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Chemical Bond Changes and Automobile Pollution Control: The Mechanism of Bond Breaking and New Bond Formation in Catalytic Converters

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Abstract. This paper systematically reviews the mechanisms and technological advancements of catalytic converters designed to achieve the efficient conversion of automotive exhaust pollutants through targeted chemical bond cleavage and formation. Studies indicate that the breaking of N–O bonds and subsequent formation of N≡N bonds at catalyst surfaces represent the core reaction pathways for nitrogen oxides (NOx) reduction. Conversely, the cleavage of C≡O bonds followed by the formation of O=C=O primarily governs carbon monoxide (CO) oxidation processes. Recently developed materials, including single-atom catalysts (SACs) and layered double hydroxides (LDHs), have significantly improved catalytic performance at lower temperatures and reduced dependence on noble metals through optimized bond activation pathways. Notably, Ru-CeO_2 catalysts achieve complete NO–CO conversion at 150°C, while atomically dispersed Rh catalysts realize full NOx conversion at just 120°C. Nonetheless, insufficient low-temperature catalytic activity and undesirable byproduct generation, particularly N_2O, remain significant technical challenges. Future research should integrate surface science and computational materials science to advance non-noble metal alternatives and develop intelligent control systems, thus enabling simultaneous progress in pollutant removal efficiency and carbon neutrality objectives.

Keywords: chemical bond breaking, NOx reduction, catalytic converter, single atom catalyst, reaction mechanism.

1. Introduction

Numerous pollutants found in vehicle exhaust, such as nitrogen oxides (NO_x), carbon monoxide (CO), particulate matter, and volatile organic compounds (VOCs), seriously impair human health and the environment.

Hydrocarbons—particularly VOCs such as unburned alkanes, alkenes, and aromatic compounds—are emitted when fuel undergoes incomplete combustion.

In China, national emissions standards such as GB 18285-2018 set limits on hydrocarbon (HC) emissions from gasoline vehicles, though reported real-world HC concentrations under idling can vary widely depending on vehicle condition and maintenance. Certain hydrocarbons—benzene, for

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instance—are known human carcinogens associated with increased risks of leukemia and lung cancer following prolonged exposure. At the same time, under the action of ultraviolet rays, hydrocarbons can react photochemically with NOx to generate photochemical smog, increasing the incidence of respiratory diseases in the population [1].

Nitrogen oxides (NO_x)—primarily nitric oxide (NO) and nitrogen dioxide (NO_2)—form during high-temperature combustion when atmospheric nitrogen and oxygen react. Diesel engines typically emit significantly more NO_x—especially NO_2—than gasoline vehicles due to differences in combustion conditions and fuel characteristics. Nitrogen dioxide can irritate the respiratory mucosa and cause bronchitis and pulmonary edema. The World Health Organization (WHO) states that healthy people will experience a significant decrease in lung function after less than 2 hours of exposure to concentrations above 4700 $\mu g/m^3$ (2.5 ppm) at rest or during mild exercise; Generally speaking, doses below 1880 $\mu g/m^3$ (1 ppm) have little effect on such individuals. One study found that 3.75 hours of exposure to 560 $\mu g/m^3$ (0.3 ppm) had a minor impact on lung function in people with chronic obstructive pulmonary disease. There have been conflicting reports about asthma patients; one study found no effects after 75 minutes of exposure to 7520 μg/m3 (4 ppm), while other studies found that 10 minutes of exercise at 560 μg/m3 (0.3 ppm) decreased FEV1 [2]. Nitrogen dioxide exposure may impair oxygen transport by oxidizing hemoglobin to methemoglobin, thereby reducing oxygen delivery; chronic exposure has been linked to heightened asthma risk in children and a potential increase in lung cancer incidence among adults.

Carbon monoxide (CO) forms when fuel combusts under oxygen-deficient conditions. Gasoline-powered engines generally emit higher CO concentrations than diesel engines, due to richer fuel mixtures and combustion inefficiencies.

