

Ammonia Decomposition in the Process Chain for a Renewable Hydrogen Supply

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DOI: 10.1002/cite.202200003

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This review article deals with the challenge to identify catalyst materials from literature studies for the ammonia decomposition reaction with potential for application in large-scale industrial processes. On the one hand, the requirements on the catalyst are quite demanding. Of central importance are the conditions for the primary reaction that have to be met by the catalyst. Likewise, the catalytic performance, i.e., an ideally quantitative conversion, and a high lifetime are critical as well as the consideration of requirements on the product properties in terms of pressure or by-products for potential follow-up processes, in this case synthesis gas applications. On the other hand, the evaluation of the multitude of literature studies poses difficulties due to significant varieties in catalytic testing protocols.

Keywords: Catalyst materials, Hydrogen, Industrial ammonia decomposition

Received: January 05, 2022; *revised:* June 10, 2022; *accepted:* June 23, 2022

1 Introduction

With a steadily growing number of scientific findings corroborating the anthropogenic climate change and drastically increasing public interest in renewable resource-based industry comes a need to replace fossil fuels in industrial processes and energy production by renewable ecofriendly ones [1–10]. While solar and wind electricity as well as hydroelectricity are already established techniques to supply renewable electric energy, fossil fuels are, i.a., also used in large-scale chemical processes, e.g., syngas chemistry.

In terms of contributing to green energy production solutions as well as simultaneously satisfying the desire for sustainable production of building block chemicals or chemical fuels, hydrogen is thought to be the most important alternative. Particularly due to the exceptionally urgent demand for a large-scale energy storage solution which is capable of buffering seasonal fluctuations, hydrogen from sustainable energy-based electrolysis seems like a palpable and economic choice for decarbonization on the path to future global energy systems, especially with regard to the decreasing costs for wind and solar technologies [11–13]. Based on the current electrolyzer technology, the production of 1 kg H₂ requires 48–55 kWh energy input [14] amounting to emissions of 26–20 kg CO₂ when considering the current German power economy (470 TWh a⁻¹ [15] and 254 Mt_{CO2}a⁻¹ equivalents [16]), which could be avoided with a process based completely on renewable energy. Still, the production of renewable hydrogen will likely be processed in significant distance to the average consumer, because cheap renewable power can be generated, e.g., in northern Africa while the

majority of the hydrogen is needed, e.g., in Europe. Storing excess renewable energy in the form of hydrogen for periods of high energy demand would minimize the CO₂ backpack compared to the regular gas-fired peaking power plants. However, the large-scale storage and transport of hydrogen in its pure form is economically not feasible and some approaches for chemical storage, i.e., in the form of hydrides, are yet of only limited practical value, while the use of ammonia as hydrogen-based synthetic fuel or hydrogen vector seems to be highly promising [17, 18].

2 Green Hydrogen as an Alternative to Replace Fossil Fuels

2.1 Hydrogen Production and Current Challenges

Hydrogen for syngas processes is commonly produced (70 Mt a⁻¹ in 2019 [19]) via steam methane reforming and partial oxidation or autothermal reforming of hydrocarbons

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with typical costs of 1–1.8 US \$ kg_{H₂}⁻¹ [6, 8, 20, 21]. Beside hazardous pollutants, i.e., SO_x, NO_x, and particulates, these processes based on natural gas, oil, and coal generate huge amounts of CO₂ (~10 t_{CO₂}t_{H₂}⁻¹ [19]). Green alternatives for H₂ production are biomass-based processes, thermal processes, electrolysis, processes using solar irradiation, or combinations of these processes [3, 9, 20, 22, 23]. Probably best known and most versatile among these techniques is the water splitting via electrolysis [8, 22, 24]. Without considering manufacturing processes for the respective technology, H₂ production can be established with lowest environmental impact in combination with electricity originating from hydropower plants, wind turbines, and photovoltaics [8, 21]. But the efficiency of production highly relies on the geographical situation, i.e., periods of wind and/or high solar irradiation of maximum longevity, and in consequence, the produced H₂ has to be stored or transported over particularly long distances to the consumer.

Storage and transportation of hydrogen have a few intrinsic obstacles [3, 5, 10, 18, 24–30]. H₂ is commonly stored under high pressure or liquified at very low temperatures. Even under high pressure, H₂ has still a low energy density (8–10 MJ m⁻³) [3, 5, 25, 27, 29] due to the low density of H₂ and the disproportionately huge weight of the vessel (at 700 bar only ~6 wt% stored H₂ vs ~94 wt% for the vessel [10]). Furthermore, pressurization is an energy-intensive process, requiring 10–13% of the net energy content of the hydrogen [26, 27, 31]. At 20 K, hydrogen can be transported as liquid but the H₂ continuously boils off (0.2–0.3% d⁻¹) [32, 33] and the energy needed for liquefaction reduces the net energy content by 30–40% [2, 18, 20, 26, 27, 34]. Further problems arise from the small molecular size of H₂ which is why it tends to leakage and can diffuse into metals which induces brittleness or blistering of, e.g., storing vessels [5, 25, 27, 30, 35]. Additionally, the flammable range of 4–75% of hydrogen demands precautions during transport, storage, and use [36, 37].

