

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Understanding glass transition from structural and vibrational properties of zero-temperature glasses¹ LIJIN WANG, NING XU, University of Science and Technology of China — We claim that the dynamical differences between the supercooled attractive Lennard-Jonesian (LJ) and purely repulsive Lennard-Jonesian (WCA) systems and the density dependence of their glass transition temperatures are understandable from properties of the $T = 0$ glasses. Below a crossover density ρ_s , the $T = 0$ LJ and WCA glasses show distinct structures, resulting in differences in their vibrational properties such as the boson peak frequency and quasi-localization of low frequency modes. These differences make LJ glasses more stable and thus have higher glass transition temperatures than WCA ones. Above ρ_s , the $T = 0$ LJ and WCA glasses are isomorphic, showing scaling collapse of the pair distribution function, density of vibrational states, and mode participation ratio spectrum. The scaling collapse helps us predict the density scaling of the glass transition temperature from dimension analysis, which is in excellent agreement with simulation results. Interestingly, the dimension analysis suggests a possibly general expression of the glass transition temperature in terms of the structural and vibrational quantities of the $T = 0$ glasses, which can fit simulation results very well over a wide range of densities for both LJ and WCA systems.

¹We thank the support from National Natural Science Foundation of China

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Date submitted: 11 Nov 2013

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