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Research Progress of Carbon Dioxide Electrocatalytic Reduction Catalysts

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Abstract. Electrocatalytic CO_2 reduction holds promise for converting the greenhouse gas CO_2 into fuels and chemicals with economic value, making it one of the critical technologies for realizing cyclic utilization of carbon resources. The core of current research lies in the development of catalysts. Among metal catalysts, single-atom catalysts exhibit outstanding activity due to their extremely high atomic utilization efficiency. By finely regulating the interaction between metal nanoparticles such as Fe, Ni, and Cu and carbon supports, the reaction pathway can be guided, significantly enhancing the selectivity of target products like CO or C_{2+} species. Doping carbon materials with heteroatoms such as nitrogen and silicon can effectively adjust their surface electronic structure and construct active sites capable of efficiently activating CO_2. Looking ahead, breakthroughs in this technology need to be advanced from multiple dimensions. People can leverage artificial intelligence to accelerate catalyst innovation, optimize the structure of electrolyzers to enhance the mass transfer process, and couple renewable energy power to effectively reduce operating costs. The way for industrial application is thus paved.

Keywords: carbon dioxide, electrocatalysis, catalyst

1. Introduction

In today's society, the excessive use of fossil fuels has exacerbated a series of problems such as global warming and air pollution. For example, there are more than 3,400 fossil fuel power plants in America. These power plants are the main sources of pollutants such as nitrogen oxides and sulfur dioxide, and also an important source of carbon dioxide emissions. These pollutants can cause acid rain, ground-level ozone and fine particulate matter pollution. Every year, the number of premature deaths and new asthma cases related to fine particulate matter and ground-level ozone caused by power plant pollution is huge. In recent years, carbon emissions have continued to increase. The report released by the International Energy Agency (IEA) indicates that global energy-related carbon dioxide emissions reached a record high of 37.4 billion tons in 2023, an increase of 410 million tons compared to the previous year, representing a growth rate of 1.1% [1]. Despite the rapid development of renewable energy technologies, chemical energy still dominates the global energy structure, which accounts for as much as 80%. As a result, it is difficult to control carbon emissions effectively and exacerbates climate change. In addition, the increase in carbon dioxide has led to a

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continuous rise in sea levels, severe ocean acidification, global warming and a series of other problems.

Energy shortage is one of the core challenges currently around the world. Its essence lies in the structural balance between energy supply and demand. It not only involves the scarcity of traditional fossil energy and geopolitical interference, but also is deeply intertwined with the phased bottlenecks of the renewable energy transition and the impact of extreme weather. This issue not only restricts economic development, but also directly affects people's well-being and global energy security.

Carbon dioxide electrocatalytic reduction catalysts are one of the core materials for addressing the global energy and environmental crisis. They can not only fix carbon and reduce emissions but also build a carbon circular economy and alleviate the contradiction between energy supply and demand. They serve as a key technical bridge connecting the "carbon neutrality goal" and "sustainable development". This process converts waste carbon dioxide into recyclable carbon resources, achieving a closed loop of "carbon capture - conversion - reuse", upgrading from "passive emission reduction" to "active carbon cycle", and fundamentally alleviating problems such as global warming and ocean acidification caused by the increase in carbon dioxide concentration. For future economic development, the reliance on fossil resources such as oil and natural gas has been reduced. Moreover, the generated products can be used as fuel or chemical raw materials, compensating for the instability of renewable energy.

This paper studies the current status of electrocatalytic reduction catalysts for carbon dioxide, aiming to summarize the characteristics and performance of different electrocatalysts and explore their influence on the catalytic performance of carbon dioxide. This article will review several common catalysts such as metal-based catalysts, carbon-based catalysts and composite catalysts, and put forward suggestions for the future development of catalysts, providing reference significance for the development of electrocatalytic reduction of carbon dioxide.

