

Topological characterization of non-rigid/rigid fluid transition in high-pressure region

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In this work, we firstly propose a topological/geometrical framework to pinpoint the Frenkel line, the viscous-to-elastic crossover line of high-pressure fluids. In this methodology, the topological information of the Voronoi polyhedrons of ideal gas state and a maximally random jammed state of hard spheres is first obtained and compared to classify the gas-like and solid-like molecules in a configuration of molecules. A neighbor-based geometrical procedure is further applied to remove the influence of the thermal fluctuations on the topological classification result. Applying the designed methodology to the fluids modeled with the Weeks-Chandler-Andersen (WCA) potential, it is discovered that the Frenkel line is the percolation transition line of the non-rigid to rigid crossover in high-pressure fluid region.