

# Glass Transitions in Polymer/Nanoparticle Composites

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## **Abstract:**

The role of surfaces on the glass transition temperature of small molecule and polymeric fluids has been a topic of considerable interest in the last two+ decades. In spite of this ongoing interest the field has remained controversial. A few experimental results have suggested that surfaces can significantly affect the  $T_g$ , while newer results suggest that surfaces play a minor role in this context. Similar, confusing results have also been found from simulations. We use detailed computer simulations and show that there should only be small effects when polymers are confined between strongly attractive surfaces. The essentially irreversible adsorption of polymer chains to a nanoparticle effectively modifies the boundary condition experienced by a polymer melt – so that the bulk polymer “sees” itself. Under these situations there should be minimal changes in  $T_g$  and in the fragility, results that seem to be more prevalent in the newer body of experimental literature. The consequences of these findings on the role of nanoparticles on the reinforcement of a polymer’s mechanical properties are also discussed.

With D. Meng, F. Starr, J. Douglas.