For storing alternatives, the U.S. Department of Energy's target for storage capacity of H₂ is 5.5–9 wt%, beside reversibility, fast kinetics of hydrogen uptake/release, low sensitivity to impurity gases, large scale producibility at low cost, and safety [2, 25, 26, 34]. Some promising alternatives are the reversible storage and transport of hydrogen as hydrides, in porous materials, with liquid organic hydrogen carrier (LOHC) like cyclohexane and methanol, or as ammonia (Fig. 1) [10, 29, 34, 35]. Within this set of possibil-

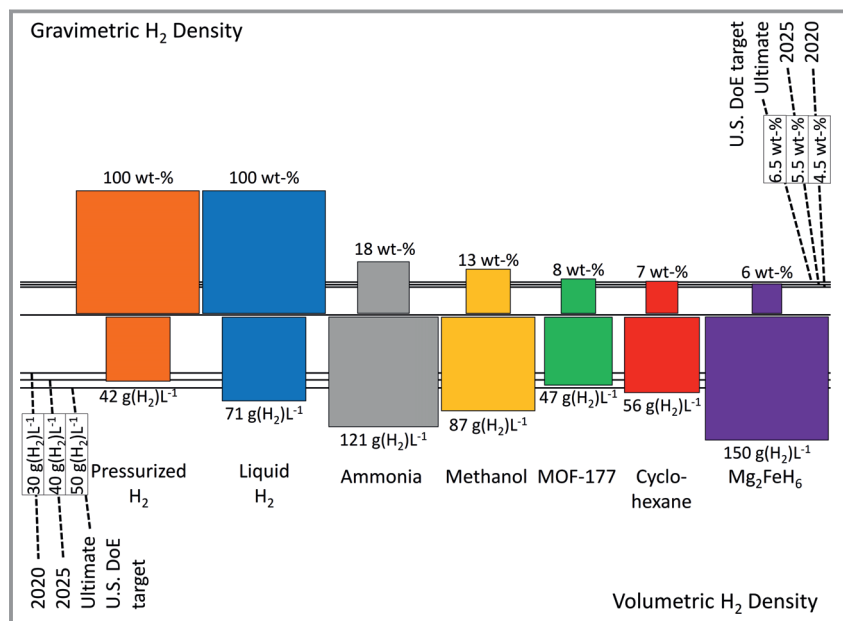


Figure 1. Volumetric and gravimetric H₂ density of selected hydrogen carriers represented as squares. Relative size of the squares shows the capacity of each hydrogen carrier compared to others and the capacity targets stated for mobile use by the United States Department of Energy [41]. Data stems from: cyclohexane (298 K, 0.1 MPa) [42], MOF-177 (77 K, 7 MPa) [43], Mg₂FeH₆ (298 K, 0.1 MPa) [44], methanol (298 K, 0.1 MPa) [35], liquid ammonia (298 K, 1 MPa) [35], hydrogen (liquid: 20 K, 0.1 MPa, pressurized: 298 K, 69 MPa) [35]. Decrease of volumetric and gravimetric capacities due to respective storage vessels has to be considered.

ities, ammonia is very interesting if it is produced from green hydrogen and renewable energy via the well-known and efficient Haber-Bosch process (Fig. 2) [17, 29, 35, 38–40], because apart from H₂ only omnipresent N₂ is connected to its production and decomposition and no storage material has to be shipped back for recycling, as, e.g., for LOHC's.

2.2 Ammonia as a Hydrogen Carrier

The gravimetric H₂ capacity of NH₃ is 17.6–17.8 wt% [10, 34, 39] and its volumetric H₂ density (121 kg_{H₂}m⁻³ in liquid ammonia [35]) is 1.4 times higher than that of liquid hydrogen [10, 35]. The round-trip efficiency of ammonia and use of the hydrogen in a fuel cell is estimated to be ~19% and is similar to that of liquid hydrogen (22% without consideration of boil off losses) [14]. NH₃ itself is a substance of already high relevance for the production of fertilizers [36, 39, 45]. A green synthesis of large amounts of ammonia (power to ammonia, P2A [1]) would have a double benefit [46].

Economic feasibility was analyzed for northern Europe by Ikäheimo et al. [1] and Australia is raising a commercial-scale ammonia plant powered with solar and wind electricity with a production capacity of 50 t d⁻¹ [19]. Furthermore, during release of H₂, the only by-product would be N₂

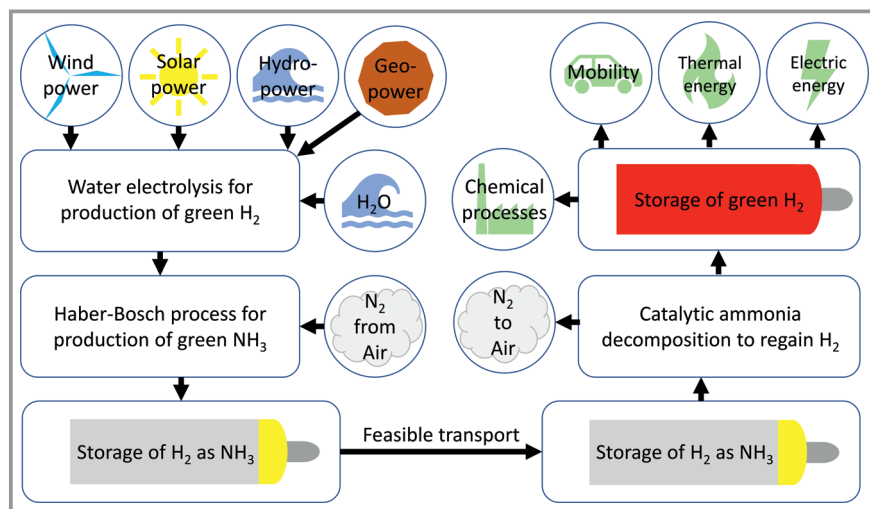


Figure 2. Flowchart of a green hydrogen economy using NH₃ as hydrogen vector.

[29, 36, 47]. Thus, there is no additional handling of greenhouse gases or materials needed.

