv 2103.03803, 2021.
[15] J. Jeong, Z. S. Davidson, P. J. Collings, T. C. Lubensky, and A. G. Yodh. Proc. Natl. Acad. Sci. USA 111, 1742 (2014).
[16] S. Zhou, S. V. Shiyanovskii, H.-S. Park, and O. D. Lavrentovich. Nat. Commun. 8, 14974 (2017).
[17] E. Romani, A. Ferrarini, and C. De Michele. Macromolecules 51, 5409 (2018).
[18] J. M. Miller, C. Joshi, P. Sharma, A. Baskaran, A. Baskaran, G. M. Grason, M. F. Hagan, and Z. Dogic. Proc. Natl. Acad. Sci. USA 116, 15792 (2019).
[19] M. Pannuzzo, B. Szala, D. Raciti, A. Raudino, and A. Ferrarini. J. Phys. Chem. Letters 10, 5629 (2019).

Machine Learning of Defects in Soft Dynamic Assemblies

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Abstract

A central paradigm in self-assembly is to create ordered structures starting from molecular monomers that spontaneously recognize and interact with each other via noncovalent interactions. In the last decades, a lot of efforts have been put in reaching perfection in generating supramolecular structures with various shapes and architectures.[1] While in the literature such assemblies are often represented as ideal (perfect) supramolecular fibers, micelles, vesicles, etc., submolecular-resolution simulations recently showed that, as a common ground, local defects that may be present, or dynamically emerge, in these structures are key in controlling the dynamic behavior of the assemblies.[2-5] However, the elusive, statistical nature of such defects poses fundamental questions: How can we unambiguously identify defects in soft and dynamic assemblies? Can use defects to compare and classify different assemblies? If yes, how? And finally, can we learn how to control defects and thus how to control the assembled materials *a priori*? Machine learning and molecular models are helping us to make the first steps in this direction.[5-8] We observe that defects and their dynamics can be used as a common ground to unify and compare self-assembled structures. This proposes new paradigms for the rational design of supramolecular materials with controllable dynamic properties.

1. Aida, T.; Meijer, E. W.; Stupp, S. I. Functional Supramolecular Polymers. *Science* **2012**, *335*, 813-817.
2. Bochicchio, D.; Salvalaglio, M.; Pavan, G. M. Into the dynamics of a supramolecular polymer at submolecular resolution. *Nature Commun.*, **2017**, *8*, 147.
3. Torchi, A.; Bochicchio, D.; Pavan, G. M. How the dynamics of a supramolecular polymer determines its dynamic adaptivity and stimuli-responsiveness: Structure–dynamics–property relationships from coarse-grained simulations. *J. Phys. Chem. B* **2018**, *122*, 4169-4178.
4. Bochicchio, D.; Kwangmettatam, S.; Kudernac, T.; Pavan, G. M. How defects control the out-of-equilibrium dissipative evolution of a supramolecular tubule. *ACS Nano.* **2019**, *13*, 4322-4334
5. De Marco, A. L.; Bochicchio, D.; Gardin, A.; Doni, G.; Pavan, G. M. Controlling exchange pathways in dynamic supramolecular polymers by controlling defects. *Chem*R*xiv* **2021**, DOI:10.26434/chemrxiv.13655864.v2
6. Gasparotto, P.; Bochicchio, D.; Ceriotti, M.; Pavan, G. M. Identifying and tracking defects in dynamic supramolecular polymers. *J. Phys. Chem. B* **2020**, *124*, 589-599
7. Capelli, R.; Gardin, A.; Empereur-mot, C.; Doni, G.; Pavan, G. M. A Data-driven dimensionality reduction approach to compare and classify lipid force fields. *Chem*R*xiv* **2021**, DOI:10.26434/chemrxiv.14039834.v1
8. Gardin, A.; Doni, G.; Pavan, G. M. On the comparability between soft self-assembled systems via machine learning of defects and of their structural dynamics. *In preparation*

Kinetics of structure formation in copolymer systems

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In a thin film, copolymers self-assemble into a variety of nanoscale structures that do not necessarily have analogs in the equilibrium phase diagram but are dictated by processing [1]. In fact, the free-energy landscape of these systems is rugged [2], featuring a multitude of metastable structures.

