2P23 Computational Chemistry Study on Characteristics of Water Molecules and Its Interactions with Bio- and Organic Molecules

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Introduction

Water is an indispensable nutrient. It plays an important role in human's life. Many experiments are focused on the interactions between water molecules and bio- or organic molecules. With the advancement of computer hardware technology and the improvement on sophisticated computer coding methods based on the increasingly efficient algorithms, there comes a remarkable enhancement on the capabilities of quantum chemistry methods to study the complex chemical systems. But generally, it costs much computational sources and time. However, our lab has succeeded in developing a program "colors"—a novel and rapid quantum chemistry molecular dynamics program, enabling the investigation of large systems within reasonable time periods. We chose to investigate characteristics of water molecule under various conditions (normal sub-critical and supercritical) as the first step of the investigation.

Method

In this study, we applied our original tight-binding quantum chemical molecular dynamics program "colors". All the parameters used for "colors" were defined by the first principle calculations, viz., Amsterdam density functional (ADF) program.

Results and discussion

In order to test and verify the accuracy of "colors" program, we calculated one single water molecule. The angel of O-H-O bond, the length of O-H bond, the charge of H and O atoms, the energy of water molecule calculated by "colors" showed good agreement with those calculated by ADF. We calculated 27 water molecules in three states. It is observed that the oxygen atoms of water molecules share some protons with each other in the normal and sub-critical states, and in the supercritical state when oxygen atom combined with hydrogen atom in other water molecule, proton transfer takes place continually. Fig. 1 shows Mean Square Displacement (MSD) of H atom in the three states. The MSD of H atom in the supercritical state is much larger, which leads to the continual proton transfer. Fig. 2 exhibits the time-dependence of O-H length, intense vibration of O-H length in supercritical state is the effect of proton transfer.

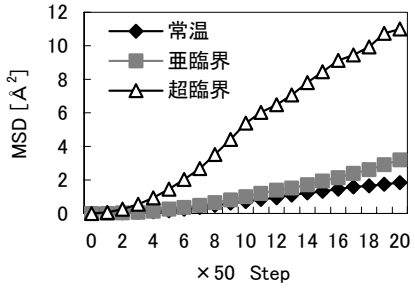

Fig. 1 : MSD of hydrogen atoms

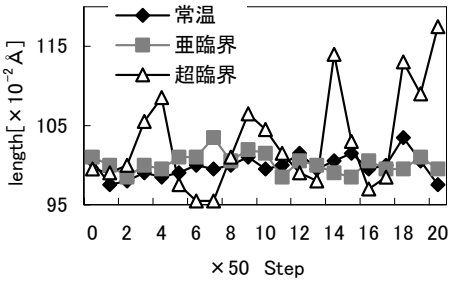

Fig. 2 : Variation of O-H length