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HDO reaction mechanism of fatty acid model over molybdenum carbide

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Abstract: Transition metal carbides could replace more expensive noble metal catalyst, such as platinum and palladium, in hydrogenation and other related reaction. Molybdenum carbide (Mo_2C) was recently used for a several reactions with Pt-like catalytic behavior, high activity and selectivity and CO and sulfur compounds poisoning resistance. Molybdenum carbide was used for hydrogenation, decomposition and hydrodeoxygenation (HDO) reactions [1-2].
It is not clear how HDO reaction over Mo_2C occurs in fatty acids formed by thermal cracking of triglycerides in bio-oil and biomass, because there are only a few microscopy experimental evidences of this system [1]. Thus, the aim of this work is to propose a reaction mechanism of acrylic acid, a molecular model for fatty acid over orthorhombic 001-Mo_2C surface. For this, DFT calculations were performed with Generalized Gradient Approximation (GGA) functional PBE with periodic boundary condition (PBC). The energy cutoff for plane wave basis set was 410 eV. Calculations were done in the projector augmented wave (PAW) approximation in Vienna Ab-Initio Simulation Package (VASP). All reactants, products, reaction intermediates, and main transition state structures were obtained until formation of propane.
Results are compatible with experimental ones. The first step of reaction is the hydrogen addition to CO group, and there is no formation of carbon monoxide and propanoic acid [1].

Key-words: molybdenum carbide, DFT, heterogeneous catalysis, HDO, fatty acid
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References:

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