Carbon monoxide has an affinity for hemoglobin that is 250 times that of oxygen, forming carboxyhemoglobin (COHb), which causes tissue hypoxia. When the CO concentration in the air reaches 4 g/m^3, it can cause death within 30 minutes. Exposure to pregnant women may cause fetal growth retardation.

Because vehicle exhaust is released at roughly human breathing height, pollutants from tailpipe emissions tend to be inhaled directly at elevated concentrations—especially in dense urban areas—contributing disproportionately to personal exposure.

Automobile exhaust pollution has become one of the focal issues of global environmental governance. According to China's Ministry of Ecology and Environment, 15.93 million tons of four pollutants were released by Chinese automobiles in 2020. These included emissions of particulate matter (PM), nitrogen oxides (NOx), hydrocarbons (HC), and carbon monoxide (CO) of 7.697 million tons, 1.902 million tons, 6.263 million tons, and 68,000 tons, respectively. The primary source of all emissions of pollutants is automobiles. To meet this challenge, countries have successively introduced relevant emission standards. China's sixth-stage light-duty vehicle pollutant emission limits and measurement methods have tightened the pollutant emission limits compared with the previous implementation standards, and increased the measurement requirements for the number of particulate matter emitted by gasoline vehicles. The EU light and heavy-duty vehicle emission standards require that all spark-ignition engine vehicles must meet the particulate matter number (PN) and mass limits (PM), and the PN is included in the threshold and tightened to 10 nanometers in diameter.

In May 2024, the European Union introduced the Euro 7 emission standards, which establish stringent technical requirements for exhaust and carbon emissions certification across vehicle categories, including mass particle and number-based particulate limits, which sets common technical requirements and management regulations for the emission type certification and market

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supervision of motor vehicles (i.e. cars, vans, buses and trucks), systems, components and individual technical components, and regulates their carbon dioxide and pollutant emissions.

The catalytic converter is the core device for exhaust gas purification, which realizes the conversion of harmful gases through redox reactions. On the catalyst surface, pollutants undergo the breaking and recombination of specific chemical bonds, NOx is reduced to N_2 and H_2O, and CO and hydrocarbons are oxidized to CO_2 and water. Catalytic converters facilitate redox reactions whereby CO and hydrocarbons are oxidized to CO_2 and H_2O, while NO_x is reduced to N_2 and H_2O. Conversion efficiency depends on catalyst composition, temperature, and precise control over reaction pathways.

Starting from the perspective of chemical bond changes, this article analyzes the pollutant conversion mechanism in the catalytic converter, reviews the technical difficulties such as precious metal dependence and low-temperature deactivation, and the key technological breakthroughs that reduce precious metals and improve low-temperature activity. It also proposes future development directions based on interdisciplinary disciplines such as artificial intelligence and materials engineering, providing theoretical support for achieving exhaust carbon emissions under the carbon neutrality goal [3].

2. Literature review

2.1. Limitations of traditional technologies and initial breakthroughs

Early three-way catalytic converters (TWCs), leveraging platinum (Pt), rhodium (Rh), and palladium (Pd), were developed to oxidize CO and hydrocarbons and reduce NO_x simultaneously, marking a pivotal advancement in automotive emissions control However, conventional TWCs face two major limitations: firstly, they become inefficient during cold starts due to ignition temperature thresholds around 250–350 °C; secondly, their reliance on platinum-group metals makes them costly —accounting for an estimated 60–70% of component cost—and susceptible to high-temperature sintering and deactivation.

Khivantsev and collaborators at PNNL explored single-atom catalysts by anchoring individual Pt atoms on cerium oxide supports, aiming to minimize metal loading while enhancing activity—a promising approach, though quantitative cost reductions remain under-explored.

2.2. Breakthrough in low-temperature active catalysts

The oxygen-rich combustion characteristics of diesel vehicles make NOx control more difficult. He Hong's team at the Chinese Academy of Sciences has achieved two major technological leaps in 25 years: first, it has developed a vanadium-based catalyst → aluminum-rich molecular sieve catalyst system, which is suitable for the NH_3-SCR system in an oxygen-rich environment. By precisely controlling the N-O bond dissociation barrier, it achieves a 95% denitrification rate at 200–300°C; second, it has built a "catalyst-carrier-encapsulation-control" full-chain innovation system, which has been applied to 5 million heavy-duty diesel vehicles and reduced NOx emissions by 2 million tons per year [4].

