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NR 87
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AU Ma, Z
   Kuloor, C
   Kreyenschulte, C
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   Malina, O
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   Jagadeesh, RV
AF Ma, Zhuang
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   Malina, Ondrej
   Haumann, Michael
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TI Development of Iron-Based Single Atom Materials for General and
   Efficient Synthesis of Amines
SO ANGEWANDTE CHEMIE-INTERNATIONAL EDITION
LA English
DT Article
DE iron catalysis; single atoms; reductive amination; carbonyl compounds;
   amines
ID REDUCTIVE AMINATION; HETEROGENEOUS CATALYSIS; MOLECULAR-HYDROGEN;
   METHYLATION; SITES

AB Earth abundant metal-based heterogeneous catalysts with highly active and at the same time stable isolated metal sites constitute a key factor for the advancement of sustainable and cost-effective chemical synthesis. In particular, the development of more practical, and durable iron-based materials is of central interest for organic synthesis, especially for the preparation of chemical products related to life science applications. Here, we report the preparation of Fe-single atom catalysts (Fe-SACs) entrapped in N-doped mesoporous carbon support with unprecedented potential in the preparation of different kinds of amines, which represent privileged class of organic compounds and find increasing application in daily life. The optimal Fe-SACs allow for the reductive amination of a broad range of aldehydes and ketones with ammonia and amines to produce diverse primary, secondary, and tertiary amines including N-methylated products as well as drugs, agrochemicals, and other biomolecules (amino acid esters and amides) utilizing green hydrogen.

Iron-based single atoms (Fe-SACs) as reductive amination catalysts have been prepared by the pyrolysis of Fe-nitrogen complexes on SiO2 and subsequent removal of silica. Applying these Fe-SACs, all kinds of amines including N-methylated products, amino acid esters, amino acid amides and selected drug molecules are synthesized starting from inexpensive and easily accessible carbonyl compounds and ammonia or amines in presence of molecular hydrogen. image
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RI MIchael, Haumann/A-7087-2013; Menezes, Prashanth/L-3651-2018; Zboril, Radek/F-5153-2015; Beller, Matthias/M-8214-2014
FU Deutsche Forschungsgemeinschaft [447724917]; Deutsche Forschungsgemeinschaft (DFG); European Research Council; State of Mecklenburg-Vorpommern [CZ.02.01.01/00/22_008/0004587]; ERDF/ESF project TECHSCALE [CZ.10.03.01/00/22_003/0000048]; European Union; Chinese Scholarship Council (CSC); Palacky University in Olomouc [03EW0015 A/B]; German Federal Ministry of Education and Research

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WC Chemistry, Multidisciplinary
WE Science Citation Index Expanded (SCI-EXPANDED); Index Chemicus (IC); Current Chemical Reactions (CCR-EXPANDED)
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TI Z-scheme configured iron oxide/g-C3N4 nanocomposite system for solar-driven H2 production through water splitting
SO APPLIED CATALYSIS O: OPEN
LA English
DT Article
DE Photocatalyst; Nanocomposites; Water splitting; Green hydrogen; Heterojunction; Redox
ID OXIDATION-STATE; G-C3N4; PHOTOCATALYSTS; COMPOSITE; DISINFECTION; PERFORMANCE; MECHANISM; EVOLUTION
AB A nanocomposite composed of alpha-Fe2O3/g-C3N4 is synthesized using a modified ultrasonication approach, which engineered a robust interfacial contact in the system. Phase formation and morphological features are confirmed via XRD and electron-microscopy techniques. XPS revealed the native oxidation states of the elements and chemisorption-mediated interactions in the system. This developed composite produced hydrogen at a rate of 1494 mu molg- 1 h- 1, which is around 6.6 times higher than the g-C3N4 system. The observed enhancement is attributed to the Z-scheme configuration, leading to the suitable band edge alignments, charge separation and extended lifetime of the carriers in the composite.
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NR 57
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J9 APPL CATAL O-OPEN
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AU Lee, EB
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Kim, SJ
Park, GR
Lee, JW
AF Lee, Eun Been
Jo, Seung Geun
Kim, Sang Jun
Park, Gil-Ryeong
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TI Fabrication of Ruthenium-Based Transition Metal Nanoparticles/Reduced
Graphene Oxide Hybrid Electrocatalysts for Alkaline Water Splitting
SO KOREAN JOURNAL OF METALS AND MATERIALS