In this talk I will consider the self-assembly of lamellae-forming diblock copolymers. First, some device-oriented structures resemble defects in a lamellar pattern and can be stabilized by "defectants" that segregate towards nonlamellar structures and reduce their free energy. These defectants can, for instance, be generated by supramolecular association "on the spot". mitigating the need to diffuse to the defect-like location [3].

Second, an alternative for fabricating defect-free structures consists in controlling the kinetics of self-assembly, in particular the early stages that template the structure at later times. I will discuss how the subdiffusive dynamics of polymers influences the short-time kinetics [4] and illustrate to what extent this information suffices to predict metastable intermediates, such as the stitch morphology [5], in the course of directed self-assembly.

[1] Process-directed self-assembly of copolymers: Results of and challenges for simulation studies M. Müller, Prog. Polym. Sci. 101, 101198 (2020)

[2] Kinetics of pattern formation in symmetric diblock copolymer melts Y.Z. Ren and M. Müller, J. Chem. Phys. 148, 204908 (2018)

[3] Directed assembly of supramolecular copolymers in thin films: Thermodynamic and kinetic advantages K.Ch. Daoulas, A. Cavallo, R. Shenhar, and M. Müller, Phys. Rev. Lett. 105, 108301 (2010)

[4] Collective short-time dynamics in multicomponent polymer melts G. Wang, Y. Ren, and M. Müller, Macromolecules 52, 7704 (2019)

[5] Kinetic pathways of block copolymer directed self-assembly: Insights from efficient continuum modeling J. Rottler and M. Müller, ACS Nano 14, 13986 (2020)

Is the concept of "function" acceptable in statistical mechanics?

Alexander Grosberg

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The talk will be an eclectic mixture of several pieces, starting from classic Gibbs paradox in statistical mechanics and including some examples from both equilibrium and non-equilibrium statistical mechanics. Through all these pieces, I will try to clarify the question posed in the title. In the end, I will come to the conclusion that the answer is not entirely clear to me.

Regulation of the phase behavior of intrinsically disordered peptides

Yani Zhao[1] , **Kurt Kremer**[2]

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Responsiveness of polypeptides and polymers in aqueous solution plays an important role in biomedical applications and in designing advanced functional materials. Elastin-like polypeptides (ELPs) are a well-known class of synthetic intrinsically dis- ordered proteins (IDPs), which exhibit a lower critical solution temperature (LCST) in pure water and in aqueous solutions. Here, we compare the influence of cis/trans proline isomerization on the phase behavior of single ELPs in pure water. Our results reveal that proline isomerization tunes the conformational behavior of ELPs while keeping the transition temperature unchanged. We find that the presence of the cis isomers facilitates compact structures by preventing peptide-water hydrogen bonding while promoting intramolecular interactions. In other words, the LCST transition of ELPs with all proline residues in the cis state occurs with almost no noticeable conformational change.

[1] Y. Zhao and K. Kremer, ArXiv: 2101.10275 (2021).

[2] Y. Zhao, M. K. Singh, K. Kremer, R. Cortes-Huerto, and D. Mukherji, Macromolecules 53, 2101 (2020).