Various technologies, such as thermal decomposition [48], microwave decomposition [49], decomposition with plasma technologies [50], decomposition with electric current/electron beam/ion beam [51–53], decomposition with solar energy [54], and electrolysis of liquid NH₃ [55], are in the scope of current research on the production of hydrogen via ammonia decomposition. Among them, thermal decomposition, usually carried out at higher temperature, is the most promising technique [56]. At the current technical state, ammonia decomposition requires a bulky reactor, which can be a drawback for mobile [10, 47] as well as for stationary applications, because of significantly growing costs for increasing reactor volumes. Microreactors for ammonia decomposition are subject of current research and would allow decentralized, small, and even mobile applications [57, 58].

2.3 Main Challenges of Ammonia as a Hydrogen Carrier

An advantage of NH₃ as future H₂ carrier is that it is already produced on Mt scale for the use primarily as fertilizer and is transported even in pipelines [10, 17, 35–37, 40, 59, 60]. Hence, safe storage and transport is common, as well since NH₃ is easily liquefied under slight pressure (8–10 bar at 20 °C) [17, 36, 39, 59, 61]. However, due to its hazards and toxicity, precautions are needed to ensure safety [10, 17, 35–37, 40, 46, 47, 59, 60]. Probably the most critical challenge is to transform ammonia back to hydrogen [46, 62]. Although catalytic ammonia synthesis is well understood, ammonia decomposition still needs comprehension and optimization, especially because there is no industrial process available so far [60]. Beside

catalytic aspects that make a difference between ammonia synthesis and decomposition [37, 60, 63], technologies using the recovered hydrogen from ammonia are particularly sensitive to NH₃ [17, 35, 46, 60]. In methanol production from syngas, ammonia impurities cause, e.g., formation of the side product trimethylamine [64–66]. Therefore, catalytic ammonia decomposition must be either 100 % complete or a post-purification process is needed. The latter, e.g., via (pressure swing) adsorption or H₂-permeable membranes [60, 61, 67, 68], adds additional costs and reduces the effectivity of using ammonia as hydrogen vector. Quantitative decomposition of ammonia in catalysis is typically observed at un-

desirably high temperatures of 600 °C and higher [10].

Therefore, one of the most significant challenges in enabling NH₃ splitting as source for subsequent syngas processes is to tailor a catalyst which is most effective with high energy efficiency, providing stable rates at low temperatures, while being highly selective, scalable, and cheap. Another important goal for hydrogen recovery from ammonia decomposition is to achieve high conversion at elevated pressures which would potentially be beneficial for follow-up processes, e.g., 30–100 bar for methanol production [64, 65, 69]. However, a higher process pressure will lower the equilibrium conversion and, therefore, significantly higher temperature and/or an extensive purification step is required subsequently. This goal is addressed by only few studies yet [70–73].

In this review, the requirements on ammonia decomposition catalysts are highlighted with regard to a potential application in an industrial utilization of NH₃ as H₂ vector for, e.g., downstream syngas chemistry processes. While a few potentially interesting materials are discussed, the challenges accompanying the identification of appropriate prospects from the available literature studies are a central topic of this article.

3 Theoretical Background

3.1 Thermodynamic Limitations

The ammonia decomposition reaction is an equilibrium reaction with ammonia synthesis as its back reaction, as shown by the formal reaction in Eq. (1). Ammonia decomposes into elemental hydrogen and nitrogen in a stoichiometric ratio of 3:1. It is an endothermic reaction with an overall reaction enthalpy of $\Delta H_0 = 92.44 \text{ kJ mol}^{-1}$, which is relatively moderate for a chemical reaction [74].



Due to the endothermicity of the reaction, ammonia decomposition is favored at an increase of temperature, as shown by the temperature dependence of the thermodynamic equilibrium in Fig. 3. At the same time, the equilibrium conversion of ammonia decreases with increasing pressure.

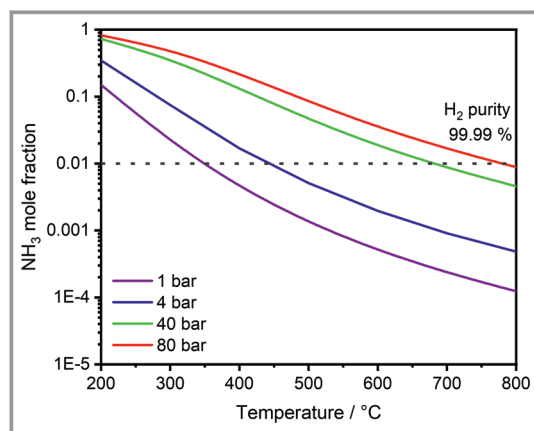


Figure 3. Equilibrium mole fraction of ammonia at 200–800 °C and different pressures of 1, 4, 40, and 80 bar (calculated with Aspen Plus software).

Therefore, a high yield or even full conversion in ammonia decomposition requires high temperatures and low pressures for a technical process. The inverse to this ammonia synthesis is favored by low temperatures and high pressures. Due to this, industrial ammonia synthesis needs to be performed at high pressures above 100 bar [75].

3.2 Reaction Kinetics

The first insights into the reaction kinetics of the ammonia decomposition reaction were mostly found during efforts to better understand the ammonia synthesis reaction. Due to the prolonged and high industrial relevance of ammonia synthesis, a lot of work has been done in this field and as the back reaction is easier accessible under lab conditions and for common characterization methods (high-pressure requirement for ammonia synthesis), ammonia decomposition has been used to investigate the single reaction steps. The same elementary reaction steps have been found for the ammonia synthesis and the ammonia decomposition reaction. A list of the single elementary steps of the ammonia decomposition reaction over a catalyst surface is illustrated in Eqs. (2)–(8) (* indicates a free adsorption site at the catalyst surface).



