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From palladium towards more sustainable metallic iron nanocatalysts for industrial hydrogenation catalysis

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PURPOSE OF THE ABSTRACT

The search for more sustainable materials and processes is one of the great challenges of our time and is mainly related to de-fossilization of energy carriers as well as chemical value-added chains and the substitution of critical materials. Regarding the latter the focus is on the substitution of expensive and rare noble metals with abundant and cheap base metals with a comparable performance. For decades Pd-Ag-based catalysts have been applied, e.g., in selective acetylene hydrogenation in the downstream processing of a steam cracker olefine stream. Such catalysts are continuously developed further. However, non-noble metal-based alternatives cannot compare in performance yet. Another window of opportunity offers the process integration, with the front-end hydrogenation as an alternative to the currently applied tail-end method. Classically, prior to the reaction the C2-cut is separated from components such as methane, carbon monoxide and hydrogen. Yet the presence of hydrogen in high amounts is advantageous, leading to a higher conversion of acetylene, suppression of the formation of oligo- and polymeric side products and therefore longer catalyst cycles and in general a simplified process integration. The major concern of this front-end integration is the higher volatility of the system and the possibility of hotspot formation or even runaway conditions. Therefore, these even more challenging conditions demand more robust and high-performing catalysts. Extensive kinetic and operational investigations under industrial conditions are necessary to understand the structure-performance-relationship and enable new catalyst innovations.[1]

We present a comprehensive catalyst innovation and kinetic study under idealized but industrially relevant reaction conditions. The ideal reactor for kinetic and operational investigations is the advanced TEMKIN reactor[2] that enables various feed compositions under industrial linear velocities and pressures. Using this system we investigated industrial reference Pd-catalysts as well as novel catalysts based on an highly dispersed eggshell catalyst with the metal organic framework $[Pd(2\text{-pymo})_2]_n$ as the active component, which competes in performance with the industrial state of the art catalysts at increased dispersion.[3] Additionally, we recently proved that metallic iron nanocatalysts are suitable alternatives to palladium hydrogenation catalysts for gas phase hydrocarbon mixtures of alkynes and alkenes.[4]

Overall, in this contribution we show the potential of innovative catalytic materials such as a Pd-MOF and base metal catalysts based on iron for catalytic hydrogenation conditions in an industrially relevant reaction system. Based on this foundation a significant advancement in more sustainable catalyst innovations for industrial applications seems feasible, especially as iron offers great potential as an abundant, cheap and sustainable alternative to noble metal catalysts for various reactions.

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FIGURES

FIGURE 1

FIGURE 2

KEYWORDS

hydrogenation | catalysis | iron | alkyne

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