

Strange story about liquid water using soft X-ray spectroscopy

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Water is ubiquitous and one of the most important materials in our life. And it is known as the most abnormal material; many abnormal properties are shown such as extremely high boiling points compared with similar compounds, etc. Many researchers take on the challenge to understand the origin of that abnormality.

Soft X-ray emission spectroscopy (XES) is a powerful tool to measure the electronic states in material. Especially, XES is very sensitive to the environment surrounding molecules. Using this spectroscopy, electronic states of liquid water were observed. Observed spectra showed double peaks assigned to the $1b_1$ state. However, different models, dynamics [1] or structure [2], are proposed to interpret these peaks, and a long debate is continuing for more than 15 years. This is a strange situation. We constructed model structure of liquid water and performed XES calculations within the framework of density functional theory [3]. Our new model can clearly reproduce experimental temperature and isotope dependence of XES of liquid water. Our conclusion is that both interpretations, dynamics and structure, are important to reproduce experimental spectra.

Next target is aqueous solutions. I introduce recent results such as ethanol aqueous solutions as an example of homogeneous solutions and water in liquid crystal membrane as an example of heterogeneous solutions.

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