While these elementary reaction steps are widely accepted in literature, it has not been possible to define a single rate-determining step (rds). This is due to the fact that the kinetics of the single steps change separately with reaction parameters like temperature, coverage of reactants on the catalyst surface, and catalyst material. Often reported rate-determining steps for ammonia decomposition are the removal of the hydrogen atoms from the ammonia molecule (Eqs. (3)–(5)) and the desorptive recombination of the nitrogen molecule (Eqs. (6) and (7)) [76–80]. The removal of hydrogen atoms has been reported as rds, e.g., on W and Mo catalysts, while the recombination of nitrogen turned out as rds for Fe catalysts. It is also possible to reach a “hydrogen poisoning” under certain reaction conditions, where the catalyst surface is highly covered with hydrogen and the reaction can only proceed when a hydrogen molecule desorbs from the surface and generates a free adsorption site. In this case, hydrogen desorption (Eq. (8)) is the rds. This has been especially reported for Ru catalysts [81].

Unlike ammonia synthesis, it is possible to obtain side products under the reaction conditions of ammonia decomposition. It has been reported that specific reaction conditions can lead to the formation of hydrazine [82, 83]. This leads to a competitive reaction pathway for the formation of hydrazine besides the main reaction steps for ammonia decomposition [82]. The formation of hydrazine as a side product is thermodynamically possible, but not a significant constraint for a potential technical ammonia decomposition process as hydrazine is quite easy to decompose in purification processes and is only formed in small amounts under specific reaction conditions [82].

3.3 Conditions Relevant for Technical and Industrial Applications

As mentioned before, ammonia decomposition is favored at high temperatures and low pressures. Any technical application where ammonia decomposition is used to produce hydrogen for a subsequent process will require nearly full conversion of the ammonia to obtain a high yield of hydrogen (> 99.9 %) and to keep the ammonia content in the produced hydrogen low, as ammonia is highly corrosive and reactive and could be a damaging impurity in the hydrogen for many subsequent processes. Due to thermodynamic

limitations, there is always a minimum required temperature to achieve a nearly full hydrogen yield (>99%) in ammonia decomposition, which increases with increasing pressure (Fig. 4). For example, at atmospheric pressure, a hydrogen yield of >99% requires a minimal temperature of around 400 °C. At the same time, for a technical process, it would be favorable to keep the temperature as low as possible to reduce the energy demand for heating. Especially due to the endothermicity of ammonia decomposition, a technical process would require a constant energy supply in heating.

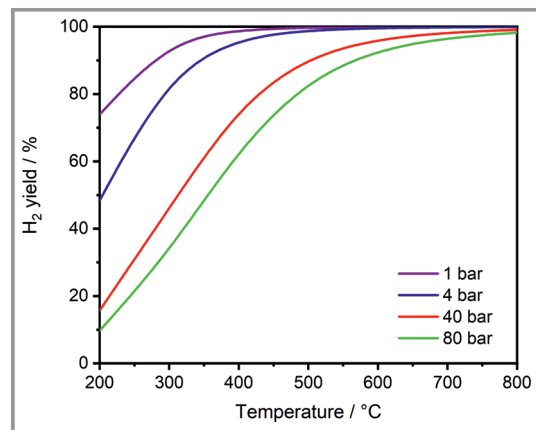


Figure 4. Equilibrium yield of hydrogen in ammonia decomposition at 200–800 °C for 1, 4, 40, and 80 bar (calculated with Aspen Plus software).

Depending on the subsequent process the hydrogen is used for, another required key parameter would be the pressure of the produced hydrogen. Currently, hydrogen for industrial use as synthesis gas is produced by cracking and steam reforming of coke, oil fractions, and natural gas at pressures of around 30 bar [75]. Most of the processes using this synthesis gas operate at the same pressure or higher. Therefore, it is desirable to obtain hydrogen from ammonia decomposition also at an elevated process pressure of around 40 bar ($p_{\text{H}_2} \sim 30$ bar). As a drawback, higher pressures can only be reached with sturdier, thicker walls of the reaction vessel, which would in turn impair the heat transfer across the reactor walls, potentially leading to significantly higher heating temperature requirements to reach the required reaction temperature inside the catalyst bed. This leaves two potential pathways for a technical ammonia decomposition process: on the one hand, a low-pressure ammonia decomposition process at about 1–5 bar, where the hydrogen is subsequently compressed according to the requirements of the following process, and on the other hand, a high-pressure ammonia decomposition process providing hydrogen directly in the desired pressure range of the envisaged ensuing processing. Which of these pathways would be the more cost-efficient way needs to be calculated specifically for each potential subsequent process.

The low-pressure decomposition process is surely interesting for applications where no elevated hydrogen pressure is required as in small-scale and/or mobile applications. A prominent example would be feeding a fuel cell with hydrogen to produce energy for an electric car. Fuel cells can operate near atmospheric pressure, and at low pressure the minimal required temperature for nearly full ammonia conversion is the lowest, which is beneficial for mobile solutions where the dimensions of the heating system have to be as compact as possible. But also for large-scale applications with higher pressure requirements it could be more efficient to keep the decomposition temperature as low as possible and compress the hydrogen to moderate pressures afterwards.

Due to the thermodynamic equilibrium, a high-pressure ammonia decomposition process would require a higher temperature for full conversion than a low-pressure process. For example, ammonia decomposition at 40 bar would need a reaction temperature above 700 °C for a hydrogen yield of >99%. For some applications, this way could actually be more efficient as a large-scale low-pressure production would require a higher reactor volume to get the identical hydrogen output of a high-pressure production and an extra compression section could also mean major expenses.

