

## **611c Influence of Local Packing on Dynamics in a Model Glassy Polymer**

*Tushar Jain and Juan J. De Pablo*

One of the long-standing goals of theoretical and experimental research on glasses has been to establish a relation between local structure and the observed dynamics. We have performed detailed structural analysis on a model glass forming polymer equilibrated using molecular dynamics and advanced Monte Carlo methods. Within the description of the energy landscape formalism, we have identified metabasins of vibration on a single particle level. We find that the residence times for vibrations are correlated with a particular Voronoi volume and number of neighbors of a particle. The local distortion around a particle, measured in terms of the tetrahedrality of the Delaunay simplices, reveals that the particles with a higher degree of local distortion are likely to transition faster to a neighboring metabasin. In addition to the transition between metabasins, we have also examined the influence of vibrations at inherent structures (IS) on the local structure, and find that the low frequency modes at the IS exhibit the greatest curvature with respect to the local structure. We believe that these results establish an important connection between the local structure of glass formers and activated dynamics, thereby providing insights into the origins of dynamic heterogeneities.