

## Palladium catalysts supported on carbonized porous silicon for H<sub>2</sub>/O<sub>2</sub> recombination

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The article presents new research on the use of catalysts for H<sub>2</sub>/O<sub>2</sub> recombination. The study emphasizes the importance of ensuring safe production, storage, and utilization of green hydrogen by recombining gas leaks. We suggest the utilization of innovative palladium catalysts for low-temperature hydrogen oxidation. These catalysts leverage molecular oxygen from the air to efficiently recombine small amounts of leaked hydrogen, resulting in the production of water. Recombination catalysts with a small amount of dispersed palladium metal on an inert support are the most efficient for production to prevent the risks of hydrogen explosion and fire. This study is focused on the development of laboratory prototypes for the H<sub>2</sub>/O<sub>2</sub> recombination catalysts. We identified a potential catalytic system through monitoring of current literature to propose efficient hydrogen recombination catalysts. We present an optimized method for coating the surface of porous silicon nanoparticles with carbon layers, and introduce a technique for the production of supported palladium recombination catalysts. The proposed catalysts efficiently facilitate the recombination of hydrogen in lean air-hydrogen gas mixtures, offering a cost-effective alternative to more expensive commercial catalysts. Furthermore, they exhibit remarkable efficiency at both room and elevated temperatures. The final remarks underscore the necessity of creating new Pd catalysts to guarantee the secure storage and usage of hydrogen.

**Key words:** porous silicon, carbonization, catalysts, palladium nanosized metal, H<sub>2</sub>/O<sub>2</sub> recombination, modern safety technology.

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### 1 Introduction

Catalysis improves engineering processes, enhances safety, and minimizes waste discharges, involving greenhouse gas emissions. Catalytic technologies are crucial for dependable manufacturing, particularly in the hydrogen (H<sub>2</sub>) energy sphere and nuclear reactors, where water is exploited for cooling and power generation in industrial settings [1-4]. Modern safety measures are widely implemented by companies in this industry to guarantee the safe handling and utilization of H<sub>2</sub>, following ISO/TR [3] and findings from [5] research. Sophisticated technology is required in the field of H<sub>2</sub> safety engineering to reduce the risks of ignition and explosion. Evidence for this can be found in investigations conducted by Saf-

fers and Molokov [5], Ono and Oda [6], and Molokov and Bragin [7].

Efficient flameless converters are essential for commercial applications that handle flammable gas mixtures [5, 8]. This is especially important for gas mixtures that contain both air and H<sub>2</sub>, where H<sub>2</sub> volumes range from 6% to 30%, regardless of whether the mixture is calm or turbulent. Passive autocatalytic recombiners (PARs) are used in nuclear power plant containments to combine hydrogen and reduce the risk of hydrogen-triggered explosions [5, 7, 9, 10]. PARs are suitable for scenarios where hydrogen accumulates slowly during a coolant loss incident. Installing PARs with catalytic properties at the power plant can lower the chances of an H<sub>2</sub> explosion should a hypothetical core meltdown occur [1, 8].

However, this approach encounters the obstacles of necessity in lowering production costs and enhancing catalyst operation stability [9]. Cost reduction for primary catalytic metals and support materials used in supported metal catalysts is crucial to hold these challenges effectively. Enhancing the turnover frequency of catalytic reactions at reduced temperatures and presenting a more effective approach for developing advanced catalysts are of utmost importance [11, 12]. It is essential to undertake further research and examine previous studies to create a wide range of robust metal catalysts, which could also find applications in PARs [9, 13].

## 2 A brief review of the literature regarding supported recombination catalysts

The investigation of  $H_2/O_2$  recombination reactions in laboratory reactors employing supported unitary Pd or Pt catalysts and/or binary Pd-Pt catalysts exposed discernible deactivation as a fluctuation of the performance due to the presence of water vapor in the reaction  $H_2/O_2$  mixture [14]. This moisture affects both the catalyst support and active metal as Pd or Pt according to results from studies [14]. Deactivation of the catalysts was pronounced when Pt was supported on alumina (Pt/ $\alpha$ - $Al_2O_3$ ) [14], but not for Pt/ASDBC, where Pt deposited on alkyl-styrene divinyl-benzene copolymer (ASDBC) [15], and for the Fe-Cr silicate cordierite with the idealized formula  $(Fe, Cr)_2Al_4Si_5O_{18}$  [16]. As the humidity increased to 2%, the deactivation became stronger and the cordierite-containing catalysts showed more pronounced deactivation. These moisture-deactivation effects were attributed to water condensation on the catalyst surface, which took place at a low reaction temperature of 60 °C while water was almost eliminated at the higher reaction temperature of about 300 °C.

