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Physics underlying the negative thermal expansion of water and the computation method with extremely high accuracy

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Density of usual substances increases monotonicallywith cooling at any temperatures. But, that of water expands with reducing temperaturebelow 4°C.A number of scientists in the world have studied for centuries what causes the negative thermal expansion and a variety of ideas have been put forward up to now. Nevertheless, none of them tells us anything about what induces the negative expansion. Recently, we have succeeded in explaining the physics underlying the density anomaly. We have shown that the soft repulsion near the hard-core contact determines mainly the thermodynamic behavior of excess internal energy of water which is much different from those of usual liquids. The behavior of the internal energy causes negative thermal expansion at temperatures below 4°C. Water has also a plenty of anomalous properties other than density anomaly. In this speech, we will also talk about why water has polymorphic structures and what determines the isothermal compressibility. Today, almost all of these anomalous behaviors of water are well reproduced by numerical simulations by using realistic water models. But, it does not mean that physics underlying these phenomena are illuminated.We can derive thermodynamic properties of any substances by using thermodynamics and statistical mechanics if intermolecular forces are known. It should be said that the Physics underlying a certain phenomenon is illuminated when the relation between the phenomenon and the shape of the intermolecular potential is elucidated thermodynamically. At the present moment, Self-consistent Ornstein-Zernike approximation will be the most appropriate method to study this kind of phenomena. We have also found a computation method which makes calculation precision 10^{10} times higher than those presented up to now. In the study of water, we need to perform numerical computations byusing models with a variety of intermolecular interactions. Therefore, we can expect that thisextremely accurate computation method will be very useful and will bring us fruitful results.

Biography:

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