

Modelling the behaviour of functional nanoparticles in polymer melts by Molecular Dynamics simulation

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Polymers hosting nanoparticles (NPs), referred to as polymer nanocomposites (PNCs), are paving the path for next-generation smart nanomaterials to meet the demand of upcoming technologies that are expected to be of remarkable industrial and societal benefit. PNCs are hybrid materials comprising a polymer matrix that hosts organic or inorganic NPs. The incorporation of NPs, usually between 1 and 5 wt%, allows one to improve the macroscopic response of a polymer, including its thermal and mechanical resistance and viscoelastic behaviour. However, formulating PNCs that are more suitable to target applications than their engendering polymers is not trivial as it depends on an intricate network of correlated factors that pivot around the interactions established at the polymer/NP interface.

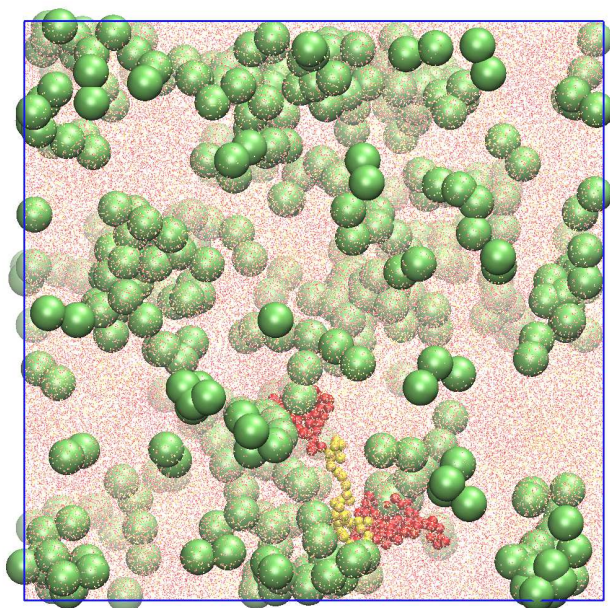


Fig. 1. Initial configuration of 800 chains of a triblock copolymer incorporating 215 nanodimers at 298 K. Blocks of type A and B are respectively shown in red and yellow, while nanodimers in light green. For clarity, only one polymer chain and nanodimers are magnified, while all other chains are point-like.

In this work, we present recent molecular simulation results that try to clarify the role of some of these factors and how they can be employed to control the behaviour of NPs and polymer chains at the small scale and influence the PNCs response at the macroscopic scale [1, 2, 3, 4]. Starting from simple models, where NPs are represented as soft spheres, we will show how manipulating the NP surface chemistry and shape anisotropy, one can better control their distribution and orientation in the polymer matrix. We will discuss how coupling NPs' functionalisation to an accurate choice of the polymer architecture can provide a powerful tool to fine-tune the material properties, including its viscosity. Finally, we will see how the use of block copolymers, able to self-assemble into ordered mesophases, offers an opportunity to drive the arrangement of functional NPs into precise nanodomains, where specific functions can be activated.

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