Energy landscapes of conformational switching in intrinsically disordered proteins and protein aggregation

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About half of the human proteome are proteins that are intrinsically disordered or contain disordered regions. By definition these proteins differ from natively folded proteins and do not adopt a properly folded structure under solution conditions. However these intrinsically disordered proteins (IDPs) also systematically differ in amino acid composition and often become folded upon binding to an interaction partner. These factors preclude solving IDP structures by current machine-learning methods like AlphaFold, which also cannot solve the protein aggregation problem, since this meta-folding process can give rise to different aggregate sizes and structures. An alternative computational method is provided by molecular dynamics (MD) simulations that already successfully explored the energy landscapes of IDP conformational switching and protein aggregation in multiple cases. These energy landscapes are very different from those of 'simple' protein folding, where one energy funnel leads to a unique protein structure. Instead, the energy landscapes of IDP conformational switching and protein aggregation feature a number of minima for different competing low-energy structures. In this talk, I discuss the characteristics of these multifunneled energy landscapes in detail, and provide examples of MD simulation studies where we elucidated the thermodynamics and kinetics of the underlying IDP conformational transitions and aggregation processes.

Molecular dynamics simulations of nanoparticles: structural aspects of lipid nanoparticles for drug delivery and interactions with biological membranes

Peter Tieleman

Centre for Molecular Simulation and Department of Biological Sciences, University of Calgary

Computer simulations using atomistic or Martini-level coarse-grained force fields in principle can give detailed insight in the structure and interactions of nanoparticles. We have used simulations to understand the structure and packing of lipid nanoparticles (LNPs) for RNA delivery, combined with experimental structural data. LNPs aren't simply hollow shells with RNA (mRNA or siRNA) but have a dense interior. Practical investigations have established a range of compositions that are essential for drug release, linked to the biological process of uptake, but the reasons for why some compositions work well remain somewhat unclear. In a separate line of research, the interactions with membranes during the uptake of nanoparticles, including ones based on a gold core, is of interest. Balancing accuracy of the simulations, sufficient sampling, and biological relevance is a challenge.

How subtle changes can make a difference: supramolecular chemistry emerges to new levels of fine-tuning

E. W. Meijer

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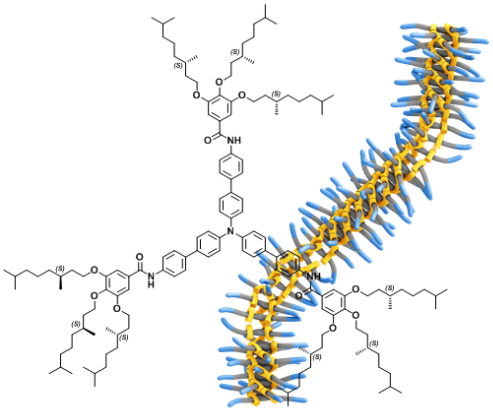
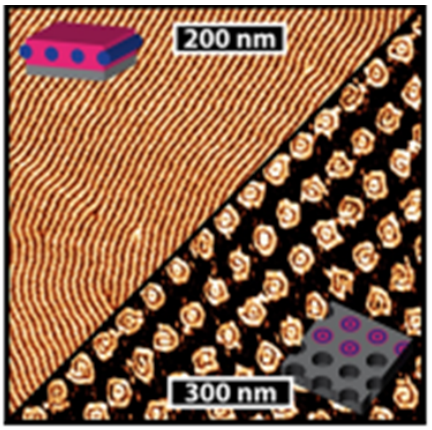
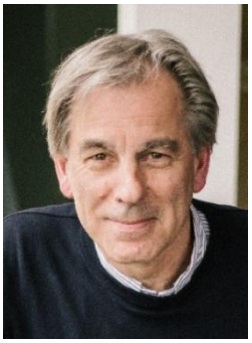
The ambition to construct complex molecular systems, materials and soft matter is driven by a need for technological evolution and our intrinsic curiosity to comprehend the origin of life. Supramolecular chemists aim to tackle this challenge using a combination of covalent and non-covalent reaction steps leading to multi-component systems with emerging complexity. Yet, such complex synthesis strategies often coincide with increasingly difficult reaction schemes and a narrow window of suitable reaction conditions. Alike small details that drive the unrepeatable crystallization of a desired polymorph or a sudden drop in reactivity of a catalyst from a different source, recently also supramolecular chemistry reached a level of fine-tuning in which underappreciated subtleties can have an unexpected major impact on a system. In the lecture, examples of our group are used to highlight the impact of subtle "irregularities" on supramolecular systems. Based on effects of pathway-complexity and minute impurities in organic solvents or the supramolecular building block we discuss potential pitfalls in the synthesis of soft matter. It is meant to sensitize for often overlooked details and to stimulate a discussion about reproducibility issues in supramolecular chemistry and soft matter.