In the end, both potential routes will require a further purification of the produced hydrogen from ammonia residuals. For the case of fuel cells utilizing hydrogen from ammonia splitting, it is often reported that the tolerance towards ammonia is minimal, i.e., below 0.1 ppm for proton-exchange membrane fuel cells [84]. This degree of purity will likely not be achieved solely by ammonia decomposition even at a low-pressure route under optimal conditions. Similar restrictions with regard to hydrogen purity apply to other industrial follow-up processes. The ammonia residuals could be detrimental to the process or lead to unpleasant impurities in the final product. Under certain conditions, NH_3 might be oxidized to N_2O , a very potent greenhouse gas, or react to other side products. In methanol synthesis, e.g., residual ammonia in the feed gas acts as a poison for the industrial $\text{Cu}/\text{ZnO}/\text{Al}_2\text{O}_3$ catalyst and leads to the formation of trimethylamine, which would lower the value of the produced methanol due to its persistent odor or might even render it unmarketable [64]. There are, however, very efficient purification processes for the removal of ammonia from synthesis gas available which are used on an industrial scale, e.g., thermally regenerated adsorbers [85]. These techniques could potentially be optimized for the product purification in an industrial ammonia decomposition process.

Furthermore, many industrial processes utilizing H_2 from NH_3 reforming would require a removal of the invariably formed nitrogen from the synthesis gas. Especially for processes with a recycle of the synthesis gas this would be essential, as the nitrogen as inert would otherwise accumulate with each recycle until the amount of actual reactants in the process gas would be minimal. A removal of nitrogen

from hydrogen could be achieved by pressure swing adsorption or cryogenic distillation as these techniques are already commonly used for gas separation on industrial scale.

4 Ammonia Decomposition Catalysts

Considering that decreasing the conversion temperature to increase the conversion efficiency is beneficial for facilitating the further development of this field, numerous efforts have been devoted to the development of highly active and robust catalysts [56,62]. According to the composition of existing catalysts, the bigger part can roughly be classified into the following categories: monometallic catalysts, multimetallic catalysts or alloy catalysts, nitride and carbide catalysts, and metal amide/imide catalysts. The majority of these material classes have been investigated on a multitude of different support materials, e.g., alumina-, magnesia-, or silica-based as well as carbon-based, to name a few prominent examples. The addition of one or more promoters to increase the catalytic activity was also studied for the majority of the available catalysts [56]. Examining the recent comprehensive review on ammonia decomposition by Lucentini et al. [56] clearly illustrates the focus of the past research on monometallic catalysts (Fig. 5).

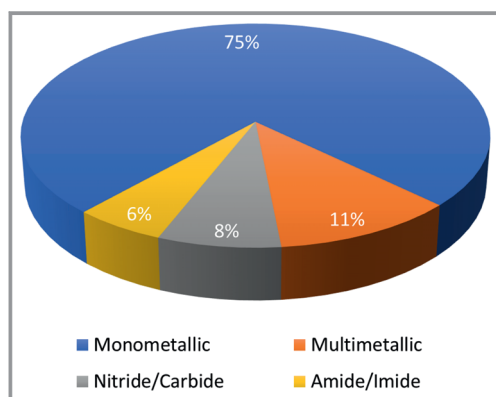


Figure 5. Evaluation of research reports on different catalyst material classes for ammonia decomposition, based on data from Lucentini et al. [56].

The following concise discussions about different catalyst materials refer to studies which have been carried out with 100% NH_3 in the feed gas, usually in a continuous plug flow-type reactor. Detailed information on by-products, e.g., hydrazine, is usually not presented in most of the available studies. Unfortunately, also long-term stability measurements or rapid ageing tests are not conducted regularly, probably as the research on this topic is still mainly focused on fundamental research and not so much on industrial applicability.

4.1 Monometallic Catalysts

Originally, ammonia decomposition and the corresponding catalysts were often investigated as part of comprehensive studies on the ammonia synthesis reaction. Accordingly, catalysts used in the Haber-Bosch process, i.e., Fe- and Ru-based materials, were among the initially examined catalyst systems [46]. Subsequent studies developed other metal-based catalysts, including Cu [86], Ni [87], Ir [88], Mo [89], Co [90], Pt [91], Pd [92], and Rh [93]. Ruthenium-based catalysts supported on different oxides, structured and unstructured carbon [17], and especially on K-doped carbon nanotubes are among the most active materials for the decomposition of ammonia reported up to now [94–96], outperforming most of the other previously reported catalysts. The Ru catalysts partially exhibit high activity at already 400 °C, the lower temperature limit for quantitative conversion according to thermodynamic boundaries. It has to be mentioned though, that in many studies there is no comment on potential methanation of carbon supports or long-term stability and only a few reports include rapid ageing tests or stability tests in the range of 200 h [96]. Furthermore, the low abundance and very high cost of ruthenium significantly impede its sustainable large-scale application. Based on the principle of microscopic reversibility, it could be expected, that an optimal ammonia synthesis catalyst would also be highly active in ammonia splitting. Alongside quite a large number of studies on iron-based catalysts, including Fe nanoparticles on carbon [97–100], silica [101, 102], or alumina supports as well as core-shell nanoparticles [103], it has now been revealed, that this is actually not the case [63]. There are reports on Nickel-based catalysts supported on transition metal oxides that exhibit satisfying mechanical properties and heat resistance [40]. Especially Ni-catalysts on Al_2O_3 show productivities that, also depending on potential dopants, might rival those of Ru-based systems. Although the required reaction temperature for sufficient activity is typically reported to be around 500–550 °C and thus higher than in case of Ru, Ni-based catalysts are regarded as a potential choice for commercial decomposition of ammonia [56, 104].

