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Molecular modeling of ultra-stable vapor deposited glasses SADANAND SINGH, DEVIN AVERETT, CHI-CHENG CHIU, JUAN J. DE PABLO, University of Wisconsin-Madison — Recent studies have shown that physical vapor deposition can be used to prepare glasses of small organic molecules with remarkably high kinetic stability and low enthalpy, particularly when compared to ordinary glasses prepared by cooling the supercooled liquid. The thermophysical properties of these new ultra-stable glasses are equivalent to those of common glasses after thousands of years of aging. However, experimental studies have so far been limited to relatively few types of molecules. We propose a molecular modeling scheme to prepare stable glasses that mimics the experimental procedure of vapor deposition. For simple disaccharides, such as trehalose, the thermophysical properties of our simulated glasses are consistent with those measured experimentally. We also prepare stable glasses of trehalose and glycerol mixtures, which are of interest for their use in stabilization of biomolecules in the glass state. Results for model binary Lennard-Jones glasses, which have been studied extensively in the literature, are also discussed. We find that the most stable glasses formed by vapor deposition are equivalent to ordinary glasses formed by cooling at a rate approximately 10 orders of magnitude slower than those accessible by ordinary cooling methods.

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