Among the catalysts with Pd, Pt, and Pd-Pt particles deposited on stainless steel wire gauze, the Pd-Pt catalyst exhibited the highest resistance to water vapor [14]. Its activity was minimally affected, whereas humidity caused a potent yet temporary deactivation of Pt or Pd particles according to [17, 18]. Previous research has indicated that Pd catalysts supported on silica exhibit superior water resistance compared to those supported by alumina [19]. Its activity remained high and stable, providing further evidence of its exceptional water resistance, both with respect to moisture already present in the reaction mixture and water molecules produced during the reaction. The Pd-Pt/ $SiO_2$  catalyst, in particular, demonstrated the best performance during extended contact with the reaction mixture [19]. Its activity remained high

and stable, providing further evidence of its exceptional water resistance, both with respect to moisture already present in the reaction mixture and water molecules produced during the reaction. According to [19], the catalytic tests revealed a slow decline in the activity of Pd-Pt catalysts supported by alumina.

However, taking into account the peculiarities of Pd, carbon layers are known to be able to modify the reactivity of Pd catalysts. On the other hand, carbon can neglect the effect of moisture. Therefore, the presence of carbon layers in the catalyst could play a crucial role in the behavior of the Pd catalyst for the hydrogen and oxygen recombination reaction. The interaction of the catalysts with moisture present in the reaction mixture (1 vol%  $H_2$  in the synthetic air) as well as with water molecules generated during the  $H_2/O_2$  recombination reaction is evaluated. The performance of the catalysts is studied in a conventional laboratory fixed bed flow reactor using dry and wet (saturated with moisture at 25 °C) reaction mixtures.

Modern advancements in materials greatly affect catalyst design, particularly in the creation of stable  $H_2/O_2$  recombination catalysts for safety systems. To address current challenges and enhance prospects for catalyst development, it is crucial to make progress in developing new modified materials for advanced metal catalyst supports and conduct systematic research.

The paper aims to prepare Pd catalysts loaded on porous silicon support and study their performance in hydrogen lean gas mixtures with oxygen, studying its action, and identifying the main directions of changes in order to estimate trends and prospects for its development.

### *The hypotheses of the research:*

H1 – The surface layer on the inert support is increasingly necessary for the strong attachment of Pd nanoparticles;

H2 – Specific properties of the inert support can be formed after the carbonization of its surface;

H3 – It is possible to accelerate the development of Pd catalysts and improve their properties on the basis of the use of carbonized porous silicon support, rational use of Pd metal according to the principle of atom economy, reduction of production costs, and improvement of methods of catalyst preparation, which would take into account specific features of catalyst production.

## 3 Methods and materials

The objectives of this paper were achieved through the use of research methods such as the kinetic method in catalytic studies and controllable Pd

sorption. Catalyst samples were prepared from a 1 M solution of palladium chloride ( $\text{PdCl}_2$ ) of at least 99.5 percent purity (on a metal element basis). Several preparation methods were used depending on the parameters. Porous silicon films were obtained by electrochemical etching [20] and mechanically ground into powder, and modified with carbon nanoscale layers as reported in [21]. The resulting porous silicon powders were dried in flowing air at  $100^\circ\text{C}$  for 6 h to produce microporous granules of the dry porous support. The catalysts were prepared by impregnation method with Pd sorption control and characterized by surface area analysis. The reference  $\text{Pd}/\text{Al}_2\text{O}_3$  catalysts with 0.5 wt% Pd were also prepared by wet impregnation method using  $\text{Al}_2\text{O}_3$  with a similar specific surface area of about  $50\text{ m}^2$  per gram.

Brunauer-Emmett-Teller (BET) surface area analysis, which is the multi-point measurement of the specific surface area of an analyte by nitrogen gas adsorption analysis, was performed at liquid nitrogen temperature using an ASAP 2020 adsorption analyzer from Micromeritics.

