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Deoxygenation and Cracking of Fatty Acids for Production of Diesel-like Hydrocarbons

Abstract

Fatty acids found in animal and vegetable fats and oils can be used to create a drop-in fuel for modern combustion engines. Thermal decomposition of fatty acids used in early conversion set-ups required lots of energy to produce fuels through a process called cracking. However, the use of metal catalysts can greatly reduce the energy needs for this process. A key step in the processing of fatty acids into diesel-like fuels is the deoxygenation of the fatty acids. Without this step, impurity build up can become a problem as well as compatibility issues with modern engines.

The role that metal catalysts play in deoxygenation and cracking of fatty acids is poorly understood on a molecular level. Investigations done on larger scales have shown a particular ability to facilitate deoxygenation by group 10 transition metals (Ni, Pd, and Pt). By using mass spectrometry, these metal catalysts are observed in the gas phase allowing for a high throughput development method with minimal sample preparation needed. In addition, due to the small sample amounts required for this method of analysis, micrograms of metals are needed, making this a much greener method for probing catalytic activity.

In this work, the mechanism of gas-phase deoxygenation and cracking of saturated fatty acids is studied using mass spectrometry and density functional theory calculations. In order to identify the key intermediates in these systems, a smaller model, propionic acid, is also used. The combination of gas-phase experiments with high-level computational chemistry can provide great insight into the most efficient way to design catalysts for production of fuel from fatty acids.