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Deoxygenation of oleic acid to produce bio-hydrogenated diesel over molybdenum oxide catalysts on supported alumina under inert atmosphere

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Deoxygenation of vegetable oil has been employed as one of important processes for highly efficient production of renewable green diesel (bio-hydrogenated diesel). Moreover, to avoiding sulfur contamination in fuel product, metal oxides, metal phosphides, and metal nitrides have become attractive. In this work, bimetal oxide catalysts over supported alumina were selected to produce diesel-liked hydrocarbons via deoxygenation of oleic acid under facile condition. All catalysts were prepared by incipient wetness impregnation and characterized by XRD, SEM, TEM and BET. Furthermore, effects of reaction time and temperature were studied in a batch reactor (300 mL in size) under N2 pressure. The results revealed that NiMo/Al2O3 catalyst exhibited a high conversion over 90% and the contribution of decarboxylation (DCO2) enhanced by increasing both reaction time and temperature. In addition, saturated hydrocarbons and stearic acid were also detected. These result indicated that dehydrogenation and hydrogenation occurred during the reaction. Therefore, all active phases (MoO3 and NiMoO4) of Ni doped Mo oxide catalyst were deeply investigated using DFT method with ethane as a model compound. The calculations emphasized that both of metal oxide phases could produce unsaturated compounds through dehydrogenation by taking hydrogen atoms out to the surface. Interestingly, the NiMoO4 phase contained numerous vacancies on the surface, and consumed less energy for the reaction in respect with MoO3. As a results of that, it would be a better phase to produce unsaturated products compared to MoO3 phase. However, the hydrogen atoms were not enough for hydrodeoxygenation(HDO) pathway because of low selectivity of C18 compared with C17 in liquid products.

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