# Theoretical Study on Depolymerization of Lignin using Supercritical Ethanol and Formic Acid

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Lignin is a lignocellulose biomass, which is the second most abundant natural polymer after cellulose, and it is mainly found in the cell wall of woody tree species. Through the decomposition of lignin, various phenolic monomers, which are the renewable energy sources, can be generated. But, lignin is very much difficult to be depolymerized due to internally self-interaction in molecular level. In this study, we investigated the decomposition of lignin using supercritical ethanol and formic acid (FA) solvents through reactive molecular dynamics (MD) simulation and density functional theory (DFT) calculation. Since the lignin is composed of several representative linkages, we modeled five major dilignol molecules (i.e., 4-O-5, b-1, a-O-4, b-b and b-O-4). In the decomposition of dilignol molecules, we found that the FA mainly provided the hydrogen for dilignol depolymerization whereas the ethanol transferred the hydrogen from FA to dilignol. Moreover, the ethanol-FA mixture solvent only required 20 kcal/mol less energy than pyrolysis for the lignin degradation.