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Tuning polymer glass formation with additives and ions[1]

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A polymer's glass transition and associated dynamic and mechanical properties are among the most important factors determining its performance in engineering applications. For this reason, decades of research have aimed to establish methods of tuning polymers' glass formation behavior. Here I describe molecular simulations providing new insight into two approaches to altering a polymer's glass formation behavior: introduction of small-molecule diluents; and introduction of charged moieties to form an ionomer. In the first case, we explore how diluent molecular properties control modifications to the host polymer's glass transition and mechanical response. Results indicate that diluents can induce a rich array of effects, necessitating development of an expanded classification beyond the usual plasticizer/antiplasticizer dichotomy. In the second case, simulations indicate that ionomer glass formation is indistinguishable from that in polymer nanocomposites, in contrast to the longstanding assumption that covalent grafting of chains to ionic aggregates in these systems leads to a qualitatively distinct effect. Taken together, these results provide new guidance towards the rational understanding and control of polymer glass-formation in a range of materials.

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