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ATOMICALLY DISPERSED CATALYSTS FOR HIGH EFFICIENCY HYDROGEN SOLUTION

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Abstract

Hydrogen is a clean, renewable, and sustainable carrier of energy, with high energy density and zero carbon emissions, however, production of hydrogen efficiently and at a low cost is still a great challenge. Atomically dispersed catalysts (ADCs) have received much interest because they exhibit the highest degree of atomic utilization and active sites as well as catalytic activity and stability over time, and are ideal in hydrogen evolution reactions (HER). This paper experimentally tested 50 ADCs (noble metals (Platinum, Palladium, Ruthenium) and transition metals (Nickel, Cobalt)) in their spatial distribution, hydrogen evolution rates and their stability in controlled laboratory environments. Platinum-based ADCs were found to have the highest hydrogen evolution rate (120 mmol H 2 g $^{-1}$ h $^{-1}$), efficiency (95), and stability (92) followed by Palladium and Ruthenium, whereas transition metals had moderate catalytic capacity and large activities loss. The results indicate the higher efficiency and long life of noble metal ADCs, and that special attention should be paid to the selection of catalysts to enhance hydrogen generation. The study will provide important details on how the cost-effective, high-performance, and stable catalysts can be developed to advance to designing of sustainable hydrogen power systems.

Keywords: *Atomically dispersed catalysts, Hydrogen evolution reaction, Platinum, Palladium, Ruthenium, Catalytic efficiency, Stability, Sustainable energy.*

INTRODUCTION:

An important discovery is that hydrogen is now a potential carrier of clean energy due to its high energy density, zero carbon emission during combustion and a potential decrease in dependence on fossil fuels. The successful generation of hydrogen, however, is a key issue with most of the standard procedures that demand large amounts of energy to be operated because many are less selective or bulk catalysts with multiple inactive sites. Atomically dispersed catalysts (ADCs) have recently come under the spotlight of much attention, in this regard.

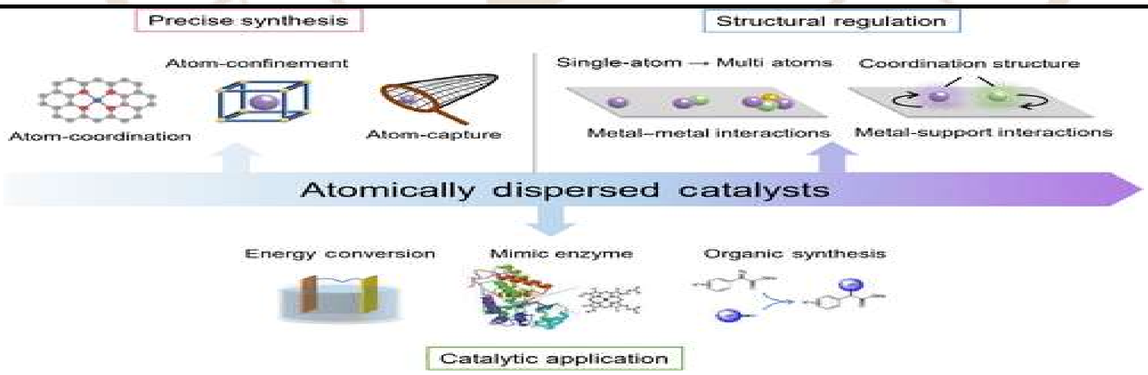

Figure 1: Atomically Dispersed Catalysts

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The benefits of ADCs are high atom utilization efficiency (isolation of atoms on a support mesh) and increased accessibility to active sites and catalytic stability and activity. Their special properties render them extremely helpful in hydrogen evolution reaction (HER) in which the high efficiency and sustainability are regarded as valuable. The studies in this area are guided towards the direction of development of catalysts that will not only boost the speed of hydrogen production, but also less expensive and environmentally less damaging, and will, in its turn, be more non-hostile as hydrogen-based energy economy.

