Challenges of catalyst development for the load-flexible and integrated production of molecular hydrogen carriers from CO_2 and water

Jens Artz[1], Chalachew Mebrahtu[1, 2], Regina Palkovits[1, 2]
[1]Forschungszentrum Jülich GmbH, Institut für nachhaltige Wasserstoffwirtschaft
Am Brainergy Park 4, 52428, Jülich, Germany
[2]Institute for Technical and Macromolecular Chemistry, RWTH Aachen University, Worringerweg 2, 52074, Aachen, Germany

Abstract

In the context of the energy transition, molecules such as methane, methanol, dimethyl ether and ammonia are ascribed a special role as energy carriers and basic chemicals. They can also serve as hydrogen carriers, provided they are subjected to reforming or cracking prior to utilization of hydrogen. To achieve sustainable and CO_2-neutral production, the utilization of renewable energy, water as a hydrogen source and CO_2 from sustainable resources (e.g. biomass or direct air capture) is preferred. However, the intermittent nature of renewable energy and dynamic material flows (e.g. waste gases, biogenic resources) poses various challenges to the overall process. Conventional chemical processes operate continuously, whereas integrating fluctuating renewable energy requires either costly storage of energy and hydrogen or load-flexible hydrogen production (e.g. via electrolysis) and chemical synthesis. Additionally, waste and recycling streams as sustainable inputs often contain impurities, which either require costly pre-treatment or robust processing technology. This in turn places high demands on the individual components of the respective technology - including the catalysts.

A main challenge for catalysts in this field is their susceptibility to the byproduct water, as it may shift the equilibrium to the reactant side via the undesired water-gas shift reaction, while also causing irreversible catalyst deactivation due to water-induced sintering of the active phase. Thus, hydrothermal stability is essential. In addition, catalysts should withstand drastic changes of harsh reaction conditions, requiring both high thermal and mechanical stability especially when they are shaped into certain dimensions providing high selectivity to desired products via pellet-diffusion and controlled contact times.

Hence, this contribution addresses these challenges and provides insights into how advanced catalyst development can overcome them. In recent work, we demonstrated the importance of impurities in the gas feed and the influence of catalyst preparation for the hydrogenation of CO_2 to methane and higher alcohols.[1,2] By integrating co-electrolysis with direct methanation, we also developed a novel concept for the production of synthetic methane from CO_2 and water.[4] Furthermore, for the production of higher alcohols, the significant influence of promoters was demonstrated[5], highlighting the importance of catalyst development on various levels, from nano- to meso- and microscopic scales.

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