



Editorial: Emerging Technologies for Materials Design and Characterization in Energy Conversion and Storage

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Editorial on the Research Topic

Emerging Technologies for Materials Design and Characterization in Energy Conversion and Storage

The increasing consumption of fossil fuels leads to energy crisis and environmental issues, which seriously affects human daily life. To date, great efforts have been made to explore sustainable, eco-friendly and renewable energy alternatives to fossil fuels. In the past few decades, various energy conversion and storage technologies, such as water splitting (Zhang F. et al., 2019; Hu et al., 2021; Wu et al., 2021), proton exchange membrane fuel cells (Edwards et al., 2008; Park et al., 2012), nitrogen reduction reaction (NRR) (Wan et al., 2019; Zhang W. et al., 2019; Yang et al., 2020b; Li et al., 2021), CO₂ reduction reaction (CO₂RR) (Ozdemir et al., 2019; Liu et al., 2020; Yang et al., 2020a; Ma et al., 2021; Wang et al., 2021), and metal-air batteries (Cheng and Chen, 2012) have shown promising potential due to the high efficiency, energy security, and environmental protection. In these fields, more attention has been paid to preparing advanced materials with outstanding performance, and developing advanced technologies for prediction, characterization and detection (Centi, 2020).

Electrocatalytic NRR to NH₃ has been regarded as an attractive alternative to the traditional Haber-Bosch process owing to its lower energy consumption under ambient conditions (Tang and Qiao, 2019; Yang et al., 2020b). The development of advanced NRR catalysts with outstanding performance and low costs is highly desired. Recently, Wang et al. reported that the ringlike V₂O₃ nanostructures could effectively convert N₂ to NH₃ under ambient conditions. Scanning electron microscopy analysis shows that the ringlike structure is uniform with outer diameter of 350–500 nm. Transmission electron microscopy (TEM) analysis confirms that such nanoring possesses a rough surface, displaying more active sites. The high-resolution TEM image of an individual nanoring indicates a contracted interplanar distance of 0.211 nm, corresponding to the (113) plane. This work presents a facile strategy to fabricate the advanced non-noble-metal catalysts for NRR. It is believed that more effective and stable electrocatalysts would be developed for boosting the NRR in the future.

Energy efficiency is another efficacious way to alleviate the energy crisis. In the field of energy-saving optoelectronics, electrochromic devices (ECDs) have shown great advantages. Among various fabrication materials for ECDs, coordination polymer (CP) shows a broad application prospect due to good cycle stability, high color rendering efficiency, and fast switching speed. Liu et al. present a comprehensive survey of the current achievements and progresses of CP in energy efficient ECDs from the aspect of influence of composition, coordination bonding and microstructure of pyridine-based CP on the performance of ECDs. This work is expected to provide the guideline for achieving a substantial enhancement in electrochromic and other optoelectronic fields.

Nevertheless, one of the paramount challenges to develop new high-efficiency energy transformation materials is the long span from experiment to practical application, due to the complexity of research objects and methods, insufficient personal accumulated experience, etc. (Luo et al.) Artificial intelligence (AI) has potential for solving the problems mentioned above. Luo et al. investigated and summarized research works on energy storage materials for capacitors and Li-ion batteries. They pointed out that machine learning (ML), as a subset of AI, algorithms can reduce test number of cycles and required experiments, which greatly reduces time consumption and accelerates every stage of development. In addition, they summarized the status and progress of AI in energy storage materials and present solutions to relevant deficiencies, such as the establishment of a database, extracting data from unstructured literature with automaticity and high efficiency and accuracy, etc. Apart from saving time, AI can predict the performance of materials, monitor reaction processes, and explore reaction mechanisms (Luo et al.; Yang et al.). Focusing on the superiority of AI in predicting experiments, Yang et al. reviewed the situation and application of AI in respects of optoelectronic materials, hydrogen peroxidation catalysts, water

electrolysis catalysts and microbial fuel cells. It indicates that the relationship between prediction and actual experiments is mutually facilitating. In other words, the efficiency of actual material processing can be promoted with accurate prediction, and the database for AI is extended.

In conclusion, the development of advanced materials and technologies for energy conversion and storage are of vital importance. Until now, various promising materials with excellent performance have been prepared, such as carbon nanomaterials [nanofibers (Zhao et al., 2018; Lee et al., 2020), nanotubes (Ma et al., 2019; Sun et al., 2020; Tuo et al., 2020; Zhang et al., 2020), graphene (Chen et al., 2020), etc.], reticular structure [metal-organic framework (Nam et al., 2018), covalent organic framework (Lin et al., 2015)], and tandem catalyst (Morales-Guio et al., 2018), etc. It is worth mentioning that traditional technologies in detection and characterization are gradually substituted with new and advanced solutions, such as computer science (AI, ML, etc.), and *in-situ* characterization (*In-situ/operando* synchrotron radiation, *in-situ/operando* morphology/spectrum, etc.). It is believed the emerging technologies for materials design and characterization in energy conversion and storage will be greatly developed in the future.

AUTHOR CONTRIBUTIONS

ZZ supervised the project. JL wrote the manuscript. ZZ, YC, and ZF revised the manuscript. All authors contributed to the article and approved the submitted version.

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Conflict of Interest: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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