Activity measurements were performed by passing a regulated gas mixture of 1 vol%  $\text{H}_2$  and 20 vol%  $\text{O}_2$ , 2 vol%  $\text{H}_2$  and 20 vol%  $\text{O}_2$ , and 0.5 vol%  $\text{H}_2$  and 20 vol%  $\text{O}_2$  diluted with argon (Ar) gas, through a fixed-bed microreactor and the effluent gas flow of 100 mL per min was analyzed using gas chromatography. A benchmark was developed to conduct catalytic experiments on palladium catalysts supported on substrates [22]. The benchmark includes three primary units: a gas mixer, a gas preheater, and a catalytic reactor, as well as a gas chromatograph (GH) as an analyzer. High-purity argon (99.999%) and oxygen (99.9%) gases obtained from Linde Gas LLC were used to prepare gas mixtures. Ar gas was used as a dilutant to ensure safe concentrations of  $\text{H}_2$  and  $\text{O}_2$  below the lower explosive limit. Gas flow into the reactor was monitored and regulated using conventional mass flow controllers. To produce  $\text{H}_2$  gas (99.999% purity), an electrolytic solution was used with a QL-H2-150 generator. The catalyst used consisted of Pd embedded in porous silicon powder, with a carbon layer coating its surface. A catalyst powder with a volume of  $1\text{ cm}^3$  was placed in the reactor. Two K-type thermocouples were placed in the reactor channels to measure axial temperature profiles. Unbiased measurements were essential to analyze the experiment's results. Thermocouples were installed before and after the catalyst to measure the inlet and outlet temperatures with an error of  $1^\circ\text{C}$ . Additionally, a pressure sensor was utilized to measure atmospheric pressure changes immediately before the catalyst. The gas mixture was preheated to the in-

let temperature with a tubular furnace. To guarantee the homogeneous composition and constant temperature of the gas, we installed static mixers in the oven to improve its mixing. The reactor and catalyst were heated through a programmable heater.

To measure the concentration of  $\text{H}_2$  and oxygen  $\text{O}_2$  in the effluent gas stream, we utilized an online GC 2010 Plus system that was outfitted with a thermal conductivity detector. The column, which was made of stainless steel 1/8-inch and 2 m long was packed with microporous carbon with supported  $\text{NiSO}_4$  used as a molecular sieve and was used in the chromatograph. The Ar carrier gas flow was kept constant at  $100\text{ mL}\times\text{min}^{-1}$  while the chromatograph was operated at  $60^\circ\text{C}$ . A 2-mL gas sample loop was used for the injection of the sample, and the peak areas on the chromatogram were measured using an electronic digital integrator. A hydrogen balance could not be obtained, as the water condensed and was removed from the system to prevent damage to the instrumentation and was therefore not measured.

## 4 Results

Previous studies suggest that Pd and Pt catalytic systems can effectively participate in the oxidation of  $\text{H}_2$  with  $\text{O}_2$ , effectively increasing reaction productivity and reducing reaction temperatures [23-25]. Previous research has investigated the effects of Pd additives on the supports and support types used in  $\text{H}_2$  oxidation with  $\text{O}_2$ . Different mechanisms of  $\text{H}_2$  oxidation have been described in the literature for this model reaction [26-28]. Our goal is to compare the catalytic activities of industrial catalysts and propose the possible reasons for the high activity. Our main aim was to evaluate the surface activity of  $\text{Pd}/\text{C}@/\text{Si}$  and to develop factors influencing it. We studied the behavior of  $\text{Pd}/\text{C}@/\text{Si}$  during the  $\text{H}_2$  oxidation process at a temperature below 373 K under ambient atmospheric conditions. Although these conditions are insufficient for the oxidation of the carbon layer, they have an impact on the surface activity and properties. The experiments were carried out under mild conditions, leading to the formation of water as the main oxidation product and its accumulation within the porous structures of the silicon. Our study showed the comparison of results obtained with the use of a  $\text{Pd}/\text{Al}_2\text{O}_3$  oxidation catalyst and we found the effect of thermal dehydration. We should note that the effect of oxidation of carbonaceous layers, as in [29], plays a determining role in the Pd dispersing, but having also negative hydrophilization effect. It shows that under the present experimental conditions, the  $\text{H}_2$  elimina-

tion capacity of the catalyst was not affected by the produced water as the  $H_2/O_2$  recombination reaction continued. It is to some extent contrary to the experimental results described in [14].