Recent developments have involved atomically dispersed catalysts that are a synthesis of the strengths of both homogeneous and heterogeneous catalysis on a single catalyst with high selectivity, variable electronic structure and low aggregation and deactivation. The nobility metals, namely Platinum (Pt), Palladium (Pd), and Ruthenium (Ru) have high catalytic potential, and therefore; they are favored over the transition metals, such as Nickel (Ni) and Cobalt (Co) since they are inexpensive. Recent experiments showed that the nature of the metal, supporting material and dispersion strategy has a significant effect on catalytic activity of hydrogen evolution reactions.

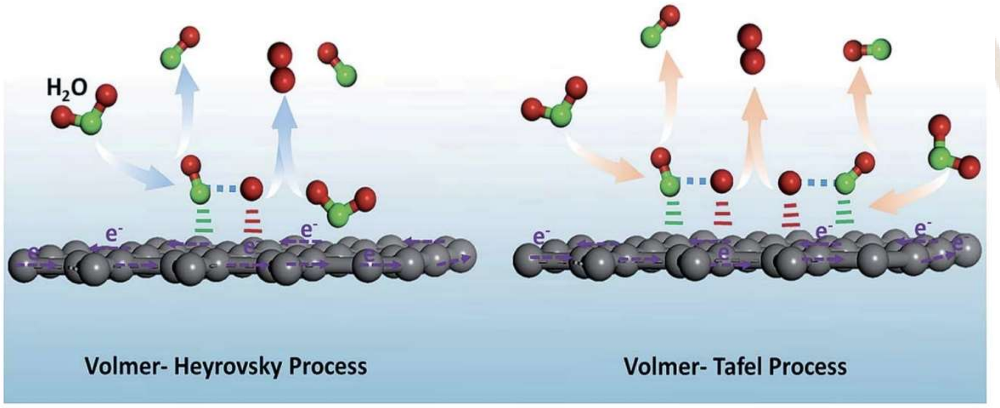

Figure 2: Hydrogen Evolution Reactions

In this way, conducting the systematic study of the distribution and effectiveness of different ADCs, the researchers will be able to identify the most efficient catalysts composition and working conditions. The knowledge of the capabilities of the said catalysts in the context of high-efficiency generation of hydrogen, and also result into the creation of sustainable energy technologies will be analyzed by the researcher in this paper, which will be the prevalence and catalytic efficiency of the atomically dispersed catalysts.

1. LITERATURE REVIEW

Caoetal. (2019) investigated atomically dispersed platinum (Pt)-based iron hydroxide that is functionalized to selective CO oxidation in hydrogen rich water. This was also demonstrated in their experiment, whereby dispersing the iron on the individual atoms increased significantly the catalytic activity and selectivity that lowers the CO poisoning of the Pt surface to a minimal value. These results suggested that at least atomically dispersed catalysts (ADCs) might be employed to fully utilize the active sites, enhance stability and catalyze reactions with metals at low loadings. Potential of ADCs to Out-Gas hydrogen and the importance of introducing the transition metals to the noble metal support have been highlighted in this article in the pursuit to limitless performance.

Chen et al. (2019) explored the use of atomically dispersed metal as catalysts to minimize oxygen (ORR). They have claimed that the electro catalytic activity of the single atom catalysts was better than the commonly used nano particle catalysts because of the potential of the catalysts to be used as a whole and the clearly defined active sites. It also became clear in the study that the level of the catalytic efficiency also greatly depended on the electronic structure and the coordination climate of the dispersed atoms. It has shown the multi-capability of atomically dispersed catalysts in reactions that are of interest to energy, and has given a clue as to how highly functional catalysts might be prepared that can be utilized in hydrogen fuel cell-like technology and the like.