4.2 Multimetallic Catalysts or Alloy Catalysts

Multimetallic or alloy catalysts are considered as one of the most promising ways for promoting the development of ammonia decomposition catalysts. Because of the well-tunable properties and potential metal-metal synergies, multimetallic or alloy catalysts can exhibit enhanced performance for the decomposition of ammonia compared to monometallic counterparts [62]. Furthermore, multimetallic catalysts bear the potential of reducing the amount of highly active but equally expensive noble metals like Ru by discovering suitable combinations of this catalyst with more common metals with retained high activity [105]. Extensive

research efforts have been devoted to investigations on different combinations of metals, including Ni-Pt [106], Ni-Fe [107, 108], Ni-Co [109], Ir-Ni [110], Co-Mo [111–113], Fe-Co [114, 115], Fe-Mo [116], and Cu-Zn [117] on different supports. Especially, Co-Mo catalysts are proposed to be one of the most attractive bimetallic catalysts for decomposing ammonia due to the significant catalytic activity and low cost [111]. Previous studies without an influence of a support material have demonstrated that the active phase in Co-Mo bimetallic catalysts is actually the nitride $\text{Co}_3\text{Mo}_3\text{N}$ [111]. However, it still seems that materials with very low noble metal content, but simultaneously similarly high activity as Ru-based catalysts at temperatures below 500 °C are not yet available.

4.3 Nitride and Carbide Catalysts

In more recent studies, carbides and nitrides of Mo, Fe, Co, Ni, Ti, V, Mn, and Cr have been identified as possible contenders for ammonia decomposition catalysts [62], especially since nitrides likely form during NH_3 decomposition, depending on the catalyst material. For example, Zheng et al. [118] prepared high-surface-area molybdenum carbide via a temperature-programmed reduction-carburization method. In contrast to previously reported Mo-based catalysts, the as-synthesized material showed a much higher H_2 production rate, which can be attributed to the existence of highly energetic sites, i.e., defects, steps, twin boundaries, and stacking faults. Choi et al. [119–121] demonstrated that vanadium and molybdenum carbides as well as tantalum carbides can be used as catalysts for ammonia decomposition. The activity of the vanadium carbides was lower than that of molybdenum carbides, and the authors proposed this might be connected to the degree of electron transfer between the metals and the carbon. Despite promising prerequisites and enormous progress in increasing the performance of nitride and carbide catalysts, this field of research still leaves a lot of room for further developments.

4.4 Metal Amides/Imides Catalysts

Apart from the above-mentioned catalysts, metal amides/imides seem to constitute promising catalysts for ammonia decomposition as well [62]. Although the first study on metal amides/imides for H_2 and N_2 evolution from NH_3 dates back to 1894 [122], this class of catalysts was rediscovered only recently, when David et al. [123] presented that sodium amide is an effective NH_3 decomposition catalyst. It is important to note that the alkali metal amides, including LiNH_2 , KNH_2 , and NaNH_2 , can show similar or even better conversion results than Ru-based catalysts. Makepeace et al. [124], e.g., discovered that lithium imide can outperform $\text{Ru}/\text{Al}_2\text{O}_3$ in the production of high-purity hydrogen from ammonia, depending on the intermediately formed stoichi-

ometry of the catalyst material. Besides, it is a possible way to improve the performance of catalysts via coupling metal amides/imides with other active metals and nitrides. A representative example is the strong promoting effect of alkali metal amides on the catalytic ammonia decomposition activity of MnN [125].

5 Comparability of Datasets from Literature and Identification of Suitable Materials

As there is no industrial process for ammonia decomposition yet, which could serve as precedence case, the identification of suitable catalyst materials or material classes for application in such processes is one of the first obstacles to clear. In the context of evaluating catalytic experiments from the literature, it has to be mentioned that a reliable comparison of different catalyst materials and their performance in ammonia decomposition from the multitude of available literature studies or comprehensive reviews on this topic [56] is complicated because of significant discrepancies in the experimental procedures, the level of detail in the description of these procedures as well as disparities in the analysis and presentation of the results. While differences in material preparation are inherent in the variety of ammonia decomposition catalyst materials, the testing procedures (exemplary illustrated in Tab. 1) and the depth of information on the applied conditions disclosed to the reader are critical to allow comparing the in part substantially different catalyst materials as reliably as possible [126]. Furthermore, a variety of reactivity determinants to describe the catalytic performance leads to a very challenging task when trying to juxtapose catalysts from several literature surveys. Noteworthy in this context is, e.g., that it became established to report activity measurement results, i.e., the conversion, in dependence of the gas hourly space velocity (GHSV). This is generally the standard in industrial application. While it is obvious, that this can also be very helpful in lab scale studies, it sometimes further complicates comparison as it is not always evident if the catalyst bed volume required for the calculation of the GHSV is only roughly approximated or determined accurately. Similarly, when the efficiency of a catalyst is discussed in terms of turnover frequencies (TOF), a comparison is only feasible, when it is obvious if a “real” turnover frequency relating to a previously ascertained number of active sites or a “quasi-average” TOF without an exact assessment of active sites is presented. Quite often there is a lack of information in the reported data hindering a direct comparison.

If the reported catalytic rates allow a transformation to a common unit, the juxtaposition of different materials is significantly facilitated. Considering the relevance of space time yield or weight time yield in industrial heterogeneous catalysis as the standard measure for catalyst performance, the transformation of reported rates to, e.g., catalyst productivity ($\text{kg}_{\text{H}_2}\text{kg}_{\text{cat}}^{-1}\text{h}^{-1}$) [17] at specific reaction condi-

Table 1. Randomly chosen results for Co-, Ru-, and Ni-based catalyst materials to illustrate the significant differences in reaction test conditions.