E.W. "Bert" Meijer *is Distinguished University Professor in the Molecular Sciences, Professor of Organic Chemistry at the Eindhoven University of Technology and co-director of the Institute for Complex Molecular Systems. After receiving his PhD degree at the University of Groningen with Hans Wynberg, he worked for 10 years in industry (Philips and DSM). In 1991 he was appointed in Eindhoven, while in the meantime he has held part-time positions in Nijmegen, MPI-Mainz, and Santa Barbara, CA. Bert Meijer is a member of many editorial advisory boards, including Advanced Materials and is associate editor of the Journal of the American Chemical Society. Bert Meijer has received a number of awards, including the Spinoza Award in 2001, the ACS Award for Polymer Chemistry in 2006, the AkzoNobel Science Award 2010, the International Award of the Society of Polymer Science Japan in 2011, the Cope Scholar Award of the ACS in 2012, the Prelog Medal in 2014, the Nagoya Gold Medal in 2017 and the Chirality Medal in 2018. In 2020 he is knighted by the king to be Commander in the Order of the Netherlands Lion. He is a member of a number of academies and societies, including the Royal Netherlands Academy of Science, where he is appointed to Academy Professor in 2014.*

Role of Ionic Strength in the formation of Supramolecular Complexes between Nanoparticles and Proteins

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Monolayer-protected gold nanoparticles can be engineered to possess physiochemical properties for specific applications e.g. biosensors. Their shape and size can be tuned but the molecular recognition properties are dictated by the chemical structure of the coating ligands, which form self-organized and multivalent binding sites for the guest species, also it is crucial for their colloidal stability. The surface of the nanoparticles interfaces with the external environment made of solvent and ions, and appropriately engineered surfaces can be used to regulate interactions between nanoparticles and proteins driven by non-covalent interactions. A theoretical description of the ion distribution around the surface of the nanoparticles still remains a relatively unexplored. Here we report a multiscale computational strategy to enhance the binding affinity of NP-protein interaction at hight ionic strength, through co-engineering of nanoparticles and protein. We study 'super-charged' proteins to provide enhanced interfacial electrostatic interactions with complementarily charged nanoparticles.

Role of defects in the charge transport of organic semiconductors

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Organic semiconductors are used in optoelectronic devices, such as organic light-emitting diodes, organic and perovskite solar cells, and organic field-effect transistors. The performance of such devices depends heavily on charge injection and transport. In many cases, organic semiconductors exhibit highly unipolar charge transport, meaning that they predominantly conduct either electrons or holes. A fundamental question is what causes this unipolarity. Using a recently developed technique to establish Ohmic hole contacts, we investigate the bulk hole transport in a series of organic semiconductors with a broad range of electron affinities and ionization energies. We demonstrate that an energetic window exists inside which organic semiconductors are not susceptible to charge trapping by defects, most likely caused by water or oxygen, leading to trap-free charge transport of both carriers. The implication for devices such as OLEDs, organic solar cells and organic ambipolar transistors is that the energy levels of the organic semiconductors are ideally situated within this energetic window. However, for blue-emitting OLEDs with a large band gap this poses significant challenge to remove or disable charge traps.

