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Special Collection: Materials Challenges for Catalysis

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Energy has played a very important role in the history of human development. In the era of traditional energy sources, our use of traditional energy sources relied heavily on human, animal, and natural energy sources; for example, people were using wood and other combustible materials to make fire for heating, cooking, and providing light. In the era of Industrial Revolution, the Industrial Revolution of the late 18th and early 19th centuries marked a major change in energy development. With the widespread use of coal, coal combustion became the main source of energy at that time, driving the development of advanced technologies, such as steam engines, trains, and textile machinery. In the oil era, the large-scale extraction and utilization of oil began to change the human energy mix in the early 20th century.[1] Oil was continuously utilized as an efficient and convenient source of energy for transportation, industrial production, and household use. In the era of nuclear energy, in the mid-20th century, nuclear energy began to gradually become an important direction for human energy development. The use of nuclear energy releases enormous amounts of energy through nuclear fission or nuclear fusion for power generation and other applications with high efficiency and cleanliness. The 21st century marks the era of renewable energy, people are increasingly concerned about environmental protection and sustainable development, and renewable energy has become a hotspot for energy development.[2] Renewable energy sources, such as solar, wind, and water, are widely utilized to reduce dependence on traditional fossil fuels, reduce carbon emissions, and achieve sustainable development. Currently, people are actively promoting energy transition and increasing the development and utilization of renewable and clean energy, as well as exploring emerging energy technologies, such as hydrogen and geothermal energy, to achieve a more sustainable and environmentally friendly energy future. For the production and conversion of renewable and clean energy sources, highly active and stable catalysts are essential.

At the beginning of human development, people already started to use some natural substances to facilitate certain chemical reactions, although they did not understand the nature of catalysts. With the development of science, the study of catalysts was gradually advanced, and in the late 18th and early 19th centuries, chemists began to study catalysts systematically and made some important discoveries. For example, in 1794, the French chemist Auguste de Louis Brière-Bertolome first observed the catalytic effect of platinum on hydrogen gas. Thereafter, he also observed the catalytic effect of platinum on the reaction of sulfur dioxide with nitrogen dioxide. The late 19th and early 20th centuries saw major breakthroughs in the field of catalysts. The German chemist Wilhelm Oswald discovered many important catalysts, such as platinum black and cuprous oxide, which were widely used in industry.[3] The French chemist Paul Serrouze and the Italian chemist Ziolio Francis Brunoli also made important contributions to the study of catalysts. The second half of the 20th century and the development of modern science and technology have led to rapid advances in the field of catalysts. Today, a variety of synthetic methods and advanced technological tools enable the design and manufacture of catalysts with high efficiency, low energy consumption, and low emissions.

A thermocatalyst promotes the rate of a reaction by providing the appropriate temperature conditions during a chemical reaction. It is usually a solid catalyst that can adsorb, dissociate, re-combine, or transfer reactant molecules, thus reducing the activation energy of the reaction and accelerating the reaction rate.[4] Photocatalysts use light energy excitation to generate electron and hole pairs and participate in catalytic reactions. Photocatalysts are mainly semiconductor materials, such as titanium dioxide (TiO_2), which can absorb photons and convert light energy into electrochemical energy, thus facilitating photocatalytic reactions.[5] Electrocatalysts facilitate electrochemical reactions by providing an effective catalytic interface and reducing the energy loss and activation energy of charge transfer in electrochemical reactions. Electrocatalysts are commonly metal catalysts, such as platinum, that provide good electrocatalytic performance in fuel cells.[6] All three catalysts play an important role in different reaction systems, facilitating chemical reactions and energy conversion processes by modulating reaction conditions and providing an effective catalytic interface to improve reaction rates and selectivity.

Commonly used catalyst materials are as follows: MOF (metal–organic framework)-based catalysts are crystalline porous materials constructed from metal ions and organic ligands. MOF-based catalysts have the advantages of high tunability and large surface area, which can provide abundant catalytic active sites and channel structures for applications in gas adsorption and separation, catalytic reactions, and energy storage.[7] Metal catalysts refer to catalysts in the form of metallic elements or alloys, such as platinum, palladium, and iron. Metal catalysts have excellent catalytic activity and selectivity, and can facilitate a variety of chemical reactions, including hydrogenation, hydrogenation, oxidation, and reduction.[8] These catalysts have different characteristics and application areas and play important roles in their respective fields. Their selection depends on the specific type of reaction, reaction conditions, and the required catalytic performance.

Existing studies often use the following methods to construct novel catalysts. The construction of multiphase interfaces can provide more catalytic active sites and reaction surfaces, which can help to improve the activity and selectivity of catalysts.[9] At the multiphase interfaces, support can interact with complexing agents, catalyst precursors, or other modifiers to form more stable catalyst structures and interfaces. The interaction between metal supports and reactant molecules has a great influence on the rate and selectivity of catalytic reactions. Metal supports can interact with reactant molecules through processes such as adsorption, diffusion, reaction, and desorption. These interactions can modulate the adsorption conformation and activity of the reactant molecules on the surface of the supports, thus affecting the rate and selectivity of the catalytic reaction. The catalytic activity and selectivity can be optimized by tuning parameters such as size, shape, and epitaxy of single metal particles.

