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Interparticle interactions of different shapes between water molecules

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We have found many interparticle interactions of different shapes between water molecules. All of them reproduce experimentally measured density-temperature relation at 1 bar with sufficient accuracy much better compared to other models available in the literature. We can expect that those will help us to understand why solid water has polymorphic structures, why liquid water has a large number of anomalies, and other thermodynamic properties of water. 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 model, orientation-dependent potential and so on have been put forward up to now to understand the physics underlying the density anomaly of liquid water, they tell us nothing about the immediate cause of the density anomaly. For example, it is not cleared yet how the tetrahedral structure induces positive thermal expansion at temperatures above four degrees celsius but negative expansion below that temperature in the tetrahedral structure model. In the network model, even though it may be plausible that water molecules partially fill cavities with reducing temperature to make liquid water condensed, but the model tells us nothing about what makes water molecules go out of the cavities at temperatures below four degrees Celsius with reducing temperature to induce negative expansion. We confirm that the excess internal energy u and its behavior play crucial roles in the anomalous behaviors of liquid water. They are determined especially near the hard core contact where soft repulsive force has large values. That is to say, the behavior of u induces positive thermal expansion above four degrees Celsius but negative expansion below that temperature. We have used a self-consistent Ornstein-Zernike approximation (SCOZA) with a potential given by multi-Yukawa terms. Because any smooth potential functions can be fitted by the multi-Yukawa terms, the method can be applied to fluids with interactions of various shapes. We also present a new simple fitting technique which makes the application of the SCOZA to any types of liquids much easier. The scheme will give not always the best fit but will be very useful in applying the SCOZA to any liquid with a smooth potential function.

Biography

Makoto Yasutomi completed his PhD at Nagoya University. He worked in University of the Ryukyus for many years as Instructor. He has published more than 30 papers in reputed journals.

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