In 2021, researchers at the University of Leeds reported a synthetic iron silicate (“LowCat”) material inspired by meteoritic iron silicates, achieving simultaneous CO oxidation and NO_x reduction below 150 °C—well below the operational temperatures of conventional catalysts [5]. In 2024, the University of Goa in India developed a Ru-CeO_2 catalyst (5% Ru loading) to achieve 100% conversion of NO-CO at 150°C. H_2-TPR and NH_3-TPD analysis confirmed that the Ru^{4+}-Ov-

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Ce^{3+} active center formed by Ru^{4+} and CeO_2 oxygen vacancies (Ov) synergistically promoted the breaking of the N-O bond, and the reaction path followed the Langmuir-Hinshelwood mechanism [6].Data Sources: [3-6].

Table 1. Comparison of low-temperature denitrification catalyst technology routes

Catalyst type	Active site	Operating temperature	NOx conversion rate	Technical advantages
Traditional TWC	Pt-O-Rh interface	>250°C	<60% (150°C)	Mature technology
Aluminum-rich molecular sieve	Brønsted acid site	200-300°C	>95%	Good sulfur resistance
Ferro silicate	Fe^{2+}-O-Si	<150°C	>90%	High thermal stability
Ru-CeO2	Ru^{4+}-Ov-Ce^{3+}	150°C	About 100%	Excellent low temperature activity

2.3. The rise of non-precious metals and biomass materials

To reduce the dependence on precious metals, researchers have developed a multi-metal synergistic system. In the CuCoCe-LDH catalyst, the Ce^{3+}/Ce^{4+} redox pair provides abundant oxygen vacancies, the Cu site activates NOx, and the Co site adsorbs C_3H_6, achieving a NOx conversion rate of >90% in the range of 150–300°C [7]. At the same time, breakthroughs have been made in biomass carrier technology. Indonesian palm oil-based B35 fuel is coupled with Pistacia shell-derived porous carbon carrier (mesoporosis 70%), and the synthesis energy consumption is reduced by 30% by optimizing the mass transfer path [8].

3. Result

3.1. Chemical bond change mechanism and reaction path analysis

3.1.1. Bond breaking and formation in key reactions

The essence of automobile exhaust purification is to convert toxic molecules into harmless substances through chemical bond recombination. Take NOx reduction and CO oxidation as an example:

NOx reduction reaction (with CO as reducing agent):

$$2NO + 2CO \longrightarrow N_2 + 2CO_2 \quad \Delta H = -623 kJ/mol \tag{1}$$

N-O bond cleavage (bond energy 607 kJ/mol) occurs, followed by N≡N bond formation (bond energy 941 kJ/mol). N-O bond cleavage requires overcoming high reaction activation energy and is the rate-determining step of the reaction. The Rh site weakens the N-O bond through d-orbital electron injection, reducing the cleavage energy barrier from 607 kJ/mol to 210 kJ/mol.

CO oxidation reaction

$$2CO + O_2 \longrightarrow 2CO_2 \tag{2}$$

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C≡O bonds (bond energy 1072 kJ/mol) and O=O bonds (bond energy 498 kJ/mol) break, subsequently forming O=C=O (bond energy 799 kJ/mol). Pt/Pd provides O_2 dissociation sites, CO is adsorbed on adjacent sites, and oxidation is completed through the Mars-Van Krevelen mechanism. Figure 1 demonstrates the visual mechanism of action of single-atom metal catalysts.