2. The source of carbon dioxide

Carbon dioxide is one of the greenhouse gases that affect the Earth's radiation balance and is an important factor contributing to global warming. Studies have shown that since the Industrial Revolution, the concentration of carbon dioxide in the atmosphere has shown a significant upward trend. In 2019, the annual average concentration of major greenhouse gases in the global atmosphere reached a new high. Take carbon dioxide as an example, its concentration was 410.5 ppm, which was 148% of the pre-industrial level [2]. At present, the concentration of atmospheric carbon dioxide is continuously rising. In 2020, the global average concentration of atmospheric carbon dioxide on the surface had reached 413 $\mu mol \cdot mol^{-1}$ [3].

Carbon dioxide (CO_2) originates from a wide range of sources, which can be mainly categorized into two major types: natural sources and anthropogenic sources. Natural sources are an inherent component of the Earth's carbon cycle. In nature, the emission and absorption of carbon dioxide are basically in a state of balance. There are four types of natural sources of carbon dioxide, through which CO_2 is released respectively via biological respiration, microbial decomposition, volcanic activity, and oceans.During their life processes, animals and plants decompose organic matter in their bodies through respiration, and then release carbon dioxide into the atmosphere. Organic substances such as the remains and feces of animals and plants are decomposed by microorganisms in soil or water, producing and releasing carbon dioxide.

When a volcano erupts, carbon elements from the Earth's interior are ejected as gases (including carbon dioxide) and enter the atmosphere. Meanwhile, the ocean acts as a massive carbon reservoir.

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When the temperature of seawater rises or the environment changes, part of the carbon dioxide dissolved in seawater is released into the atmosphere.

Anthropogenic sources are the key to human activities disrupting the balance of the carbon cycle. The combustion of fossil fuels is the main anthropogenic source of carbon dioxide, which includes the burning of coal, oil and natural gas. In some industrial production processes, carbon dioxide can be directly emitted without burning fuel, such as cement manufacturing, steel smelting, chemical production, and so on. In addition, some indirect factors have also led to an increase in the concentration of carbon dioxide. Forests have the function of absorbing carbon dioxide. However, in recent years, the forest area has sharply declined due to forest fires, the government's policy of developing agriculture and land, and illegal deforestation. As a result, many green plants have been damaged, which has reduced the absorption of carbon dioxide [4]. Also, burning trees or clearing land will directly release carbon dioxide. In daily life, the disposal of waste also increases carbon dioxide. In landfills, the organic components of domestic waste are decomposed by microorganisms to produce methane. After further oxidation in the atmosphere, methane is converted into carbon dioxide. Waste incineration treatment will directly release carbon dioxide.

3. CO2 electrocatalyst

3.1. Metal catalyst

Atomic-level dispersed metal catalysts have the highest atomic utilization rate among commonly used catalytic systems, among which single-atom catalysts (SACs) are the earliest proposed and widely studied atomic dispersed catalysts. Compared with bulk metal structures, SACs exhibit excellent electrocatalytic activity due to their unique geometric properties, electronic properties and uniform active sites. Metallic iron (Fe) has a relatively low hydrogen evolution overpotential and a strong CO adsorption energy, which leads to H2 being the main product in the electrocatalytic CO_2 reduction process. Loading FeNPs onto carbon materials can inhibit the precipitation of H_2 and improve the selectivity of CO_2 (RR). Fe/C composites can optimize the CO_2 RR activity by selecting the type of Fe and modifying the carbon carrier.

Similar to metallic Fe, pure metallic Ni has weak CO_2 reduction activity due to its strong CO adsorption energy and low H_2 precipitation overpotential, and thus has been less reported in CO_2 reduction. Researchers synthesized Ni-PCNF catalysts with Ni nanoparticles uniformly dispersed on carbon nanofibers through electrospinning technology, in which the average diameter of Ni NPs was approximately 5 nm [5]. After being compounded with nitrogen-doped porous carbon nanofibers (PCNF), the local electron density of Ni NPs changes, accelerating the transformation between *COOH and *CO intermediates and the desorption of *CO intermediates, and enhancing the catalytic activity of CO_2 RR. In addition, the porous structure of Ni-PCNF enhances the effective utilization rate of Ni active sites, thereby significantly increasing the current density and Faraday efficiency for converting CO_2 to CO.

