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Configurational entropy of glass-forming systems from graph isomorphism YUXING ZHOU, SCOTT MILNER, The Pennsylvania State University — The configurational entropy plays a central role in the thermodynamic scenarios of glass transition, such as Adam-Gibbs theory and random first-order transition theory. By definition, the configurational entropy S_c is the difference between the entropy of liquid and the vibrational entropy with structural rearrangement restricted, both of which can be obtained by means of thermodynamic integration. On the other hand, S_c is essentially a measure of the number of basins in the energy landscape, and therefore it can also be estimated by explicitly enumerating inherent structures. To this end, we first coarse-grain the vibrational motions by mapping configurations to Voronoi diagrams and then categorize them using canonical labelling. The Voronoi graph entropy is calculated as $S_G/k_B = -\sum p_i \log(p_i)$, where p_i is the probability of finding distinct graph i. We find for an n-particle subsystem of glass-forming hard-disk/sphere fluids, $S_G(n)$ scales linearly with n, and S_c can be estimated from the slope.

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