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Interparticle interaction between water molecules

Makoto Yasutomi

University of the Ryukyus, Japan

Abstract

Why does liquid water have a maximum density at 4°C? Although the question has long been studied by many different authors so far, it is not still cleared what thermodynamic mechanisms induce them. Thermodynamic properties of liquid water are determined by the interparticle interaction. We will obtain the interaction which reproduces experimentally measured density-temperature relation at 1 bar and radial distribution function. The accuracies in a temperature range of $-20<T(^{\circ}C)<100$ are much better compared to other models available in the literature. We have used a self-consistent Ornstein-Zernike approximation with a screened power-series closure. We have considered a fluid of spherical particles with a pair potential given by a hard-core repulsion plus a tail. The tail is composed of a soft repulsion and an attraction. We will also elucidate the thermodynamic mechanism which causes density anomaly of liquid water and discuss why solid water has polymorphic structures. Our results show that even though such ideas as second critical point hypothesis, a simple two-state model, liquid-liquid phase transition model, clathrate model, network model, tetrahedral structure, and orientation-dependent potential would be important to some properties of water, those are not the immediate cause of the density anomaly.Instead, the author believes that those ideas would be formed as a result of negative thermal expansion. We show that the density anomaly is induced by the behavior of the excess internal energy especially near the hard-core contact where the soft-repulsion has large values. The behavior causes positive expansion above4°C, but negative expansion below4°C.