Monometallic catalysts are easy to prepare and characterize, they have better controllability, repeatability, and higher atomic utilization, and the development and utilization of metal resources is more sustainable.[10] Constructing alloys can change the electronic structure and surface properties of metal and support to improve catalytic activity and selectivity.[11] In summary, multiphase interfaces, metal–support interactions, and both monometallic and alloy catalysts are very important factors in catalyst design. By reasonably regulating these factors, the catalyst performance can be optimized and the efficiency and selectivity of catalytic reactions can be improved.

In the 21st century, energy catalysis research still faces many challenges. There is a need to develop catalysts with high selectivity and activity to achieve efficient conversion of specific reactions. For example, in petroleum processing, improving the selectivity of catalytic cracking and hydrogenation reactions can improve product quality and reduce waste generation.[12] During energy conversion, catalysts are often subject to extreme conditions, such as high temperature, high pressure, and oxidation environment, and are prone to deactivation and decay. Therefore, researchers need to find catalyst materials with good stability and long lifetime. Source catalysis research also requires the development of environmentally friendly catalysts and reaction conditions to reduce the production of pollutants and energy consumption. The development of green catalytic technologies, such as the use of renewable energy and waste resource utilization, is essential to achieve sustainable energy systems.

Revolutionary catalytic materials with high activity and robust stability are a key nexus for efficient storage and clean utilization of renewable energy. Reasonable design and synthesis of metal-based, metal-free, and crystalline/amorphous materials is key for improving the activity and stability of catalysts.[13] Moreover, establishing the exact relationship between the active center/phase structure and the catalytic activity is also an essential requirement for the design of advanced catalytic materials.[14] To further trigger catalytic activity, selectivity, and stability of active structures, it is crucial to introduce active supports to strengthen the catalytic properties via tuning the local electronic structure and surface chemical status of catalysts.[15] Advanced theoretical simulations and specific *in situ* spectroscopy characterizations also need to be developed to unravel the actual morphology and manner of the catalytic active sites.

This thematic issue dedicated to Materials Challenges for Catalysis contains five groups of research articles:

- mixed metal oxide (MMO) catalysts,
- single-atom catalysts,
- two-dimensional ultra-thin materials,
- carbon materials,
- electrocatalysts.

The first group of articles is dedicated to mixed metal oxide (MMO) catalysts. Liu and Wang focus on *Low-temperature oxidative dehydrogenation of propane over NiV mixed oxides derived from LDH precursors.*

The second group of articles concerns single-site catalysts, a very hot field in heterogeneous nanocatalysis. In the first article of this group Ham and colleagues report *Direct CC bond scission of xylitol to ethylene and propylene glycol precursors using single-atom catalysts (SACs) anchored on MgO–*. An up-shift in the DOS for the surface M_1 atoms in all investigated SACs compared to the surface atoms of their respective SCCs results in M_1 higher d-band center and stronger adsorbate(s) binding. This study highlights the importance of SACs for boosting the atom efficiency of costly metals while also offering a new strategy for tuning the activity of catalytic reactions.

The third group of articles deals with two-dimensional ultra-thin materials. In the first article, Chu and Lu focus on *Durable Ni_3N porous nanosheets array for non-noble metal methanol oxidation reaction*.

In the second article, the groups of Zhang and Li present *Perspectives on two-dimensional ultra-thin materials in energy catalysis and storage*. These authors investigated in details the research and application of 2D ultra-thin material-based catalysts for heterogeneous catalysis. Various catalysts based on 2D ultra-thin materials, such as MXenes, GO, black phosphorus, and h-BN, are discussed in detail for catalytic processes in the fields of electrocatalysis, photocatalysis, and energy catalysis.

The fourth group includes two articles on carbon materials. First, Liu and co-workers report *Synthesis of Co_9S_8@CNT hydrogen production composites by one-step pyrolysis of monomolecule precursor*. This area has long been central in energy storage and conversion.

Then, in the second article of this group, Zhou and Jiang report *High-efficiency oxygen electrocatalyst for Zn–air batteries on CoMn alloy encapsulated in N-doped carbon architectures*. This study opens a new way for designing high-efficient bifunctional electrocatalysts for application in renewable energy facilities.

Finally, the fifth group contains two articles focusing on electrocatalytic materials. In the first article of this series, Kimata and Yamaki discuss *Platinum nanoparticles prepared by ion implantation exhibit high durability for fuel cell applications*.

Then, Huo and co-workers focus on *In-plane heterostructured MoN/Mo_2N nanosheets as high-efficiency electrocatalysts for alkaline hydrogen evolution reaction*.

We hope that this Special Topic will be relevant and interesting for readers both in and outside the field.

We thank all authors who contributed to this Special Topic.

AUTHOR DECLARATIONS

Author Contributions

Baojun Li: Writing – original draft (lead); Writing – review & editing (equal). **Seungho Cho**: Writing – review & editing (equal). **Yanyan Liu**: Writing – review & editing (equal). **Didier Astruc**: Writing – review & editing (equal).

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