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SPECIAL ISSUE: Energy Transitions towards Carbon Neutrality

Advanced materials and energy technologies towards carbon neutrality

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The rapid development of human society has led to much increased consumption of energy, which results in global energy shortage as well as serious environmental concerns due to the use of non-sustainable fossil fuels. For example, the heavy relay on the use of coal and oil leads to carbon emission which is a major factor for global warming and climate change. Developing green and sustainable energy paths becomes more urgent than ever. In this regard, energy sources like sunshine, wind, and water are important to build a clean and sustainable future. For example, one could generate electricity from sun by solar cell devices. Later, such electricity can be stored either in the form of charges by batteries or supercapacitors, or stored in the form of chemicals by electrochemical catalysis conversion, which can be transported over a long distance or stored for a long time for end use. The efficiency of these new energy technologies and devices including photovoltaic, energy storage, and energy conversion, is key which determines whether they can be large-scale implemented. High-performance materials play central rules in determining the efficiency of these technologies and therefore largely influence the use of these clean energy technologies and paths toward global mission of carbon neutrality.

In this Special Issue focus on Energy Transitions towards Carbon Neutrality, we collected 27 papers discussing these important energy processes and showing how advanced materials and their manufacturing affect the efficiency of these technologies including solar cells, electrocatalytic devices, and energy storage devices.

Solar cell is a device which can absorb solar light and convert it into electricity by using active components including perovskite materials [1–5], organic molecules [6,7], and inorganic materials [8,9]. Defects in active materials or charge transport layers, and the quality of the interface between different components are important factors need to be optimized to improve the photoelectric conversion efficiency (PCE) of solar cells. Yi *et al.* [1] reported the use of a multi-functional phosphor-ethanolamine to suppress defects in SnO_2, which is an electron transport layer, and increase the PCE of flexible perovskite solar cells. To reduce nonradiative recombination loss at defects, Wang *et al.* [2] used cesium stearate, which is an anionic surfactant, to passivate defects and enhance the tolerance to light and moisture for metal halide perovskite solar cells, reaching a PCE of 23.41%. Considering that ion migration is a problem in improving the stability of perovskite solar cell, Bai *et al.* [4] have developed an organic anion anchoring strategy to suppress ion migration with improved device stability for 1320 hours. In another study, Wen *et al.* [3] have provided a perspective on the monolithic all-perovskite tandem solar cells and put forward future important targets for this type of devices including improving performance and stability, scaled fabrication, and device structure optimization. It is known that poor stability is a major concern for the commercialization of perovskite solar cells. In the review by Zhou *et al.* [5], the authors have discussed strategies to improve the stability of metal halide perovskites including engineering of composition, crystallization, interface, and defect, as well as the mechanism involved. In another study, Guo *et al.* [6] have fabricated all-small-molecule organic solar cells based on a benzotriazole-based π-bridge unit which can change the energy band alignment at the interface, leading to improved efficiency and reduced energy loss. Interestingly, Yue *et al.* [7] have reported that weakly crystalline materials perform better than highly ordered ones in terms of PCE of organic solar cells, due to their improved miscibility and charge transport, which is controversial to what researchers understood previously. Li *et al.* [8] reported a dual effect of NH_4F additive in the preparation of Sb_2S_3 for solar cell performance, including regulating the band gradient and modifying the surface of the electron transport layer. Silicon is an active material for commercialized solar cells. He *et al.* [9] reported that light soaking can enhance the performance of silicon heterojunction solar cells.

After generation of electricity from sunshine by solar cells, one way to store such electricity is to convert it into energy-containing chemicals like hydrogen (as energy carrier) based on electrocatalytic or photoelectrochemical synthesis. Another strategy is to use electricity to convert CO_2, which is a green house gas, into value-added chemicals. In terms of electrocatalytic water splitting to generate hydrogen *via* the hydrogen evolution reaction, Pt is the catalyst with the best intrinsic performance, but with problems of high cost and low abundance. In the work by Li *et al.* [10], the authors anchored low-amount of Pt species on defect-rich $W_{18}O_{49}$ nanowires which show good performance in acidic electrolyte. Ma *et al.* [11] have prepared ternary PtRuTe alloy nanofibers showing efficient and durable hydrogen oxidation performance in alkaline media,