Among the metallic materials used for CO_2 reduction, copper (Cu) has a unique catalytic activity for CO2 reduction and can convert CO_2 into C2+ products. Existing research indicates that Cu NPs catalysts based on graphene carriers can effectively anchor the key reaction intermediates in the CO_2RR process by taking advantage of the strong interaction between Cu and carbon-based defects, thereby selectively regulating the products. In addition, by rationally regulating the particle size and oxidation state of Cu NPs and combining with appropriate carbon-based carrier materials, the Cu/C composite electrocatalyst can significantly improve the selectivity of C2+ products [6].

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3.2. Carbon-based catalyst

Carbon-based metal-free catalysts have become a research hotspot due to their low cost, high electrical conductivity and environmental friendliness. They have significant potential for the capture and conversion of CO_2 under mild conditions. When they were used as CO_2 reduction catalysts, they also have advantages such as high cost-effectiveness, large specific surface area, excellent electrical conductivity and controllable physical and chemical properties. However, pure carbon-based materials lack the activity of CO_2 reduction reaction (CO_2RR). One reason is that the electrical neutrality of carbon atoms is not conducive to the adsorption of CO_2. The other cause is that the activation of CO_2 requires overcoming a higher energy barrier. The lattice configuration of carbon materials affects the CO_2 electro-reduction pathway and efficiency. The root cause lies in the differences in adsorption energy between the surfaces of different carbon materials and key intermediates such as * COOH and *CO. According to the spatial dimension, carbon materials can be classified into 0D fullerenes, 1D carbon nanotubes, 2D graphene and 3D porous carbon. Among them, 0D materials promote CO_2 contact through high specific surface area and rich edges, while 1D materials shorten the electron transfer distance by high aspect ratio (the hollow structure can also enhance the CO_2 diffusion capacity) [7]. 2D materials become ideal matrices due to their planar structure and high mechanical strength, but these three types of materials are prone to stacking. Although 3D materials can prevent agglomeration and facilitate CO_2 diffusion through porous frameworks, they have the problem of relatively small specific surface area. In addition, although carbon nanotubes (CNTs) are widely used in electrocatalysis, their pure CO_2RR activity is relatively poor. However, nitrogen atoms can be used as dopants to improve the local charge distribution of CNTs and enhance their CO_2 adsorption and reaction activity due to their atomic radius being close to that of carbon and their electronegativity (3.04) being higher than that of carbon.

In addition to morphology regulation, doping the carbon skeleton with heteroatoms is also an effective means to enhance the catalytic performance of CO_2 reduction. Introducing heteroatoms such as B, N, S, P, and F, which have different electronegativity from carbon, can regulate the surface charge distribution of carbon materials, break the pure carbon electrical neutrality, and thereby form active sites that can adsorb and activate CO_2. Among them, the co-doping of nitrogen atoms with other heteroatoms (such as the co-doping of nitrogen-silicon, nitrogen-sulfur, and nitrogen-boron) can significantly enhance the electrochemical CO_2 reduction activity of metal-free carbon materials. For instance, Dai Liming's team prepared porous silicon-nitrogen co-doped carbon (Si-NC) nanomaterials through self-sacrificing template-assisted pyrolysis. Compared with single-doped Si-C and NC materials, the bifunctional catalytic activities of CO_2RR and OER of Si-NC under neutral conditions were significantly enhanced. It is confirmed that the co-doping of silicon and nitrogen can enhance the intrinsic activity of carbon-based catalysts. Moreover, the CO_2 complete decomposition system with Si-NC as the electrode achieved a total energy efficiency of 75% and a solar-chemical energy conversion efficiency of 12.5% under the drive of photovoltaic cells [8].

