Reaction mechanism of palm oil conversion to biofuel using Ni$_2$P catalyst

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Abstract: Fatty acids are important reaction intermediates in catalytic reduction of triglycerides. In this work, we conducted a detailed investigation of the hydrodeoxygenation of butyric acid (Fatty acid model) on Ni$_2$P surface to understand the performance of Ni$_2$P catalytic support in biomass conversion by using density functional theory calculations. Our model predicts that the main reaction can be classified into 2 pathway: hydrodeoxygenation (HDO) pathway and decarbonylation (DCO) pathway. In HDO pathway, the first step of the reaction is butyric acid hydrogenation and followed by the dissociation into surface OH and butanal. The second step of the reaction is butanal hydrogenation into butanol via the surface butoxyl intermediate. The third step is butanol dissociation into surface OH and butyl, which is further hydrogenated into butane. The rate determining step of HDO pathway is the butanol conversion to butane. In DCO pathway, the reaction starts with butanal dissociation into surface CO and propyl, which is further hydrogenated into propane. The results show that the DCO pathway is more favorable than the HDO pathway on Ni$_2$P surface. Our results provide the basis for exploring the intrinsic nature of Ni$_2$P catalysts in the hydrodeoxygenation of oxygenates involved in the refining of biomass-derived oils.

Keywords: Reaction mechanism; Palm oil conversion; Ni$_2$P surface