Predictive Modelling of Structure Formation in Semiconductor Films Produced by Meniscus-guided Coating

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Abstract: Meniscus-guided coating methods, such as zone casting, dip coating and solution shearing, are scalable laboratory models for large-area solution coating of functional materials for thin-film electronics. Unfortunately, the general lack of understanding of how the coating parameters affect the dry-film morphology upholds trial-and-error experimentation and delays lab-to-fab translation. In this contribution we present a modelling study [1] focusing on the prediction of dry-film morphologies produced by meniscus-guided coating of a crystallizing small molecular solute. Our model reveals how the interplay between coating velocity and evaporation rate determines the crystalline domain size, shape anisotropy and regularity. If coating is fast, evaporation drives the system quickly past supersaturation, giving isotropic domain structures. If coating is slow, depletion due to crystallization stretches domains in the coating direction. The predicted morphologies have been experimentally confirmed by zone-casting experiments of the organic semiconductor 4-tolyl-bithiophenyl-diketopyrrolopyrrole. Although here we considered a molecular solute, our model can be applied broadly to polymers and organic-inorganic hybrids such as perovskites.

[1] Jasper J. Michels, Ke Zhang, Philipp Wucher, Pierre M. Beaujuge, Wojciech Pisula, Tomasz Marszalek,

In honor of the 65th birthday of Kurt Kremer, a special Special symposium will be held on "Recent progress in the understanding of entangled systems"

Topological tuning of DNA mobility in entangled solutions of supercoiled plasmids

Jan Smrek

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Ring polymers in dense solutions are among the most intriguing problems in polymer physics. Because of its natural occurrence in circular form, DNA has been extensively used as a proxy to study the fundamental physics of ring polymers in different topological states. Yet, torsionally constrained—such as supercoiled—topologies have been largely neglected so far. The applicability of existing theoretical models to dense supercoiled DNA is thus unknown. Here, we address this gap by coupling large-scale molecular dynamics simulations with differential dynamic microscopy of entangled supercoiled DNA plasmids. We find that, unexpectedly, larger supercoiling increases the size of entangled plasmids and concomitantly induces an enhancement in DNA mobility. These findings are reconciled as due to supercoiling-driven asymmetric and double-folded plasmid conformations that reduce interplasmid entanglements and threadings. Our results suggest a way to topologically tune DNA mobility via supercoiling, thus enabling topological control over the (micro)rheology of DNA-based complex fluids.

J. Smrek, J. Garamella, R. Robertson-Anderson, D. Michieletto, Sci. Adv., Vol. 7, no. 20, 2021

Kremer–Grest Models for Commodity Polymer Melts: Linking Theory, Experiment, and Simulation at the Kuhn Scale

Ralf Everaers

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The Kremer–Grest (KG) polymer model is a standard model for studying generic polymer properties in molecular dynamics simulations. It owes its popularity to its simplicity and computational efficiency, rather than its ability to represent specific polymers species and conditions. In a recent publication we have shown that by tuning the chain stiffness it is possible to adapt the KG model to a minimal model for specific polymer melts. In particular, we have provided mapping relations from KG to SI units for a wide range of commodity polymers. The connection between the experimental and the KG melts is made at the Kuhn scale, i.e., at the crossover from the chemistry-specific small scale to the universal large scale behavior. We expect Kuhn scale-mapped KG models to faithfully represent universal properties dominated by the large scale conformational statistics and dynamics of flexible polymers. In particular, we observe very good agreement between entanglement moduli of our KG models and the experimental moduli of the target polymers.

[1] Characteristic time and length scales in melts of Kremer–Grest bead–spring polymers with wormlike bending stiffness, C Svaneborg and R Everaers, Macromolecules, 2020

[2] Kremer–Grest Models for Commodity Polymer Melts: Linking Theory, Experiment, and Simulation at the Kuhn Scale, Ralf Everaers, Hossein Ali Karimi-Varzaneh, Frank Fleck, Nils Hojdis, and Carsten Svaneborg, Macromolecules, 2020