Catalyst material	Temperature [K]	GHSV [$\text{L}_{\text{g}_{\text{cat}}}^{-1}\text{h}^{-1}$]	Flow rate [L h^{-1}]	Conversion [%]	Productivity [$\text{kg}_{\text{H}_2}\text{kg}_{\text{cat}}^{-1}\text{h}^{-1}$]	Reaction time [h]
Co@SiO ₂ [127]	600		15	71	12	4
Co@La-MgO [128]	550	22		100	3	45
Co@MWCNTs [129]	500	6		75		20
Ru@K-CNTs [130]	500	150		29	6	10
Ru@K-CNTs [96]	500		3	100	8	200
Ru@MgO-CNTs [95]	450	60		100		200
Ni _{2.7} Al _{0.3} O ₄ [102]	600	36		93		70
Ni ₂ Mo ₃ N [131]	525	6000		98		30

tions would be favorable, as it also would allow a rough classification of the NH₃ decomposition catalyst performance in relation to similar catalytic processes.

Taking this up, we collected available data from literature studies on catalytic decomposition of 100 % NH₃ in which either the productivity was reported directly, or reaction rates which allowed a transformation to productivity. To at least rudimentarily classify the multitude of different catalyst materials in terms of potential applicability in industrial processes, we mapped the reported productivity of several different active components, i.e., ruthenium [70, 94–96, 130, 132–146], other noble metals like palladium and platinum [130, 137, 147], nickel [102, 128, 130, 132, 137, 138, 148–154], cobalt [90, 102, 115, 127, 128, 155, 156], iron [102, 128, 130, 157–159], molybdenum-based nitrides, carbides or sulfides [118, 160–163] as well as bimetallic catalysts [90, 115, 147, 164, 165], at distinct temperatures (Fig. 6). This criterion is rather straightforwardly accessible from the mentioned studies. A comparison of the number of studies reporting a certain productivity of the respective material in a defined temperature range reveals that catalyst materials based on noble metals other than Ru as well as Fe-based catalysts seem to exhibit comparably low productivities at any investigated temperature, while Co- and Ni-based materials and especially catalysts comprising Ru show partially very high productivities at temperatures around 500–550 °C. Mo-based catalysts have mainly been scrutinized at higher temperatures around 600 °C. It has to be mentioned, though, that the total number of suitable reports significantly varies across the individual materials and the majority of literature studies was not regarded due to a lack of reported reaction rates.

Based purely on the evaluation of preferably high productivities of the available catalyst materials in the temperature region below 550 °C, the targeted region for the low-pressure NH₃ decomposition route, nickel- and cobalt-based catalysts might constitute promising materials for large-scale applications as a significant fraction of the reported

productivities exceed those of other transition metals. As ruthenium is by far the most popular active material in fundamental studies on NH₃ decomposition and has been investigated in combination with a myriad of different supports, promoters, and other modifications, the productivity map spreads out across almost the entire investigated temperature region. It is likely safe to assume that there would be suitable Ru-based catalysts for an industrial NH₃ cracking process with regard to high productivity at a given temperature as long as the material costs and an upscaling of the catalyst production process can be kept in check. This also applies particularly to Ru support materials, as the highest productivities were reported for the well-known combination of promoted ruthenium on carbon nanotubes.

For future endeavors to interrelate a large spectrum of catalyst materials for, e.g., evaluating the feasibility of application in a desired reaction, it would be very beneficial, if there were more studies containing screening of materials under a set of consistent reaction parameters, or, better yet, a general concept or procedure for testing heterogeneous catalysts, if of course the parameters are applicable to the respective material. In this context, a basic strategy towards consistent data set generation in heterogeneous catalysis has been elaborated by Trunschke et al. [126]. If the challenge to thoroughly benchmark and compare catalyst materials had been overcome, it would make the selection of suitable catalysts for in-depth investigation in terms of meeting the decidedly high requirements for an application in industrial processes, particularly in connection with subsequent synthesis gas applications, significantly more convenient. The preliminary survey of the productivities in this review suggests that well-structured catalytic studies of Co- and Ni-based catalyst materials, including in-depth analyses of the catalyst material, kinetic studies, and long-term stability tests, might be promising. It does, however, also not exclude, that more recent approaches to develop highly active catalyst materials, e.g., nitrides, amides, or mixed oxides, might yield rewarding results as the number of studies on