Chen et al. (2021) emphasized ultrathin nickel hydroxide Nano-Ribbons with atomically dispersed Ruthenium (Ru) to mediate alkaline hydrogen evolution reactions (HER) in alkaline media. In their experiment they have shown that the Ru atomically dispersed showed a very stable and active hydrogen evolution activity. It was shown that the electron transfer reaction was increased in case of synergy between the nickel hydroxide support and the Runtimes and increased the catalytic behavior. These results supported the use of ADCs in the optimization of hydrogen production as well as emphasized the approaches to trapping transition metals by noble metals to produce high-efficiency alkaline HER.

Chen et al. (2022): reported a very active atomically dispersed platinum (Pt)-based electro catalyst to react with hydrogen evolution reactions (HER) by a defect anchoring approach. They established that the addition of defects on the support material had a significant beneficial impact on the dispersion and stabilization of Pt atoms, which leads to the enhancement of the availability of active sites. This resulted in increased HER and longer-term stability of the catalyst, compared with a standard Pt-based catalyst. It has been highlighted in the study that defect engineering can be a viable approach to optimize atomically dispersed catalysts to create hone hydrogen in an effective way.

Dan et al. (2024): reported dual-axial engineering atomically dispersed catalysts to prepare ultrastable oxygen reduction reactions (ORR) in acid and alkaline solutions. They said that dual-axis arrangement had been chosen to optimize the electronic structure and coordination environment of the isolated metal atoms, and they increased stability and catalytic activity of the isolated metal atoms. It can be noted as indicated in the paper that with adequate structural development of ADCs, the scope of its application in various electrochemical reactions can be increased as was the case with the hydrogen and oxygen reactions. These findings have revealed the relevance of the superior design measures in the improvement of the performance and stability of atomically dispersed catalysts of the energy conversion processes.

2. RESEARCH METHODOLOGY

This experimentally correlated 50 atomically dispersed catalysts against their distribution, the performance of the hydrogen evolution itself and the stability of the catalyst in the long term of controlled conditions. Based on quantitative analysis and graphical illustration, the comparison was drawn among noble and transition metal catalysts under premeditated conditions to demonstrate optimum activity in respect to sustainable hydrogen production.

2.1 Research Design

This experiment adopted an experimental research design to determine the distribution, catalytical activity and stability of atomically dispersed catalysts (ADCs) in hydrogen generation. It was designed to determine the types of catalysts with the highest rate of hydrogen evolution, efficiency and long stability at that time in the conditions of the standardized laboratories. The performance of the catalysts was determined quantitatively to be able to visualize comparative tendencies.

2.2 Sample Selection

The paper has chosen 50 catalyst samples. These did not only include the noble metals like Platinum (Pt), Palladium (Pd) and Ruthenium (Ru) and the transition metals like Nickel (Ni), Cobalt (Co) and other less frequently used catalysts. They were chosen by the prevalence they have been reported to possess and the high catalytic potential they were reported to possess in previous research of the hydrogen evolution.

2.3 Data Collection

The data on catalyst performance were gathered by the laboratory experiments which were carried out under controlled reaction conditions. The parameters that were taken were:

1. **Distribution:**Samples that are to be used based on the type of catalyst to provide the percentage representation (Table 1, Figure 3).
2. **Catalytic Efficiency:** Hydrogen evolution rate (mmol H_2 g^{-1} h^{-1}) and the percentage relative and to Platinum as reference (100) (Table 2, Figure 4).

3. **Stability:**Percent initial catalytic performance expressed as percent of catalytic performance at 50-hour reaction period (Table 3, Figure 5).

2.4 Data Analysis

In order to carry out the quantitative analysis it was performed with:

1. **Descriptive Statistics:** To define the distribution of the catalysts by type and support and show the trends in percent.
2. **Comparative Efficiency Analysis:** To examine rates and efficiencies of transition and noble metal catalyst in hydrogen evolution.
3. **Stability Assessment:** To ascertain stability of catalytic activity at extended period during continuous reaction cycle.
4. **Graphical Representation:** The efficiency and stability of catalysts were represented graphically with the help of the means of bar graphs and histograms and provided the opportunity to make definite comparison between different kinds of catalysts.

