# MAGNETO-ELASTIC COUPLING IN COARSE-GRAINED COMPUTER SIMULATIONS

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Creating functional magnetic soft matter required many years of preliminary work spent on investigating fundamental properties of all its components. The main ingredients of such materials are (1) magnetic single-domain nano-sized or multi-domain macron-sized particles of various shapes and (2) magneto-passive fluid or gel that serves as a carrier. Among the most known examples are ferrofluids, magnetorheological suspensions, ferrogels, etc.). The third possible ingredient can be used to stabilise or functionalise magnetic nanoparticles, as well as to cross-link them in various shapes or form gel-like networks. For more than 50 years scientists all over the world have been actively investigating these systems both experimentally and theoretically, starting from simple systems and increasing the complexity in the due course. The synthesis of magnetic soft matter nowadays is extremely elaborated and allows to design new materials on the nanoparticle level. What is still missing, is the fundamental knowledge about the mechanisms which control the self-assembly and/or phase behaviour of magnetic soft matter and its macroscopic response.

In the present contribution I will describe our attempts to fill this gap in the understanding of the inter-scale relationship in magnetic soft matter, reporting the results of coarse-grained molecular dynamics simulations of magnetic gels, filaments and composite magnetoelastomers (see, Figure 1.). The main idea of this work is to show how using molecular dynamics one can trace back the relationship between the internal structure and the macroscopic magnetic and elastic response of these systems. Along with demonstrating the advantages of our approach and the main results obtained for bottom-up design of magnetic soft matter, we will also discuss the limitations of coarse-grained modelling.

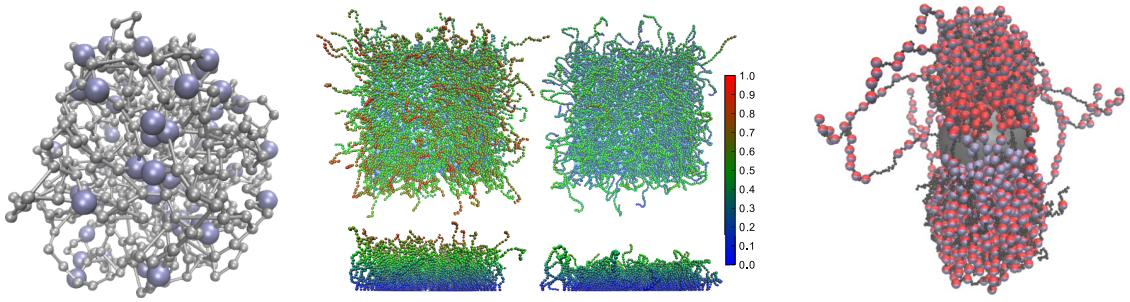


Fig. 1. Simulation representation of magnetic gel (left); filament brush (middle); composite elastomer (right).