Structure and Dynamics of Polymer Nanocomposites: Multiscale Simulation Approach

Our primary goal is to develop an understanding of the nonlinear elasticity of elastomer-based nano-composite materials. We aim at disentangling the different contributions to the visco-elastic properties. The key question is: **how can the reinforcement of polymers by filler particles be understood at a fundamental level?** To achieve the goal of understanding and ultimately controlling the reinforcement, it needs to be related to both the molecular scale interactions and the structuring of the filler particles within the polymer matrix on a mesoscopic level. We will study tunable model systems made of hard silica particles of controlled surface chemistry in a polymer matrix, and will simulate the (linear *and* nonlinear) visco-elastic properties of different particle-polymer systems, systematically varying the relevant parameters. The relevant parameters are notably the filler/matrix composition, the polymer network structure and the particle/polymer interaction. The projected insights into these systems are essential to the development of e.g. environmentally more friendly ('green') tires, elastomeric sealants and other advanced rubber materials.

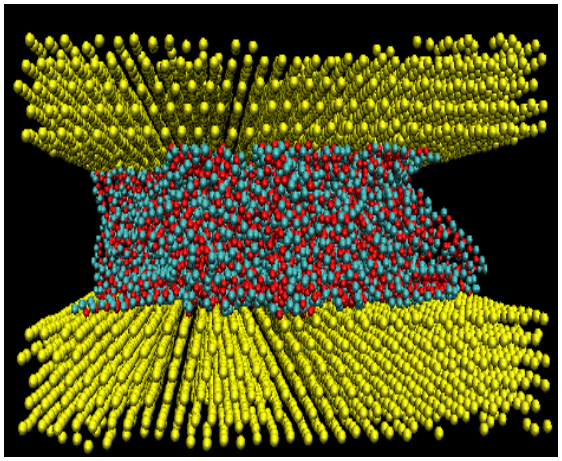

Figure 1: Schematic level of proposed atomistic (length scales 1-10 nm) molecular dynamics, used to study elastomer films of various thicknesses between nanoparticle surfaces, and