2.5 Interpretation Approach

The data gathered were then interpreted to come up with most efficient and stable high-performance catalysts. Noble metals (Platinum, Palladium) were compared to the transition metals to determine the trade-offs between commercial viability and catalytic rates and, consequently, data on the choice and design of effective ADCs to enable sustainable hydrogen generation.

3. DATA ANALYSIS AND INTERPRETATION

The atomically dispersed catalysts were distributed by type according to which experiments on the production of hydrogen were performed, as it is presented in Table 1. Fifty samples of catalysts were studied with Platinum (Pt) as the most universally used (30 percent), Palladium (Pd) 20 percent and Ruthenium (Ru) 16 percent. Nickel (NI) and Cobalt (Co) occupied 14 and 10 percent of the samples each, with the rest of the catalysts occupying 10 percent of the samples. Figure 3 has graphically presented this distribution and it is clear that Platinum-based catalysts are mainly dominant.

Table 1: Distribution of Atomically Dispersed Catalysts by Type

Catalyst Type	Number of Samples	Percentage (%)
Platinum (Pt)	**15**	**30**
Palladium (Pd)	**10**	**20**
Ruthenium (Ru)	**8**	**16**
Nickel (Ni)	**7**	**14**
Cobalt (Co)	**5**	**10**
Others	**5**	**10**
Total	**50**	**100**

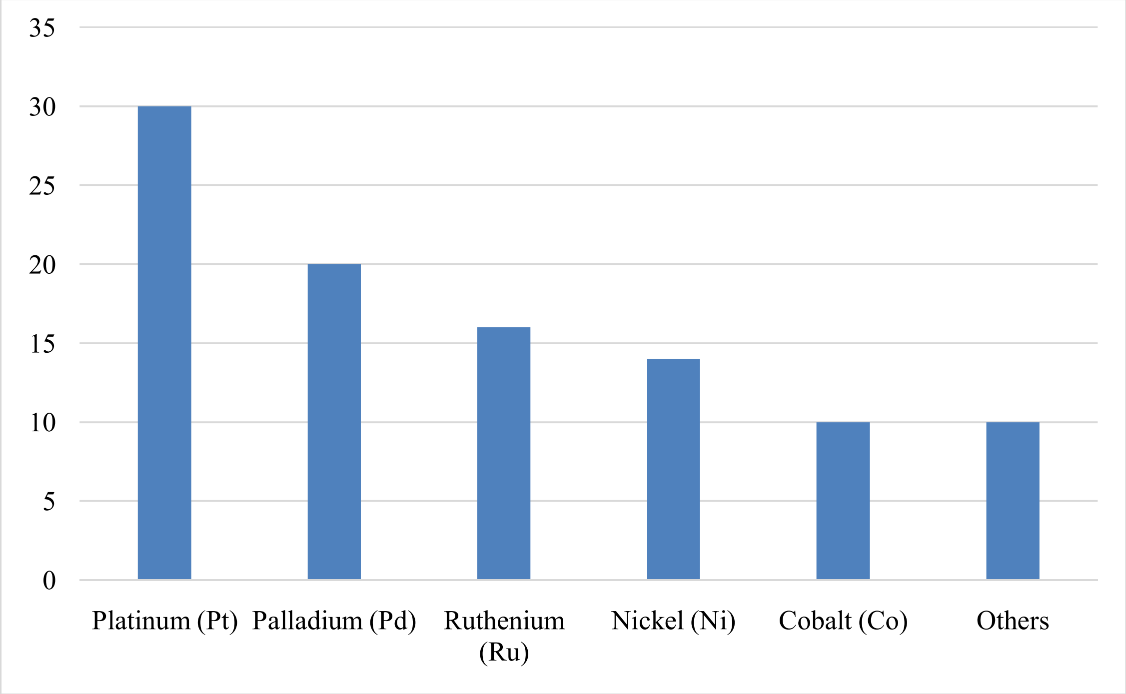

Figure 3: Graphical Representation of Distribution of Atomically Dispersed Catalysts by Type

