**PROPERTIES OF POLYMERS AND POLYMER NANOCOMPOSITES VIA SIMULATIONS ACROSS SCALES: FROM ATOMS TO MACROSCOPIC PROPERTIES**

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**ABSTRACT**

Nowadays, computαtional approaches can be used in order to provide a direct insight at the properties of complex polymer-based materials across multiple spatiotemporal scales. Molecular simulations in particular have the advantage of accurately describing the chemistry of the systems under study, and of predicting their behavior at the molecular level. However, the study of polymers via molecular simulations is a very challenging field, due to the broad spectrum of the underlying length and time scales. Here, we present a hierarchical multi-scale methodology for predicting the macroscopic properties of polymer-based nanostructured systems, that involves atomistic and coarse-grained simulations. The coarse-grained (CG) models are derived through a “bottom-up” data-driven strategy, using information from the detailed atomistic scale, for the given chemistry. The systematic linking between the atomistic and the chemistry-specific CG scale, allows the study of a broad range of molecular weights, for specific polymers, without any adjustable parameter [1-3]. At the same time, machine learning (ML) algorithms have been developed to re-introduce atomic detail in the CG scale, and thus obtaining atomistic configurations of high molecular weight polymers [3].

We apply the entire methodology to (a) cisPB polymer melts [4], and (b) cisPB/silica nanocomposites [5]. For both systems we provide a detailed study of their dynamical and rheological macroscopic properties. For the polymer melts, we report predictions about the self-diffusion coefficient of polymer chains, the relaxation modulus and the zero shear-rate viscosity, as a function of molecular length probing the transition from oligomers, to Rouse-like, up to the well-entangled systems.

Concerning the polymer nanocomposites, we examine the structure and the dynamics of polymer chains at the polymer/nanoparticle interphase, by probing directly the density and the conformations of polymer chains, as well as and the segmental and terminal dynamics of the adsorbed, “bound” layer. In all cases the results are compared against experimental data and theoretical predictions.

**KEYWORDS:** Molecular simulations, polymer nanocomposites, machine learning methods

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