Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Molecular modeling of a stable glass – the case of trehalose SADANAND SINGH, DEVIN AVERETT, JUAN DE PABLO, University of Wisconsin - Madison — Recently, a new class of glasses –stable glasses- has been identified in experiments using physical vapor deposition of indometahcin (IMC) and 1,3,5-(tris)naphthylbenzene (TNB) [1,2]. These glasses have been shown to exhibit lower enthalpies (by as much as 10J/g), higher glass transition temperatures, higher onset temperature when subjected to plasticization and higher densities (by $\sim$2%) than traditional, ordinary glasses. We propose a molecular simulation method to generate stable glasses of an atomistic model of trehalose. The results of simulations are in good agreement with experiment: simulated stable trehalose glasses have an enthalpy that is 9.3 J/g lower and a density that is 1.6% than traditional, ordinary glasses. The plasticization of stable glasses formed by our method shows an increase of the onset temperature from 378K to 450K. Further analysis shows that these glasses have higher mechanical strength and higher Q6 crystal order parameter than ordinary glasses. The molecules farthest from the substrate layer are observed to be more mobile than those in the bulk; a mechanism for stable glass formation is proposed that relies on this enhanced surface mobility. [1] S. F. Swallenet al., Science. 2007, 315, 353-356, [2] K. L. Kearns et al., J Chem. Phys. 2007, 127.

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Date submitted: 08 Dec 2009 Electronic form version 1.4