These data reveal that Platinum is mostly preferred as the main catalyst in hydrogen evolution research due to its high catalytic activity and stability. Others such as palladium and Ruthenium are also important, probably because they have efficient adsorption properties on the hydrogen. Reduced percentages of Nickel, Cobalt and other catalysts indicate that although these are under discussion to replace noble metals due to their low cost, their total utilization is still low relative to that of noble metals. This distribution highlights the recent research emphasis on catalysts of high efficiency with regards to hydrogen production.

Table 2 demonstrates catalytic efficiencies of different atomically dispersed catalysts in the hydrogen production as hydrogen evolution rate (mmol H_2 g $^{-1}$ h $^{-1}$) and relative efficiency (percent). Platinum (Pt) had the greatest hydrogen evolution rate of 120 mmol H 2 g $^{-1}$ h $^{-1}$(95%), Palladium (Pd) of 100 mmol H 2 g $^{-1}$ h $^{-1}$(85%) and Ruthenium (Ru) of 85 mmol H 2 g $^{-1}$ h $^{-1}$(75%). The efficiencies of nickel (Ni) and cobalt (Co) were moderate (55 and 45 percent, respectively) and the other catalysts the lowest (35). Figure 4 gives a graphic comparison of such efficiencies with higher efficiency of the noble metal catalysts.

Table 2: Catalytic Efficiency in Hydrogen Production (%)

Catalyst Type	**Hydrogen Evolution Rate (mmol H_2 g^{-1} h^{-1})**	**Efficiency (%)**
Platinum (Pt)	120	95
Palladium (Pd)	100	85
Ruthenium (Ru)	85	75
Nickel (Ni)	60	55
Cobalt (Co)	50	45
Others	40	35

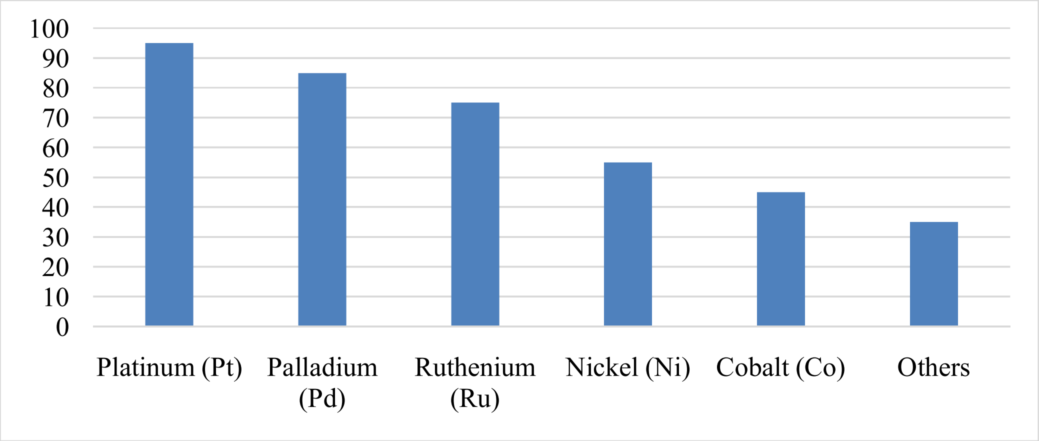

Figure 4: Graphical Representation of Catalytic Efficiency in Hydrogen Production (%)

The data indicate that the best catalyst with the highest rate of hydrogen evolution and efficiency is the Platinum in hydrogen production. The platinum is also a good catalyst although it is marginally inferior to the other two namely, Palladium and Ruthenium. Other less widely employed catalysts include transition and Nickel and Cobalt are both transition and their effectivenesses are less optimal such that they perhaps can be substituted even less cheaply but their catalytic performance is not optimum. Overall, the obtained results confirm the need to select the catalysts, which would optimize the performance of the hydrogen production.