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which is a key problem in anion exchange membrane fuel cells. Metal-phthalocyanine is a type of alternative catalyst to metal nanoparticles, and Jeong *et al*. [12] have reviewed molecular structures of metal-phthalocyanine catalysts and their application for various electrocatalytic reactions including oxygen and CO_2 reduction and hydrogen and oxygen evolution. In the research paper by He *et al*. [13], the authors prepared two-dimensional mesoporous Mo-Co-O catalysts composed of crystalline Mo_4O_{11} and amorphous cobalt hydroxide which show improved oxygen evolution reaction performance due to abundant holes, oxygen vacancy, and enhanced adsorption of reaction intermediates. In another study, Tang *et al*. [14] have prepared a single-atom zinc-nitrogen-carbon catalyst and reported the electrocatalytic reduction of oxygen to produce H_2O_2 by a two-electron transfer reaction with improved catalyst atom utilization efficiency and reduced waste generation, with the H_2O_2 selectivity of 80% after 10,000 s continuous opperation. In the work by Li *et al*. [15], the authors reported the regulation of spin states in amorphous materials like Mo-doped CoS to the low-spin state, which optimizes the adsorption free energy of oxygen reduction intermediates and improves the performance of zinc-air batteries in terms of cycle stability, discharge voltage, mass-energy density, etc. Photoelectrochemical water splitting is also an appealing technology for energy conversion. In this technology, fast migration and spatial separation of photogenerated charges are key to improve the device efficiency. Wan *et al*. [16] have made a $CdS/PbTiO_2/TiO_2$ heterostructure catalyst with combined interfacial electrical and ferroelectric fields which can efficiently separate charges and lead to two orders of magnitude improvement of photocatalytic hydrogen production. In addition, Yang *et al*. [17] have doped Al into the lattice of $LaTaON_2$, which maintains the light absorption property, inhibits the defect concentration, and increases the surface hydrophilicity of the catalysts, leading to much enhanced photocatalytic water oxidation performance. Yin *et al*. [18] have prepared a CoO_x/Ni:COOH bilayer-protected n-Si photoanode which is stable under oxygen evolution with improved onset potential and photocurrent density. Besides fundamental studies on the structure-performance relationship, large current operation and electrolyzer assembly are prerequisites for the practical implementation of these electrocatalytic technologies in industry. Along this direction, Liu *et al*. [19] have systematically reviewed key components and engineering strategies of membrane electrode assembly in advanced polymer electrolyte water electrolyzer, and proposed future directions of this field.

Besides water splitting, other electrocatalytic reactions have also drawn much attention recently. For example, ammonia is an alternative energy carrier to hydrogen with the advantages of easy storage and transportation. In the Review by Lee *et al*. [20], the authors have reviewed catalysts for electrochemical ammonia oxidation including their fundamental mechanism, poisoning species, Pt and non-noble metal-based catalysts, and their performance. In another review, Ge *et al*. [21] have discussed the use of non-noble electrocatalysts for biomass derivatives' oxidation reaction at the anode side which can produce more value-added products than common oxygen evolution reaction to produce oxygen. Electrocatalytic CO_2 reduction is another promising technology to produce value-added chemicals. In the article by Ma *et al*. [22], the authors prepared nano-porous Cu-In heterostructures which can electrochemically reduce CO_2 into syngas with controllable H_2/CO ratios in the range of 0.47 to 2.0, where the interface induced by charge redistribution leads to the formation of two different copper active sites. In the review by Qiu *et al*. [23], the authors discussed the classification and synthesis of dual-atomic-site catalysts and their uses for CO_2 reduction. Photocatalysis is also promising to reduce CO_2 which basically converts solar energy into chemicals. In the research paper by Wang *et al*. [24], the authors studied how gold nanoparticles can induce the formation of oxygen vacancy on the surface of semiconducting Bi_2WO_6, which results in improved light absorption, optimized adsorption energy of reactants, and separation and transport of photogenerated carriers.

In addition to converting electricity to chemicals, one alternative important technology is to store electricity in energy storage devices like batteries, supercapacitors, etc. Zhou *et al*. [25] have reported the use of defective Te-doped $ReSe_2$ with expanded interlayers grown on MXene for potassium ion batteries with improved reversible capacity, rate capability, cycle life, flexible full battery operation, etc. In the review by Song *et al*. [26], the authors discussed the use of planar micro-supercapacitors for flexible on-chip electronics, covering stretchable, self-healing, stimulus-responsive, thermosensitive, biodegradable, and temperature-tolerant features. In another review by Xia *et al*. [27], the authors discussed carbon-based electrodes in energy storage devices which may combine energy storage and catalytic effects to improve the device performance.

To sum up, the 27 invited papers in this special issue cover clean energy generation, conversion, and storage with an aim to realizing green and sustainable development for carbon neutrality. It is clear that advanced materials and material manufacturing play dominating and irreplaceable roles in the implementation of these technologies. Here we want to take this chance to sincerely thank our authors who contribute to this Special Issue of Energy Transitions towards Carbon Neutrality and wish these high-quality research and review articles can inspire more ideas in these important research areas.

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