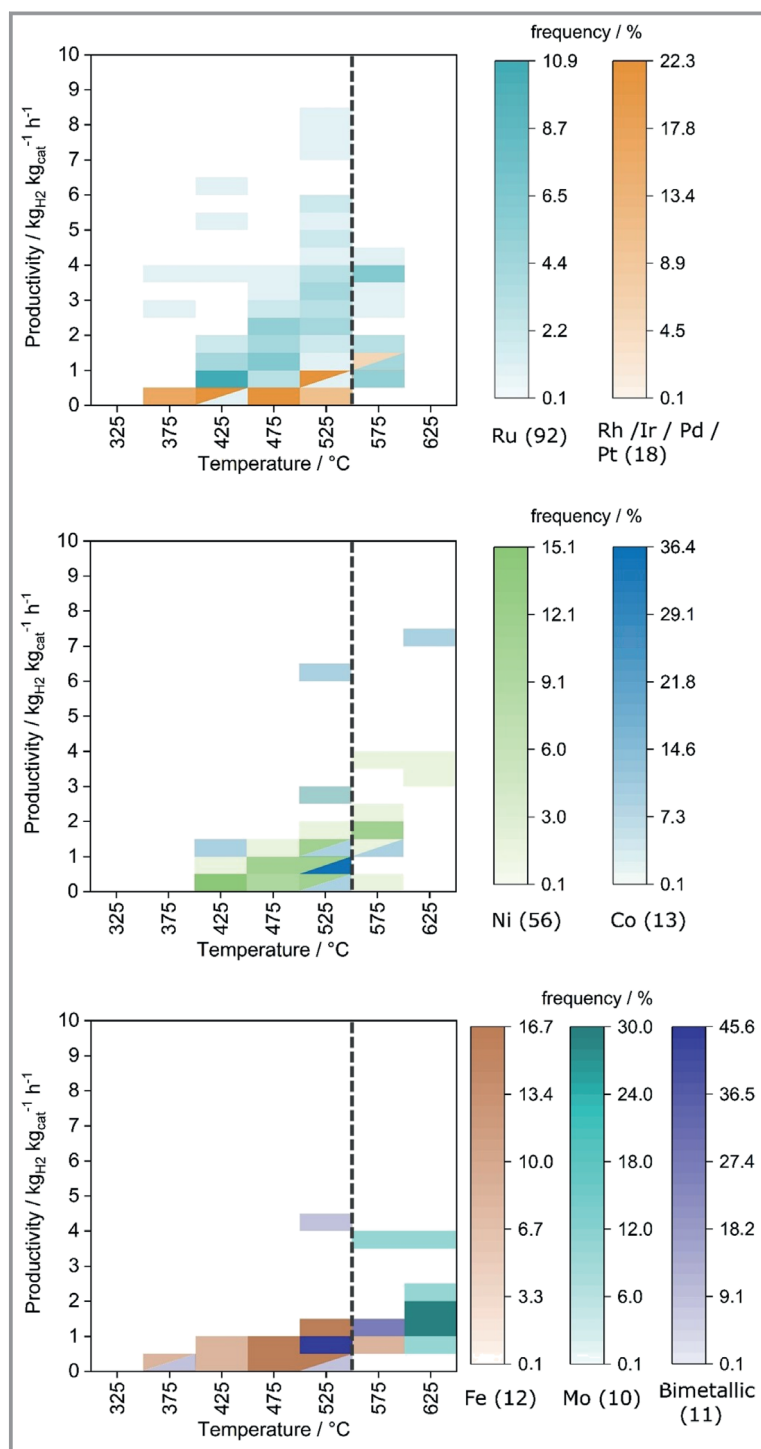


Figure 6. Productivities of different catalyst material classes at distinctive temperatures from suitable literature studies. The dashed line marks 550 °C as an upper T-limit. The color gradient indicates a percentage-weighted frequency of reports on the respective productivities, the total number of identified data sets per material class is given in brackets next to the material identifier.

these materials and the related insight is still continuously growing, meaning these materials are somewhat under-represented on the productivity map. Apart from thor-

oughly benchmarking catalysts, recent advances in the coupling of theoretical and experimental approaches likely have the potential to contribute to identifying suitable catalysts [166–168]. In this context, an innovative multidisciplinary approach not only involving necessary standardized catalyst testing protocols, as proposed by Trunschke et al. [126], but also novel strategies for research data generation, unification of data formats, and big-data management, assisted by AI-based structure-function predictions for a more rational catalyst design would be of great assistance to cross paradigmatic boundaries between theory and experiment. This transformation of the general mindset of current catalysis research and handling of research data into a new dimension is often termed digital catalysis. It is thought to be the most significant booster for innovations and the future of catalysis research and is, e.g., discussed in detail by the research initiative NFDI4Cat [169].

6 Conclusion

The catalytic decomposition of ammonia is a well-known reaction that has been studied thoroughly, albeit not to the extent of ammonia synthesis. This likely is in tandem with a current lack of a large-scale industrial application, which is however to change since ammonia is widely discussed as potential hydrogen vector or storage system in the context of green hydrogen technologies and infrastructure. While a huge variety of catalyst materials was examined in lab-scale experiments, a reliable comparison of the catalysts and a detailed estimation of the suitability of the respective catalysts in an industrial process is complicated by the broad spectrum of approaches in catalytic testing and data analysis. A defined analysis protocol or testing procedure within well-defined boundaries would simplify literature study evaluation. There are several materials which seem to be very promising, but the demands on an industrial ammonia decomposition catalyst are quite high, i.e., space time yields in the same range as commercial ammonia synthesis catalysts, very high selectivity to reach the required purity levels, and sufficient long-term stability while maintaining economic viability. The versatility of promising catalyst systems and possibility to tune material properties that come with such a wide range of materials provide a good starting point for catalyst development. However, there is an urgent need to set up an industrially feasible ammonia decomposition already in the near

future to tackle the upcoming hydrogen demand in a more sustainable industrial network. Despite the multitude of investigations on this topic, fast and structured screening of potential candidates is still required to break down the variety of possible catalysts to those applicable in an industrial process. To solve the ammonia challenge scientifically, an understanding of the descriptors for the catalyst materials and a study of the dynamic phenomena is required. A structured, multidisciplinary approach such as, e.g., proposed by the NFDI4Cat initiative would seem very promising to approach this and further future major challenges in catalysis research.

The authors thank the Federal Ministry of Education and Research, Germany (Bundesministerium für Bildung und Forschung, BMBF, Verbundvorhaben Carbon2Chem[®], support code: 03EW0004C and TransHyDE Forschungsverbund AmmoRef, support code: 03HY203A) for funding. Open access funding enabled and organized by Projekt DEAL.

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