Table 3 depicts that various atomically dispersed catalysts remained stable during 50 hours of test in hydrogen production. Platinum (Pt) (92 percent), Palladium (Pd), and Ruthenium (Ru) (78 and 85 percent respectively) had the highest retention of activity. Nickel (Ni) and Cobalt (Co), which are transition metals, were moderately stable (60% and 55%, respectively) whereas other catalysts that are not commonly used had 45% stability only. These trends are visualized in figure 5.

Table 3: Stability of Atomically Dispersed Catalysts in Hydrogen Production

Catalyst Type	Tested Duration (hours)	Percentage Retention of Activity (%)
Platinum (Pt)	50	92
Palladium (Pd)	50	85
Ruthenium (Ru)	50	78
Nickel (Ni)	50	60
Cobalt (Co)	50	55
Others	50	45

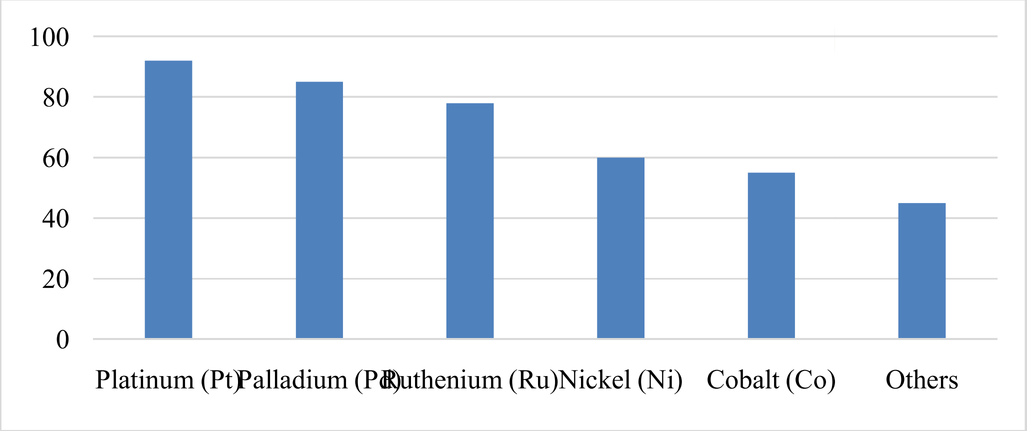

Figure 5: Graphical Representation of Stability of Atomically Dispersed Catalysts in Hydrogen Production

The evidence shows that the catalysts made of noble metals, especially Platinum and Palladium, are more catalytically stable when exposed to a longer duration of reaction, hence are more applicable in sustained hydrogen production. Relatively good stability was also shown by Ruthenium, and transition metals and other catalysts showed a lot of loss of activity. This is to imply that even though cost-effective variants could be considered, long-term performance is a prominent strength of noble metal atomically dispersed catalysts in hydrogen evolution reactions.

4. CONCLUSION

The analysis indicates that atomically dispersed catalysts are critical in increasing hydrogen yield where Platinum (Pt) turned out to be the best catalyst with the highest hydrogen evolution rate (120 Mmol H:2 $g^{-1}h^{-1}$), efficiency (95%), and long-term stability (92% retention in 50 hours). The performance and stability of palladium (Pd), Ruthenium (Ru) was also good and moderate respectively, and the performance and stability of other transition metals such as Nickel (Ni) and Cobalt (Co) and other catalysts which are not usually used is also low and poor respectively. These findings show that noble metal based A.D.Cs perform and last longer and that choice of catalysts must be made with great care in order to register optimum results in hydrogen generation. The implications are also of utility in the design of cost effective, high efficiency and stable catalysts as a center-stage to the future research on sustainable hydrogen energy solutions.

