On the Versatility of Polymer Brushes and Multi-Block Copolymers for Nano-Technologies and Bio-Engineering

Fabien Leonforte[1], **Marcus Müller**[1].

[1] *Institüt für Theoretische Physik, Georg-August-Universität Göttingen, Germany*
leonforte@theorie.physik.uni-goettingen.de

Development and processing of functional materials is one of the main issue in micro- or nano-technologies. A growing number of technological applications are in need of e.g. adhesives that could stick on every type of surfaces, super-hydrophobic, anti-friction or anti-fouling coatings, or adaptive materials that could respond to some variations induced by their environment.

Because of their versatility as surface coatings as well as their ability to provide experimental and theoretical models, polymer brushes have been widely used in order to address problems like fine tuning of interactions between surfaces [1], reversible tuning of adhesion and wetting [2-4], or control of the motion of nano-objects [5]. They can also be fabricated on the nano and macroscale for electronics [6] and microfluidic devices [7]. Furthermore, new experimental *grafting from* techniques have allowed to turn inorganic surfaces to organic, biologically friendly ones that provide broad release, selectivity and attachment capabilities, including under the control of an external stimulus. Such functionalization of stimuli-responsive brushes, like multi-component *pH*- and thermo-responsive mixed brushes [8,9], is therefore extremely relevant for biological purpose like control release of drug delivery.

However, despite their apparent simplicity, the properties of functionalized and adaptive polymer brushes are difficult to address theoretically and experimentally (e.g. due to their use in *in-situ* applications, or because of the coupled constraints induced by the nanoscale, the changing environment and the induced response of the material). Their promising applications thus necessitate to capture the relevant parameters that can alter their stimulated response to environmental modifications, as well as to anticipate and optimize the architecture of the adaptive materials in relation to the used stimuli (electric field, solvent, temperature, salinity, magnetic field, optical triggering...). Therefore, a detailed understanding of such systems is critically dependent on the bi-directional passing of relevant and pertinent parameters between experiment, theory and modeling.

From the simulation side, the complex environment triggering response of polymer brushes is difficult to model and one has often to balance between (i) the resolution of the molecular details and involved mechanisms, (ii) the computational efficiency, and (iii) time and length scales of same order than the experiment. Using a coarse-grained model with soft interactions and a spectrum of complementary techniques, e.g. Monte-Carlo, Multiple-Dissipative-Particle-Dynamics and Single-Chain-in-Mean-Field simulations, we study the structure and dynamics of multi-component polymer brushes under different environmental conditions. During this talk, we will discuss the ability of our model to access experimentally relevant invariant degrees of polymerization and capture the salient features of stimuli-responsive polymer brushes, and films of multi-block copolymers as well, without loss of computational efficiency and with the aim to open new strategies in the design of smart, polymer-based surfaces.

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