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Multiscale investigation of low molecular weight glass formers JAYEETA GHOSH, ROLAND FALLER, UC Davis — Ortho-terphenyl (OTP), a very well known and well investigated organic glass former, is used as a model to study the static and dynamic properties of low molecular weight glass formers. Molecular dynamics is applied to simulate 800 molecules in atomistic detail. The model is able to provide very good agreement with experimental observations. Our simulation gives the glass transition temperature ($\sim$260K) slightly higher than the experimental value (243K) but is much closer to that value than comparable simulations. Radial distribution functions calculated at temperatures above and below the glass transition temperature show that there are no remarkable changes in structure at the molecular level. We study the in-homogeneity at the local level around each molecule and compare static and dynamic heterogeneities. From the radial distribution functions we develop a structural coarse grained model. With this coarser model in which each ring of OTP is considered as one super atom, OTP should provide similar structural and dynamic properties above and below glass transition temperature. Future work on this multiscale approach includes applying the Density of States Monte Carlo technique to this real glass forming organic molecule. This novel Monte Carlo technique has been used for a binary Lennard Jones mixture as model glass former. This would be the first approach to apply it to a real glass forming liquid. We will eventually be able to study the effect of confinement on the transition.

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