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Design rules for rational control of polymer glass formation behavior and mechanical properties with small molecular additives[1] JAYACHANDRA HARI MANGALARA, DAVID SIMMONS, The University of Akron — Small molecule additives have long been employed to tune polymers' glass formation, mechanical and transport properties. For example, plasticizers are commonly employed to suppress polymer T_g and soften the glassy state, while antiplasticizers, which stiffen the glassy state of a polymer while suppressing its T_g, are employed to enhance protein and tissue preservation in sugar glasses. Recent literature indicates that additives can have a wide range of possible effects, but all of these have not been clearly understood and well appreciated. Here we employ molecular dynamics simulations to establish design rules for the selection of small molecule additives with size, molecular stiffness, and interaction energy chosen to achieve targeted effects on polymer properties. We furthermore find that a given additive's effect on a polymer's T_g can be predicted from its Debye-Waller factor $<u^2>$via a function previously found to describe nanoconfinement effects on the glass transition. These results emphasize the potential for a new generation of targeted molecular additives to contribute to more targeted rational design of polymers.

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