A Large-Scale Molecular Dynamics Simulation of Compressed Ice

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Water, albeit an extremely simple chemical, is the most important for human life and the growth of our society. It is a vital resource for our health, food, and energy production. As the demand for water steadily continues to increase, researchers have begun to dedicate an incredible amount of resources to study it. It should be noted that in order to solve wide-scale and societal problems regarding water, we must also try to understand it on a molecular level. While the structure of liquid water remains elusive, quenched water and disordered ice is an excellent starting point. In this study, a large-scale molecular dynamics simulation of compressed ice 1h has been performed to study the formation of high-density amorphous ice and very high-density amorphous ice. While the mechanism for this phase transition is known, the results of this study provide a much more detailed description of the local structural changes that occur during amorphization. Topological data analysis has been used in tandem with molecular dynamics results to properly characterize the medium-range order of high-density and very high-density amorphous ice.