#### 4.1. Comparative characteristics of produced catalysts.

As mentioned above, the costs of the catalysts depend on the percentage of Pd metal in it, the working temperature, and the catalytic performance. The current price of Pd metal as of September 21, 2023, is \$1,266.28 per ounce or oscillates around \$42.33 per gram, according to Macrotrends (2023) [30]. It should be noted that the temperature window of the reaction depends on the composition of the reaction mixture. With the increase in hydrogen content, the reaction temperature window shifts to higher reaction temperatures. The prepared catalysts are composed of porous silicon and contain supported Pd, with an approximate surface area of 50 square meters per g. These catalysts containing 0.1%, 0.25%, and 0.5% Pd effectively enhance the  $H_2/O_2$  recombination reaction in gas  $H_2-O_2-Ar$  mixtures. According to the data presented in Figure 1, the following conclusions can be drawn. To achieve 100% efficiency in the conversion of  $H_2$ , it is necessary to maintain a temperature range between 50 °C and 132 °C. Increasing the concentration of Pd in the catalyst lowers the temperature required for high levels of  $H_2$  conversion. Tempera-

ture hysteresis during the conversion of hydrogen gas depicted in Figure 1 may be result from free radical reactions taking place at medium-low temperatures. These species of radicals facilitate a recombination reaction of hydrogen and oxygen through a pathway that enables a combination of homogeneous and heterogeneous reactions. The radical chain reactions in which hydrogen and oxygen species participate have been observed to be highly exothermic [28]. The catalyst initiates the reaction by releasing  $\cdot OH$  and  $\cdot HO_2$  radicals into the gas flow, which promotes an increase in the reaction performance. Under low temperatures and atmospheric pressure,  $H_2$  recombines with  $O_2$  in a rapid radical chain oxidation process resulting in significant  $H_2$  conversion.

In ref. [26], it explained the process of heating the gas volume around the catalyst surface and the temperature on the catalyst surface. This surface heating can result in an exponential increase in radicals, leading to an almost complete conversion of  $H_2$ . Moreover, the radical recombination of  $H_2/O_2$  can take place spontaneously under these conditions, requiring no external heating. High hydrogen conversion level persists for a specific duration during the cooling process, explaining the observed hysteresis loop within the given temperature range. Furthermore, the supported Pd catalysts can demonstrate proficient radical generation at lower temperatures [22].

**Table 1** – Comparing characteristics of  $H_2/O_2$  recombination catalysts

$H_2-O_2-Ar$ mixture	Temperature at 100% $H_2$ conversion for selected catalyst, °C			
	Pd amount in Pd/C@Si, wt%			0.5 wt% Pd/ $Al_2O_3$
	0.1	0.25	0.5	
0.5 vol% $H_2$ + 20 vol% $O_2$	85	33	25	70
1 vol% $H_2$ + 20 vol% $O_2$	100	45	30	95
2 vol% $H_2$ + 20 vol% $O_2$	121	70	52	132

Under operating conditions, the Pd metal nanoparticles are stable enough to maintain a steady performance over 25 reaction cycles of subsequent heating from room temperature to the temperature at the highest conversion and subsequent cooling to room temperature (Figure 1).

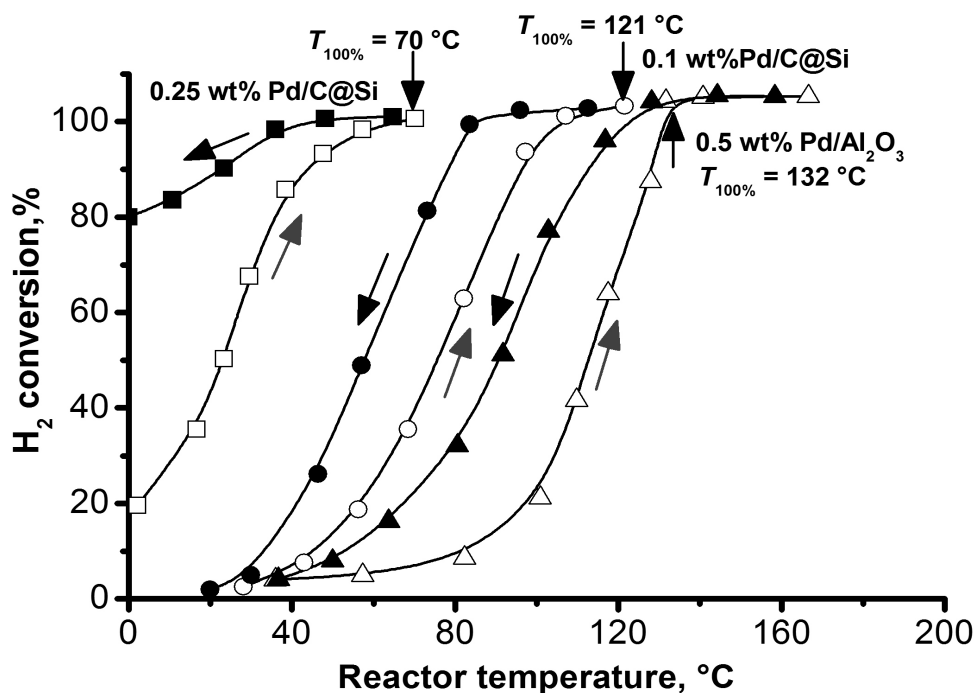
Table 1 shows that the saving of Pd metal can be achieved by using the Pd for the preparation of Pd/C@Si catalysts instead of the reference 0.5 wt% Pd/ $Al_2O_3$  catalyst. As can be seen from Fig. 1 and Table 1, the Pd/C@Si catalysts have higher activity than the Pd/ $Al_2O_3$  catalyst, and higher  $H_2$  conversion

