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Hydrolysis of Cellulose in Supercritical Water: Quantum Simulation

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Abstract **–** Among several fabrication processes of cellulose nanofibers (CNF), we focus on the hydrolysis of cellulose in supercritical water. In order to analyse the detailed chemical reaction, a series of quantum molecular dynamics simulation were performed based on the density functional theory coupled with the tight binding model (DFTB). After locating the vapor-liquid critical point of the DFTB water system, we explored the hydrolysis reaction of cellulose using a simplified system consisting of a cellobiose and 100 water molecules. We observed cleavage of a β-glycosidic bond at a high temperature (1000 K). The charge analysis suggests that the oxygen atom at the cleavage site gives an electron to a water molecule approaching with sufficiently large velocity.

Keywords**:** cellulose nanofiber, hydrolysis, supercritical water, MD simulation, DFTB