Hydrodeoxygenation in aqueous phase with hydrogen of bio-derived phenols on nano-sized ruthenium clusters

The catalytic deoxygenation of phenolic compounds has become a major area of interest in recent years because they are produced during the pyrolysis of lignin and are present in biofuels. Hydrodeoxygenation (HDO) of lignin monomers requires the initial hydrogen insertions into unsaturated aromatic ring to weaken the C–O linkages, which followed by successive desired C–O cleavage and undesired further hydrogen–insertions that occurs in parallel. The catalytic pathways for lignin–monomer HDO have been studied, but the generalized reaction pathway and mechanistic interpretation among these typical lignin monomers have not been established. So, we generalized the reaction pathways for typical lignin–monomers (phenol, anisole, catechol, and guaiacol) in depicting parallel and sequential H–insertions and C–O cleavages during HDO in aqueous phase with hydrogen of these model compounds on nano–sized Ru clusters. The purpose of this study was to generalize the reaction pathways for lignin–monomers during HDO in aqueous phase with hydrogen of these model compounds on nano–sized Ru clusters.