LA English
DT Article
DE microwave-assisted process; ruthenium; transition metal; nanoparticles;
water splitting
ID EARTH ABUNDANT ELECTROCATALYSTS; HYDROGEN EVOLUTION REACTION; RECENT
PROGRESS; OXYGEN; EFFICIENT; ALLOYS; OER
AB Green hydrogen has attracted significant attention as one of the future energy sources because no greenhouse gases are emitted during production and its energy density is much higher than fossil fuels. Precious metals such as platinum (Pt) and iridium (Ir)-based catalysts are commonly used for water splitting catalysts. However, because of high cost of these precious metals, the mass production of green hydrogen is restricted. In this study, water splitting catalysts based on relatively inexpensive ruthenium (Ru), cobalt (Co), and iron (Fe) were synthesized. The metal nanoparticles were anchored on reduced graphene oxide (rGO) by a microwave-assisted process. The nanoparticles were uniformly distributed on the rGO supports with sizes of about 1.5 and 2 nm in Ru/rGO and RuCoFe/rGO, respectively. This promoted the reaction by further increasing the specific surface area of the catalysts. In addition, it was confirmed by EDS mapping results that the nanoparticles were made of RuCoFe alloy. Among the prepared catalysts, Ru/rGO was excellent toward the hydrogen evolution reaction (HER), which required an overpotential of 50 mV to reach a current density of -10 mA cm-2. In addition, RuCoFe/rGO, which contained the RuCoFe alloy, was the best for the oxygen evolution reaction (OER), and it required 362 mV at the current density of 10 mA cm-2.
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NR 37
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U1 4
U2 18
PU KOREAN INST METALS MATERIALS
PI SEOUL
PA KIM BLDG 6TH FLOOR, SEOCHO-DAERO 56 GIL 38, SEOCHO-GU, SEOUL 137-881,
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TI Electronic and Surface Modifications of Ni-Co-Fe Oxides: A Catalyst with
Maximum Exposure of Fe Active Sites for Water Electrolysis
SO ACS APPLIED ENGINEERING MATERIALS
LA English
DT Article
DE sequential deposition; electronic modification; catalyst support
interaction; abundant active sites; sustainable electrodes
ID OXYGEN EVOLUTION REACTION; NICKEL FOAM; ELECTROCATALYSTS; NANOSHEETS;
PERFORMANCE
AB The production of green hydrogen through water electrolysis is a crucial component of sustainable energy systems. One key challenge is the development of cost-effective electrocatalysts with high performance. Here, we report on the fabrication of a multilayered electrode by coating a nickel foam with nickel-cobalt-iron (Ni-Co-Fe) oxide layers (NiCoFe@NF/SD). The detailed physical and electrochemical characterizations demonstrated that the topmost layer is rich in Fe active sites. The electronic shuffling between the different layers creates an optimal environment for intermediate adsorption-