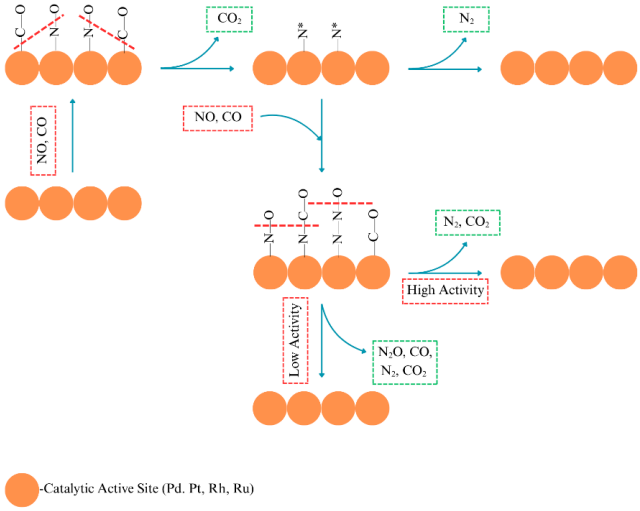

Figure 1. Noble metal catalysis for NOx and CO pollutant conversion

Picture credit: Original

3.1.2. Thermodynamic and kinetic constraints

The exhaust gas purification reaction is subject to both temperature effects and competitive reactions:

The O_2 conversion rate follows a volcanic curve distribution with temperature. Taking the CuCoCe-LDH catalyst as an example, the conversion rate in the 150–250°C range increases from 40% to 95%, and drops to 80% after exceeding 300°C due to the reverse shift of equilibrium. This phenomenon stems from the contradiction between low-temperature kinetic limitations (low N-O bond breakage rate) and high-temperature thermodynamic inversion ($\Delta G>0$).

At the same time, there is also the influence of side reaction interference. The water-gas shift reaction consumes the effective reducing agent CO, resulting in a 10–15% decrease in NOx reduction efficiency. The N_2O generation reaction produces a greenhouse effect, which is 298 times stronger than CO_2. Experiments show that when the temperature exceeds 400°C, the N_2O selectivity increases from 5% to 30%.

3.1.3. Regulation of bond activation pathways by catalytic materials

Different catalysts regulate chemical bond breaking through different active site designs:

Pt/Rh TWC: The Pt-O-Rh interface promotes N-O bond cleavage at the Rh site and facilitates N≡N formation at the interface, although this process requires high temperatures (>350°C).

CuCoCe-LDH: In the Cu^{+}-Ov-Ce^{4+} site, oxygen vacancies (Ov) provide electrons to reduce NO→N_2O→N_2 in steps, and 90% conversion can be achieved at 200°C.

Single-atom Rh/CeO_2: Atomically dispersed Rh^{+} activates NO via bridge adsorption, thus avoiding the formation of N_2O intermediates.Data Sources: [3,5,7,9].

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Table 2. Comparison of bond activation mechanisms of key catalytic materials

Catalyst type	Active site	Bond change path	Transformation efficiency
Pt/Rh TWC	Pt-O-Rh interface	N-O breaks at the Rh site → N≡N is formed at the interface	NOx≤90% (T>350°C)
CuCoCe-LDH	Cu^{+}-Ov-Ce^{4+}	NO→N_2O→N_2 (Ov provides electrons)	NOx>90% (200°C)
Ferro silicate	Fe^{2+}-O-Si	CO oxidation and NO reduction synergistically	NOx>90% (<150°C)
Rh/CeO_2	Isolated Rh^{+}	NO→ N≡N formation	NOx 100% (120°C)

3.2. Technological progress and material innovation

3.2.1. Three-way catalyst upgrade and precious metal reduction

Traditional three-way catalysts (TWCs) are evolving towards lower platinum content and fully palladium-based compositions. The Pd/Rh bimetallic catalyst developed by BASF optimizes the distribution of precious metals through the palladium core-rhodium shell structure, reducing the amount of Rh by 40%.

The revolutionary breakthrough comes from single-atom catalysts (SACs) technology. Pacific Northwest National Laboratory (PNNL) uses high-temperature atom capture (800°C) to immobilize Rh atoms on CeO_2 supports, forming atomically dispersed active centers. At 0.1% Rh loading, 100% NOx conversion can be achieved at 120°C, and the amount of precious metals used is only 1/32 of that of traditional catalysts. The key to this technology is to inhibit the migration of metal atoms and avoid activity attenuation caused by high-temperature sintering [9].

