Ionic polymer nanocomposites under deformation

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Polymer nanocomposites have received special attention from academia and industry during the last 30 years, due to their improved properties in comparison to polymer blends. Nanoparticle (NP) dispersion is necessary for effective reinforcement in the matrix and is a prerequisite for property "tuning" and enhancement. One way to provide NP dispersion is to let the interaction between NPs and chains to be of an ionic nature. The presence of oppositely charged ions at the polymer/nanofiller interphase can promote dispersion. This relatively new class of ionic nanocomposites combines filler reinforcement with the reversibility of ionic interactions. Despite the improved mechanical performance, the reversible feature of ionic bonds, that can break and reform under certain conditions has led to smart materials for self-healing, shape-memory, piezoelectric, and mechanochromic applications due to their ability to respond directly under a certain chemical or physical stimulus [1, 3].
We set out to investigate the dynamics, structure, entanglements, and viscoelastic properties of ionic nanocomposites by means of coarse-grained molecular dynamics simulations. To this end, we study model systems consisting of bead-spring polymer chains and spherical nanoparticles –roughly with the same size as polymer radius of gyration– both in equilibrium [2] and subject to a deformation field.

References

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