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# MD simulations of $1,4$ - polybutadiene at graphite surfaces

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Polymer dynamics in confinement is both of fundamental interest concerning our understanding of the glass transition, as well as of high technological importance for the performance of composite materials. The results here presented are concerned with atomistic MD simulations of a chemically realistic model of a 1,4-polybutadiene melt (55% trans and 45% cis content) confined between two walls of graphite. The focus of our study is to investigate the effects of confinement on the chain dynamics in the melt and to reveal to what extent the walls are influencing structure and dynamics of the melt. As an example, Fig. 1 depicts the conformation that a chain adopts at an interface by forming trains, loops and tails. It is evident that the chain dynamics of an adsorbed chain may be strongly constrained in comparison to a chain which is not adsorbed at an interface.
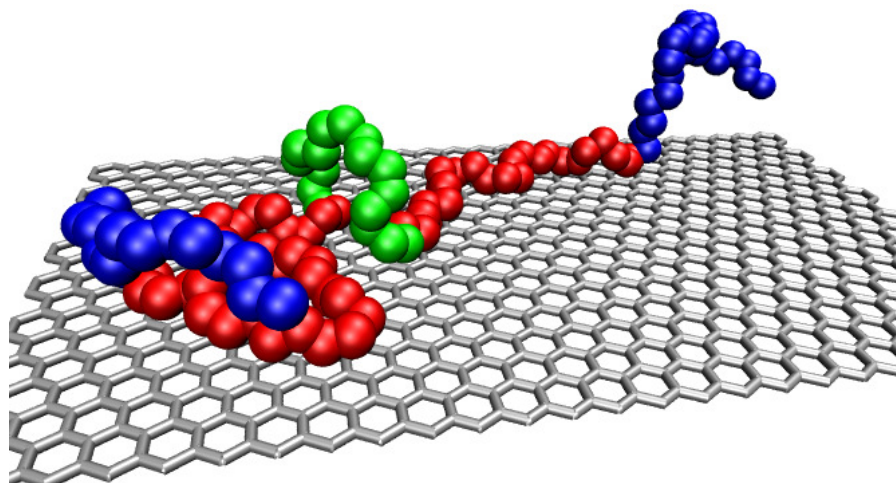


Figure 1: The conformation that a chain may adopt at an interface by forming trains (red beads), loops (green beads) and tails (blue beads). The snapshot was taken at $T = 353$ K ($\approx 2T_g$). The grey lattice represents the crystalline graphite interface

The physical properties here investigated are density profiles, the incoherent scattering function and collective dielectric relaxation. The results presented are key to a better understanding of the glass transition process in a confined polymer system.

## References

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