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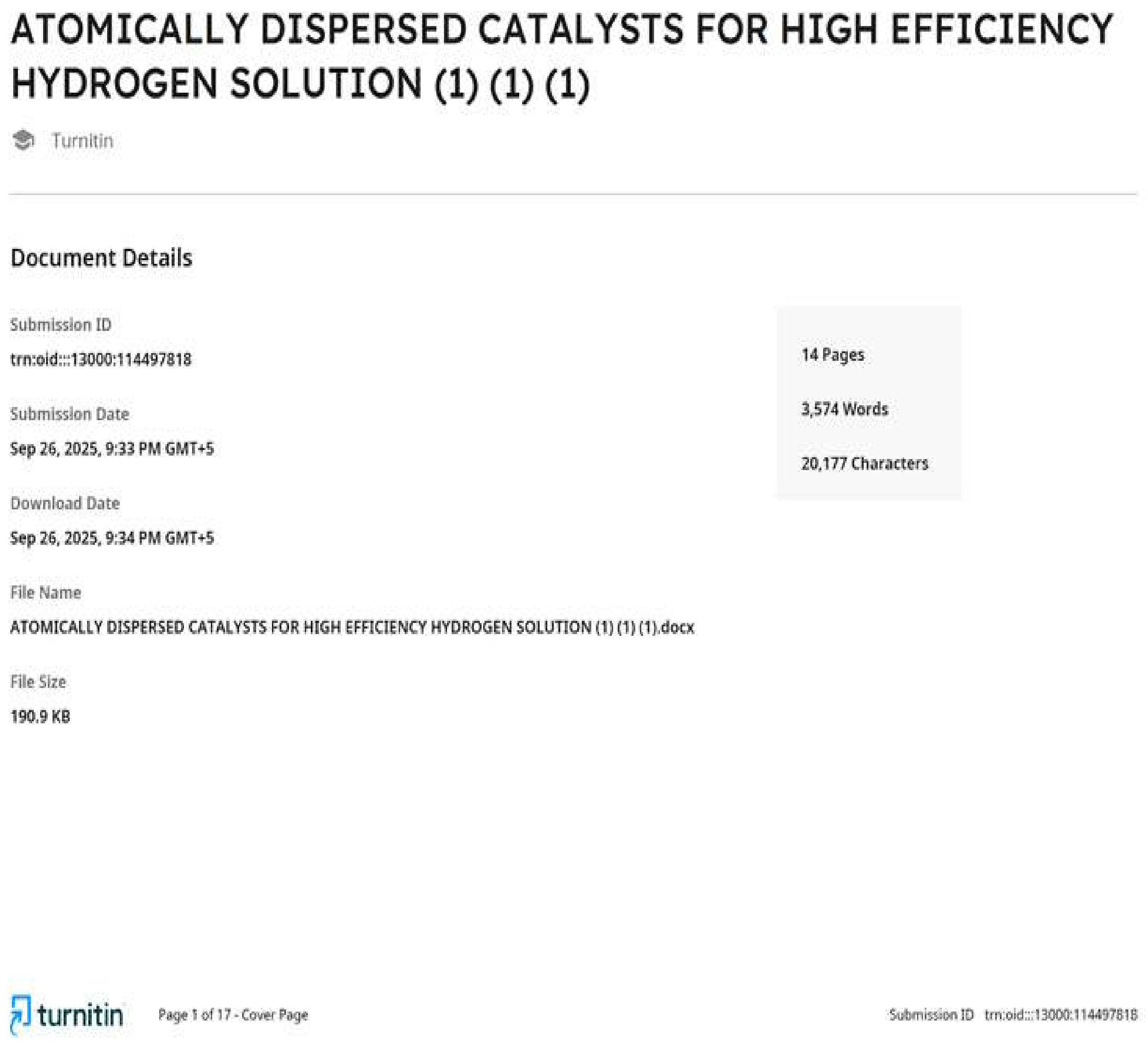

