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Modeling Amorphous Materials via Randomly Generated Networks SAMUEL CUPP, JUSTIN OELGOETZ, Austin Peay State University — Materials research today relies heavily on experimental research to drive the discovery of new materials. Theoretical work is used to explain properties and interpret experimental data but is far less commonly used as a predictive tool. In covalent glass/amorphous materials research, the input to these calculations is often an initial structure formed based off experimental data. The major hindrance to performing theoretical calculations is the time-consuming task of manually adjusting the amorphous network, which is used as initial starting points for geometric optimizations. For purely computational approaches to make predictions, the process of producing amorphous networks must be automated. We previously implemented a Monte Carlo approach to create amorphous networks from constituent atoms and used the Metropolis algorithm to determine characterizations of these networks. We use MOPAC to calculate energies and physical properties. We are currently enhancing our program to use the Cation-Interlinking Network Cluster Approach and have implemented a method for randomly generating a glassy network built from base fragments. We calculate the pairwise distribution functions and average energy for these networks by averaging over MOPAC-optimized random networks. Our next steps are to fully implement the Metropolis method for CINCA and investigate differences in runtime and accuracy between the old and new methods.

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