3.3. Composite catalyst

The mechanism of electrocatalytic CO_2 reduction reaction (CO_2RR) is complex, and single-component catalysts often fail to meet the ideal catalytic performance requirements. Constructing composite electrocatalysts of metal nanoparticles (NPs) and carbon materials is a common strategy for achieving efficient CO_2RR [9]. The outstanding CO_2RR catalytic performance of this composite system usually stems from the synergistic effect between metal nanoparticles and carbon-based

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carriers: on the one hand, the metal components can effectively adsorb and activate CO_2 molecules, significantly reducing the formation energy barrier of intermediates and electrochemical overpotential; On the other hand, the high specific surface area and hierarchical porous structure of carbon carriers can provide rich active interfaces for catalytic reactions, effectively alleviate the diffusion limitations of reactants and products, and thereby enhance the performance of CO_2RR [10]. Although high-temperature carbonization can further enhance the electrochemical active area and conductivity of carbon materials, metal nanoparticles are prone to aggregation and agglomeration under high-temperature conditions, resulting in a decrease in specific surface area and catalyst deactivation. Therefore, the rational regulation of active sites is the key to preparing highly stable electrocatalysts.

4. Prospects of electrocatalytic carbon dioxide

The electrocatalytic reduction technology of carbon dioxide is an important direction for achieving "negative carbon" emissions and green energy conversion. At the technical level, the key to current research lies in enhancing the selectivity and efficiency of reactions. In the future, with the help of artificial intelligence and high-throughput computing, it will be possible to design and screen new types of catalysts such as single-atom alloys and metal-organic frameworks more quickly, thereby achieving highly selective preparation of high-value products like ethylene and ethanol. Meanwhile, the continuous improvement of the electrolyzer structure such as optimizing the gas diffusion electrode and membrane electrode components will significantly enhance the mass transfer efficiency, drive the current density to an industrial-grade level, and lay the foundation for large-scale application.

The task of reducing costs is arduous but the direction is clear. Firstly, it is necessary to gradually replace expensive precious metal catalysts and develop resource-rich non-precious metal or molecular catalysts to control material costs from the source. Secondly, it is necessary to enhance the integration with renewable energy sources such as wind power and photovoltaic power, and utilize "green electricity" during periods of low cost or even negative electricity prices for production. This not only reduces electricity consumption costs but also enhances the green attributes of the products. Furthermore, the investment in equipment as well as the operation and maintenance costs can be further amortized through system integration and scale-up.

5. Prospects of electrocatalytic carbon dioxide

Electrocatalytic carbon dioxide reduction is an important technical approach to achieving the "negative carbon" goal, with the core lying in the development of efficient, stable and economical catalyst systems. At present, metal catalysts and carbon-based metal-free catalysts each have their own characteristics: single-atom catalysts demonstrate unique advantages due to their maximum atomic utilization rate and uniform active sites; Fe and Ni-based materials can effectively regulate the reaction pathway and enhance the efficiency of CO generation through carrier modification. Cu-based catalysts have attracted much attention due to their special selectivity for multi-carbon products such as ethylene and ethanol. Carbon-based materials can break through the limitation of intrinsic electric neutrality, construct highly active interfaces, and significantly enhance the adsorption and conversion capacity of CO_2 through heteroatom doping and structural design. The composite catalyst ingeniously combines the intrinsic activity of metal components and the structural advantages of carbon materials, which forms a synergistic catalytic effect and becomes a

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current research hotspot. However, the agglomeration tendency of metal nanoparticles during high-temperature preparation remains a bottleneck which restricts their long-term stability.

Furthermore, the development of this field requires a multi-pronged approach. People can leverage artificial intelligence and high-throughput computing to precisely design new catalysts. Also, it is useful to optimize the structure of electrolyzers, which can enhance reaction efficiency and current density. It is necessary to promote the integration of non-precious metal catalysts with renewable energy-based electricity. A solid foundation will be laid for the large-scale practical application of CO_2 resource utilization by making joint efforts from both the material source and energy consumption end.

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