

Single-Atom Carbon-Based Catalysts in High Oxidation Reactions for Water Remediation: From Materials to Reaction Pathways

Abstract

SACs are widely recognized as the most advanced catalysts for environmental remediation due to their high efficiency, 100% metal atom utilization, near-zero secondary pollution, and robust structures. Recently, the use of persulfate in advanced oxidation processes (AOP's) with carbon based SACs has raised great interest in the decomposition of novel contaminants in wastewater, due to its high and versatile ability to generate reactive oxygen species (ROS). However, the detailed and critical review of the relationship between carbon based SAC structures and the resulting generated ROS is still very limited. In this article, we provide a systematic overview of the basic understanding and intrinsic mechanisms between the single metal atom (SMAT) active sites and the produced ROS during an AOP. First, the types of emerging contaminants are discussed; presenting the pre-existing pollutants that must be degraded. Then, the preparation and characterization methods for carbon based SAC are discussed. The basic material structure-ROS type relationships for persulfate based AOPs are discussed in detail to explain the catalytic mechanisms. Finally, we conclude with the current state of development of carbon based SAC in an AOP and suggest the future prospects of rational design, synthesis, and catalytic performances for carbon SAC in AOP in future research.

Keywords: Single-atom catalysts • Emerging contaminants • Advanced oxidation processes • Persulfate activation • Reactive oxidant species

Introduction

Water quality is typically assessed by looking at the levels of inorganic, organic, microbial, and heavy metals in the water. Recently, however, some unknown pollutants have been identified as emerging contaminants, which are not listed as harmful to the environment [1]. We have gained limited knowledge of the emerging contaminants because they rarely appear [2]. Emerging contaminants usually range in concentration forming/l to $\mu\text{g/l}$, but they are non-degradable under natural conditions and build-up in the food chain (Macro Invertebrates). As a result, their release into the environment has posed a significant risk to human health and the environment. As a result, several treatments have been developed to remove emerging contaminants, including phase-changing technologies (PCTs), biological processes

(BMPs) and advanced oxidation (AOP) processes [3]. AOPs have the highest potential due to their high generation of reactive oxidizing (ROS) species (H_2O_2 , H_2O_3 , H_2O_4 , H_2O_5 , H_2O_6 , H_2O_7 , H_2O_8 , H_2O_9 , H_2O_{10} , H_2O_{11} , H_2O_{12} , H_2O_{13} , H_2O_{14} , H_2O_{15} , and H_2O_{16}). These reactive oxidizing species have high oxidation potential, allowing them to efficiently attack and degrade emerging contaminants.

Pesticides

Pesticides (also known as pesticides) are physical and chemical agents that are used to protect agriculture from harmful insects, weeds and microorganisms, depending on the target species. There are four classes of pesticides that are conventionally used: Insecticides Aldicarb Marathon Athmectin Rotenone

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Herbicides Atrazine Clopyralid Alachlor Oxyfluorfen Fungicides Oxypropion Micatin Chlorothalonil Methylthobuzin Maintaining good soil Bactericides [4, 5].

Semiconductor acids (SACs) based on carbon

The development of scalable, controllable, and reproducible synthetic strategies for the preparation of carbon based SACs is essential for the industrialisation of carbon-based SACs for persulfate based AOPs due to its high surface energy [6]. Here is a summary of the topics covered in this review Summary of Carbon Based SACs Preparation Classification and Representative Structures of Emerging Contaminants. *eco-Environment & health* 2(2023) Surface energy of isolated single metal atoms The isolated single metal atoms always migrate and aggregate with each other to form nanoparticles or clusters [7]. However, only when the interaction between the individual metal atom and the carbon carrier is strong enough to anchor the individual metal atom to the carbon carrier can carbon based SAC be obtained [8]. The as-processed catalysts have various chemical and electronic structures that allow the induction of radical or non-radical pathways in persulfate based AOP's [9]. The characterizations of the structure of these carbon based SACs allow us to reveal the relationship between structure and catalytic pathway, the focus of this review, to realize rational design of high performance catalysts and eventually industrial application [10].

Description

The purpose of this review is to provide an overview of recent progress in the development of carbon-based catalytic converters (SACs) in persulfate based AOPs for the degradation of emerging contaminants. First, the types of emerging contaminants are clarified and the corresponding typical contaminants are described. Second, this article provides an overview of the progress in the synthesis and characterization in recent years in the production and characterization of carbon based SACs. Thirdly, the relationship between the types of generated oxidative residues in persulfate activation and the underlying single atom active sites of carbon based catalytic converters are systematically summarised and discussed. Fourthly, brief conclusions and perspectives on the design

of carbon base catalytic converters with controllable catalytic active sites towards targeted catalytic properties in persulfate base AOPs from the design principle, the synthesis strategy, and the distinction between single metal active sites.

Conclusion

In conclusion, we summarise recent research on emerging contaminants type, carbon based SAC synthesis and characterization, and their environmental applications. In particular, we compare the catalytic mechanism of persulfate based AOPs to the structure of carbon based SACs from the perspective of the generation of reactive oxygen species (ROS). Previously, excellent carbon based SAC were well prepared and characterized with superior catalytic performance over their nanoparticle/cluster counterparts for the degradation of emerging contaminants. Excellent catalytic performance benefits from the unique geometrical and electronic structure of the single atom active sites in carbon based SAC. The single atom active site can influence the adsorption by persulfate, regulate the electron transfer from the active site to persulfate and determine how persulfate cleaves to generate different types of ROS. The difference in the generation of ROS ultimately impacts the reaction pathway and the difference in ROS ultimately affects the reaction pathway and catalytic performance. Although carbon-based SACs are believed to be of great potential in the application of persulfate-based AOPs, there are still some aspects that require more attention in future research strengthen the coordination environment. For instance, introduce additional heteroatoms to create a more stable interaction between the metal atoms and the carbon carriers. Form numerous small cavities to stabilize individual metal atoms. For instance, use more cavities in MOF to anchor multiple metal atoms. Finally, it is important to note that different metal atoms have varying interaction strengths and loading dynamics with the carbon carriers, which may lead to significant differences in their upper limit of loading.

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