can be achieved at lower reaction temperatures. The Pd/C@Si catalyst with 0.25 wt% Pd contains less Pd, and so it is more affordable than the 0.5 wt% Pd/ $Al_2O_3$  catalyst. This is because it needs less amount of the expensive Pd metal when it is being made. Additionally, the 0.25 wt% Pd/C@Si catalyst performs better over a wider range of temperatures and can recombine more  $H_2$  at lower temperatures.

The work stability in terms of prolonged use of the 0.5 wt% Pd/C@Si catalyst in the heating-cooling cycle regime, which combines work at low and high temperatures in one cycle, was investigated. We found

that the temperature at about 100% H<sub>2</sub> conversion over the 0.5 wt% Pd/C@Si catalyst under moisture effect does not change for up to 100 consecutive cycles. The deactivation problem solution can be a thermal heater integrated into or external to the water heating jacket, which ensures rapid and accurate

heating of the catalyst in the reactor by turning it on after the selected operating time. However, it is necessary to further evaluate the effect of the reaction flow of the reaction mixture of 1 vol% H<sub>2</sub> and 20% vol% O<sub>2</sub> in Ar, which simulates different regimes of PAR work.



**Figure 1** – Representative comparison of H<sub>2</sub> conversion over Pd catalysts vs. reactor temperature. The reaction gas mixture contains 2 vol% H<sub>2</sub> and 20% vol% O<sub>2</sub> in Ar. White symbols measured at heating regime, while black symbols measured at cooling regime

## 5 Discussion

Earlier in [21], we showed by TEM imaging that the Pd nanoparticles formed over the carbonized surface layer on the porous silicon. That study informs on 2-4 layers of carbon on the surface of porous silicon, the carbonization technology is repeated here for the preparation of the support for Pd catalysts. The comparative characteristics of H<sub>2</sub>/O<sub>2</sub> recombination catalysts presented in this paper are focused on improving the performance and working stability for the development of safety systems. In this context, our results correlate with those reported in [15]. Defining the main directions of increasing the stability of the H<sub>2</sub>/O<sub>2</sub> recombination catalysts, we paid special attention to promising areas of surface hydrophobization for the development of the stable passivate layer over highly porous matter discussed in [31, 32].

We considered approaches to improving the situation with the deactivation of Pd metal with the reaction product mentioned in [32], which can be done by stimulating the formation of surface easily removable, low-bonded surface water forms. Therefore, the porous silicon support modification, even with carbon nanoscale layers, plays a crucial role in our study. Further research should focus on identifying effective Pd nanoparticles to increase the effectiveness of carbon layers with supported Pd interaction for energy dissipation. This surface layer on the inert support is increasingly necessary for the strong attachment of the Pd nanoparticles because Pd atoms have a reasonable affinity to bind to carbon layers [33, 34]. These Pd atoms can bind strongly to unsaturated and defect surface sites on the carbon layers [35].

Incorporating thermal imaging techniques can significantly contribute to this endeavor. While pre-

vious studies [36-38] have explored this matter, they primarily focused on heat quantity and considered other dehydrogenation reactions. However, further research on the aforementioned topic is necessary, and in order to thoroughly understand the reaction, one should use the aid of thermal analysis, operando and kinetic studies.

Returning to the reasons of better characteristics for the supported Pd catalysts, it should be noticed that the high catalytic activity and stability are due, in part, to the presence of a hydrophobic surface layer on the porous silicon support, which is significant for catalysis, particularly in reactions involving gaseous reactants, reaction products or where water might be present as an impurity. This crucial hydrophobic layer prevents water accumulation and enhances catalyst effectiveness, particularly in real-world scenarios, as outlined below.

