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Investigating the Glass Transition Temperature of Water using a Variety of Models and Methods via Molecular Dynamics Simulation JOHN MURYN, Baldwin-Wallace College, GARY LEUTY, MESFIN TSIGE, Department of Polymer Science, The University of Akron — In everyday life, we think of solid water existing as crystalline ice. The majority of water in the universe, however, exists as an amorphous solid or "glassy" form. This glassy form has garnered significant interest and sparked sizable debate in recent years over the nature and conditions surrounding the transition from liquid to amorphous solid, not the least of which centers on the determination of the glass transition temperature. Previous experimental studies have suggested a glass transition temperature below the temperature at which water undergoes homogeneous nucleation, thus making experimental determination of the glass transition temperature difficult because of the need to avoid ice formation. In this study, we have used molecular dynamics simulation to study the structure, order and dynamics of water molecules at small timescales and under rapid cooling conditions to elucidate the formation of the amorphous solid and better understand the glass transition. Constant-pressure and constant-volume simulations have been performed in order to examine convergence or divergence of water dynamics under differing conditions. In addition, the van der Waals energy of simulation systems has been examined in an attempt to identify the glass transition temperature in a way that, to our knowledge, has not previously been used. Results suggest a glass transition temperature higher than previous widely accepted values but comparable to more recent results.

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