Design of Ni-based Mixed Metal Catalysts for Hydrogen Production from Biomass : A DFT Study

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Xylose is a potential feedstock for hydrogen source. One of the challenging issues for hydrogen production from Xylose is the slow C—C bond breaking reaction of Xylose, which reduces the hydrogen extraction efficiency. In this study, we first analyzed the reaction mechanism for the conversion of Xylose to ethylene glycol and glycerol via the C—O and C—C dissociation of Xylose on the surface of small Ni cluster catalysts using first principles-based density functional theory (DFT) calculation. We determined the most favorable reaction pathway and rate determining step for the conversion of Xylose by calculating the reaction energy, reaction barrier, leading to the understanding of the descriptor that can represent the reactivity. Next, we designed the Ni-based bimetallic cluster catalysts (Ni_2M/MgO) by substituting a single Ni atom of Ni_3/MgO with noble metal M (M=3d, 4d, 5d transition elements) and investigated the catalytic activity. We correlated the descriptor and catalytic activity by varying the composition of bimetallic cluster catalysts and found the promising candidates such as Ni_2W/MgO for enhanced C—C bond cleavage catalysis.