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Non-equilibrium dynamics at polymer surfaces and interfaces

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The ability to predict the rheological and flow properties of polymer blends and other multi-phase systems relies critically on the ability to understand how the interfacial dynamics affect the overall properties. Continuum theories tend to break down in the near interfacial region since they do not account for local molecular orientation and other related effects. We have shown, using MD simulations, that the behavior at interfaces tends to be controlled by the stress transfer between the two phases and this is dependent on the local chain structure and conformation at the interface. Studies on nanoparticles added to polymer blends also illustrates the importance of controlling the interfacial region. To account for all these effects we have formulated a dynamic self-consistent field theory that couples local chain conformation to a constitutive equation that describes the rheological properties of the system. We illustrate this approach by studying the effect of slip at polymer/polymer interfaces.