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Rotation of water molecules in plastic phase at extreme conditions from first principles molecular dynamics method TOMOFUMI TASAKA, KAZUO TSUMURAYA, Meiji University, Kanagawa JAPAN — Water has a variety of polymorphs in wide ranges of temperature and pressure. Ice VII phase transforms to ice X with increased pressure. However the ice VII transforms to a superionic phase at higher temperatures around 2000K and pressure 30GPa in which the protons migrate in the body centered cubic lattice of oxygens. The ice VII transforms into rotator phase (so called plastic phase at lower temperatures around 600K and 5 to 50GPa. The formation of the phase has been confirmed only with the empirical potentials, whereas the experimental confirmation has been postponed until now. The present study elucidates the mechanism of the rotation of the water molecules and the correlation between the molecules during the rotation with the first principles molecular dynamics method. The water molecules rotate around each oxygen atom to conserve the ice VII positions of the protons.

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