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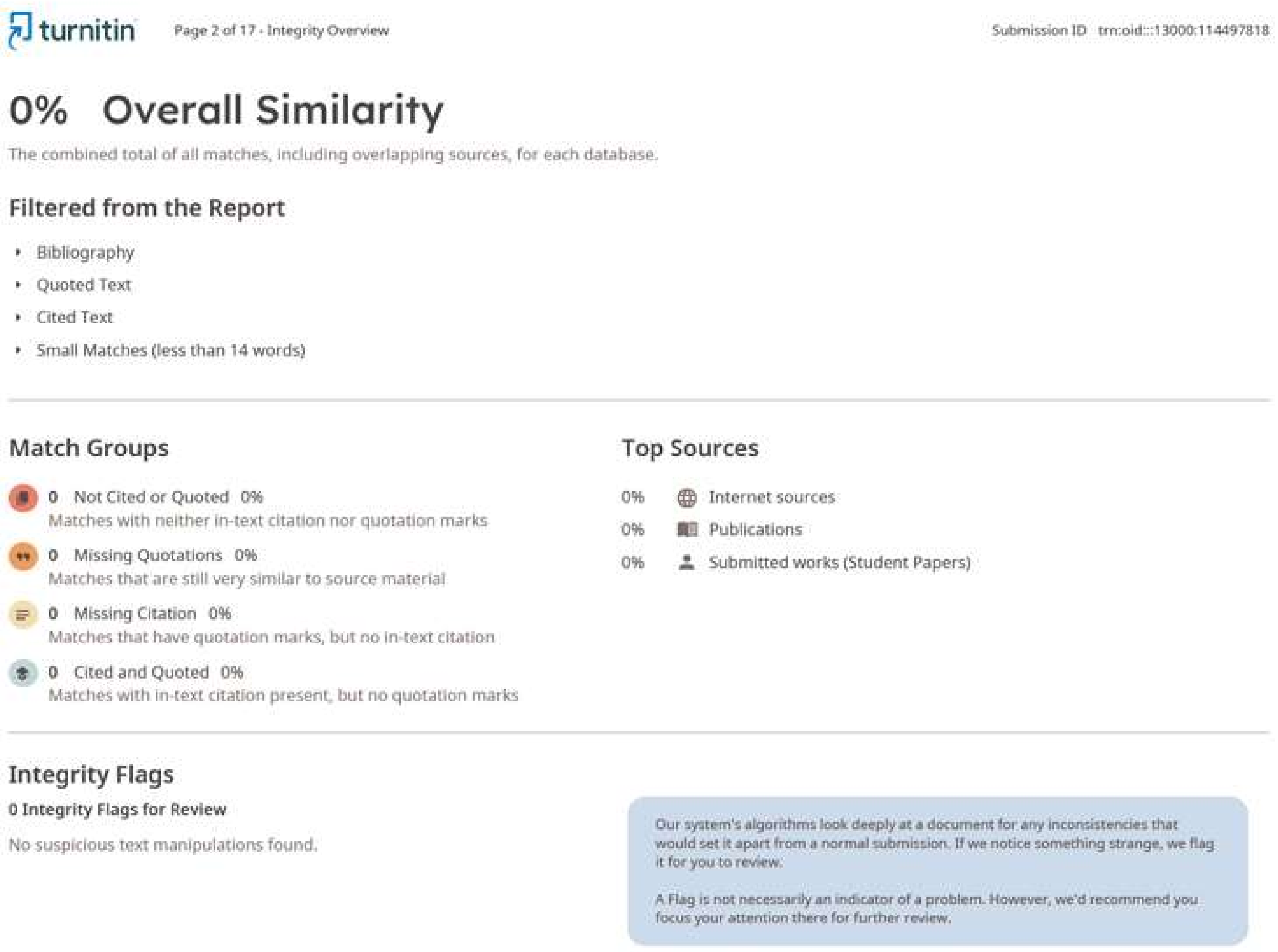

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