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Density of States Simulations of Confined Glasses ROLAND FALLER, JAYEETA GHOSH, UC Davis — Glassy systems under confinement have been studied with great enthusiasm and effort for the last decades. They are relevant both fundamentally and technically because there is still debate about the nature of glass transition in small geometries which is important for lithographic processes in the semiconductor and other industries. In this work we are using the Wang-Landau approach also known as Density of States Monte Carlo to study glassy systems in bulk and under confinement. We apply the technique to a model binary Lennard Jones glass as well as the small organic glass former Ortho-terphenyl (OTP). For Lennard Jones glasses we use a well tested model. For OTP we start from a united atom model and then derive systematically a coarse grained representation by replacing each phenyl ring with a bead and using the Iterative Boltzmann Inversion. The properties of bulk Lennard Jones model show very good agreement with literature values. The atomistic and coarse grained representations of ortho-terphenyl in the bulk are in good agreement with experiments. Unsupported freestanding films show a lower glass transition than the bulk value.

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