**Water Repulsion:** The hydrophobic carbon surface layer on which supported the Pd atoms repels water. In general, all hydrophobic materials do not have an affinity for water and tend to repel it. This property is beneficial in situations where water is a common component or a reaction product or an impurity in the reaction mixture. The hydrophobic surface prevents water from adsorbing onto the catalyst's surface and interfering with the catalytic reaction. Without this hydrophobic layer, water could occupy active sites on the catalyst, blocking or slowing down the desired reactions. Accumulated water negatively impacts on the catalytic reaction temperature and has a cooling effect.

**Maintaining Catalytic Activity:** The effectiveness of catalytic oxidation/reduction reactions involving palladium catalysts relies on the availability of active sites on the catalyst's surface. Water accumulation can block these active sites, which can lead to a decrease in catalytic activity. By repelling water, the hydrophobic layer ensures that the active sites remain accessible for reactants to interact with the Pd metal, as an active component of the catalyst, allowing the reaction to proceed at its intended rate.

**Improved Catalytic Stability:** Water can also lead to the corrosion and deactivation of some catalysts. Palladium, for instance, can form oxides when exposed to water or deep in it, which can reduce its catalytic activity. The hydrophobic layer helps protect the Pd surface from such corrosive reactions, thereby contributing to the long-term stability and durability of the catalyst in the presence of moisture or the water as a reaction product.

**Real-World Applications:** In real-world scenarios, moisture is often present, and its removal from a reaction mixture can be challenging or energy-

intensive. By having a hydrophobic surface layer on porous support, Pd catalysts are more practical for use in industrial and environmental applications where moisture cannot be completely eliminated. For example, in hydrogenation/oxidation/recombination reactions or catalytic converters in vehicles or PARs, where exhaust gases can contain water vapor, palladium catalysts with hydrophobic support properties maintain their effectiveness.

In summary, the hydrophobic surface layer on the porous support of Pd catalysts is crucial for repelling water and ensuring the availability of active sites over Pd metal for catalytic reactions. This property is particularly valuable in real-world applications where moisture is present, as it helps maintain the catalyst's activity and stability in the presence of water or other hydrophilic impurities. It enhances the efficiency and practicality of Pd catalysts in a wide range of industrial and environmental processes.

## 6 Conclusions

We presented some state-of-the-art findings regarding the use of  $H_2/O_2$  recombination catalysts. The results indicate the need for advanced solutions to ensure optimal fire/explosion safety. This can be done by recombining  $H_2$  gas leaked when stored or used. Implementing  $H_2/O_2$  recombination catalysts to combine small amounts of leaked hydrogen with  $O_2$  to form water is an effective method. It is noteworthy that supported catalysts with a low palladium metal content effectively distributed over catalytically inert support are the most effective catalysts for preparation. The preparation process for laboratory  $H_2/O_2$  recombination catalysts indicates the need for a hydrophobic surface layer to avoid water accumulation and negatively affect the effective adsorption-desorption regime of the catalysts' working. These selected catalysts can be a prototype for creating highly effective catalysts for the hydrogen recombination process. An optimized method for obtaining protecting carbon layers on the surface of porous silicon nanoparticles is the thermal decomposition of sugars on the catalytic surface, based on which we developed a wetting perception method for the preparation of palladium catalysts. The proposed catalysts highly efficiently recombine hydrogen with oxygen in gas mixtures simulated gas air-hydrogen mixtures, which allows the widespread use of such catalysts, without the need to use more expensive analogues. The catalysts' recombining action of  $H_2$  in the simulated air-hydrogen mixtures causes high conversion of  $H_2$  at room and elevated temperatures. The modified surface plays a proper role in ensuring the resistance to moisture

with a sufficient capacity resource. The high cost of Pd metal, lack of info, and insufficient understanding of the catalytic working of most small and medium-sized Pd nanoparticles hinder the development of effective catalysts. The main problems attracting attention in the catalysis with Pd nanoparticles are the following: deactivation under the action of water, high costs of catalytically active metals, such as Pd, industrial risks, which is associated with long operating cycles, and operational changes in hazardous conditions. Therefore, based on the above, the main improvements of catalysts should be the development of small Pd nanoparticles with high activity and long catalytic action, decreasing costs of catalysts and supports, rational use of costly Pd metal, low-

ering the reaction temperature for the targeting sector, improving the methods of the preparation of Pd catalysts, which would take into account the specific features of their future application. Consequently, we stated key priorities in accelerating the development of new H<sub>2</sub>/O<sub>2</sub> recombination catalysts to be used by companies to improve the safety of H<sub>2</sub> storage and application.

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