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Why does liquid water have a maximum density at 4°C?

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Abstract

Even though anomalous behaviors of liquid water around 4°C have long been studied by many different authors up to now, it is not still cleared what thermodynamic mechanisms induce them. The thermodynamic properties of substances are determined by inter-particle interactions. We analyze what characteristics of pair potential cause density anomaly using a thermodynamically Self-Consistent Ornstein-Zernike Approximation (SCOZA). The SCOZA is known to provide a very good description of the overall thermodynamics and a remarkably accurate critical point and coexistence curve. We consider a fluid of spherical particles with a pair potential given by a hard-core repulsion plus a Lennard-Jones type tail (HC-LJ system). We show that the soft-repulsion near the hard-core contact determines the behavior of excess internal energy which plays a crucial role in the anomalous behaviors of the system. Our results show that even though such models as second critical point hypothesis, a two-state model, liquid-liquid phase transition model, clathrate model, network model, and orientation-dependent potential would be important to some properties of water, those are not the immediate cause of the density anomaly in liquid water. We present also a core-softened potential which reproduces experimentally measured density-temperature curve in the wide temperature range much better compared to other models presented up to now. Although our study is restricted to liquid phases of water, it provides us with important insights into the thermodynamic properties of solid water.