3.2.2. Breakthrough in low-temperature denitrification materials

In response to the cold start problem of diesel vehicles, new low-temperature denitrification materials continue to emerge:

Ru-CeO_2 catalyst: Goa University used a solution combustion method to prepare 5% Ru-CeO_2, and achieved 100% NO-CO conversion at 150°C through the coordination of Ru^{4+} and CeO_2 oxygen vacancies. In situ FTIR confirmed that the reaction followed the Langmuir-Hinshelwood path: NO and CO were co-adsorbed on the Ru^{4+}-Ov site to form N-O⋯Ru^{4+} and C-O⋯Ce^{3+} coordination structures, and the N-O rupture energy barrier was reduced to 60 kJ/mol [6].

3.2.3. Non-precious metals and biomass carriers

Layered double hydroxide (LDH) materials have become a research hotspot due to their adjustable composition. CuCoCe-LDH achieves wide temperature window denitrification through the synergistic effect of three metals: Cu^{+} activates NO molecules, Co^{2+} adsorbs C_3H_6 reductant, and Ce^{4+}/Ce^{37} redox couple provides oxygen vacancies. The three work together to make the NOx conversion rate >90% in the range of 150–300°C [7].

Biomass-derived materials have significant advantages in reducing costs and carbon emissions:

Porous pistacia shell carbon: Derived from pistacia shells, this carrier (70% mesoporous structure) designed for Indonesia's B35 fuel has a specific surface area of 1,200 m^2/g, enabling a

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20% reduction in precious metal loading and a 30% reduction in energy consumption during synthesis [8].

Rice husk silicon-based carrier: The University of Nigeria uses rice husk ash to extract porous SiO_2 to prepare a monolithic honeycomb catalyst, with a denitrification rate of 95% at 200–300°C and a 2-fold increase in sulfur resistance [10].

4. Conclusion

In conclusion, despite significant advancements in catalytic technologies, several critical challenges persist in automotive exhaust treatment systems. Low-temperature catalytic inactivity leads to substantial emissions during vehicle cold-start phases, with traditional catalysts failing to maintain adequate NOx conversion efficiency below 200°C. The generation of harmful byproducts like N_2O, possessing a greenhouse gas potential vastly higher than CO_2, and NH_3 leakage from selective catalytic reduction (SCR) systems exacerbate environmental concerns. Furthermore, the reliance on precious metals, whose costs have surged dramatically, and dependency on imported rare-earth materials pose substantial economic and supply chain risks. Hybrid vehicles also present unique durability issues due to fluctuating temperatures, causing significant deterioration in the catalyst lifespan.

Addressing these bottlenecks, innovative multidisciplinary solutions emerge as promising strategies. Precision-designed single-atom catalysts, leveraging carrier defect engineering, dramatically lower reaction activation barriers, thus enhancing catalytic performance at lower temperatures. Dynamic surface reconstruction technologies, exemplified by CuCoCe-LDH, effectively expose new active sites during reactions, substantially improving low-temperature catalytic activity. Additionally, utilizing biomass-derived materials like porous pistacia-shell carbon significantly reduces costs and achieves carbon-neutral synthesis processes.

Looking forward, the integration of cross-disciplinary technologies such as electrocatalytic auxiliary systems, AI-driven intelligent controls, and modular catalytic units will redefine future exhaust gas treatment approaches. Electrocatalysis, exemplified by PDMS-Cu_2O/C electrodes, offers promising avenues for pollutant conversion and carbon capture. AI-enabled systems like Bosch's AIDrive enhance real-time catalytic efficiency, minimizing harmful byproducts and improving conversion rates. Modular design facilitates maintenance efficiency and scalability, significantly lowering lifecycle costs. Together, these integrated technological advancements represent a comprehensive approach to meeting stringent environmental regulations and achieving sustainable development goals.

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