desorption during the oxygen and hydrogen evolution reactions. The NiCoFe@NF/SD electrode exhibits high catalytic performance due to the presence of intrinsically reactive active sites, as well as high structural, chemical, and mechanical durability with a low overpotential of 210 and 166 mV for the oxygen and hydrogen evolution reactions, respectively, to deliver a geometric activity of 20 mA cm(-2). In a two-electrode configuration, NiCoFe@NF/SD as cathode and anode requires a relatively small input voltage of 1.56 V to deliver a current density of 10 mA cm(-2) and sustained a current density of 100 mA cm(-2) for over 90 h with no noticeable degradation. This work offers a simple approach for the rational design of electrodes to produce green hydrogen through water electrolysis.
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NR 66
TC 4
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PU AMER CHEMICAL SOC
PI WASHINGTON
PA 1155 16TH ST, NW, WASHINGTON, DC 20036 USA
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TI Developing Practical Catalysts for High-Current-Density Water Electrolysis
SO ADVANCED ENERGY MATERIALS
LA English
DT Article
DE electrocatalyst design; green hydrogen production; high current density; industrial application; water electrolysis
ID EFFICIENT OXYGEN EVOLUTION; HYDROGEN EVOLUTION; ACTIVE-SITES; HIGH-PERFORMANCE; ACIDIC WATER; OXIDATION; IRON; ELECTROCATALYST; ELECTRODES; STABILITY
AB High-current-density water electrolysis is considered a promising technology for industrial-scale green hydrogen production, which is of significant value to energy decarbonization and numerous sustainable industrial applications. To date, substantial research advancements are achieved in catalyst design for laboratory-based water electrolysis. While the designed catalysts demonstrate remarkable performance at laboratory-based low current densities, they suffer from marked deteriorations in both activity and long-term stability under industrial-level high-current-density operations. To provide a timely assessment that helps bridge the gap between laboratory-scale fundamental research and industrial-scale practical water electrolysis technology, here the current advancements in various commercial water electrolyzers are first systematically analyzed, then the key parameters including work temperature, current density, lifetime of stacks, cell efficiency, and capital cost of stacks are critically evaluated. In addition, the impact of high current density on the electrocatalytic behavior of catalysts, including intrinsic activity, long-term stability, and mass transfer, is discussed to advance the catalyst design. Therefore, by covering a range of critical issues from fundamental material design principles to industrial-scale performance parameters, here the future research directions in the development of highly efficient and low-cost catalysts are presented and a procedure for screening laboratory-designed catalysts for industrial-scale water electrolysis is outlined.
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AB The energy crisis is a daunting global problem that calls for innovative and supportable solutions to ensure future energy security and environmental stability. To counter this energy uncertainty, accelerating renewable-driven hydrogen production stands as a vital option to foster carbon-neutral energy infrastructure. This review conveys an overview of worldwide hydrogen generation techniques (steam methane reformation, thermochemical, biological, and electrolytic), highlighting the key features, indicating the pros and cons, and unraveling the potential environmental consequences. Herein, the conventional gray and cutting-edge green hydrogen production technologies are compared, with a focus on sustainable water electrolysis utilizing renewable energy sources. The existing difficulties with conventional electrolysis, including the usage of expensive catalysts in both cathode and anode, are discussed along with the possible gateway with cost-effective and sustainable electrocatalysts. This review focuses on the potential of three types of 3d transition metal-based molecular catalysts-cobaloximes, iron porphyrins, and nickel bis-phosphines-for hydrogen evolution reactions (HER), stressing their strategic synthetic designs, mechanistic routes, and catalytic parameters. Despite their high activity and selectivity, these molecular systems confront stability and scalability issues, limiting their practical applicability. To address this, the immobilization of these catalysts into solid matrices is studied, simplifying their integration into membrane electrode assembly (MEA) water electrolyzers for industrial-

scale renewable-driven hydrogen production. To bridge the gap between lab-scale investigations and commercial implementation, several design components of the MEA stack are examined, such as flow patterns and scaling methodologies. A comprehensive approach to catalyst development and deployment is ensured by highlighting the significance of Life Cycle Assessment (LCA) and Techno-Economic Analysis (TEA) in assessing environmental sustainability and economic viability. The review closes with a call for multidisciplinary research and innovation to improve electrochemical water-splitting technology and accelerate the transition to an enduring hydrogen economy.
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TI γ-FeOOH Nanosheet with Enormous Cationic Defect: Efficient and Durable
Bifunctional Electrocatalyst Suitable for an Industrial-Scale AEM
Electrolyzer
SO ACS APPLIED ENGINEERING MATERIALS
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DT Article
DE gamma-FeOOH nanosheet; cationic defect; electrocatalysts; AEM
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ID HYDROGEN-PRODUCTION; WATER ELECTROLYSIS; EVOLUTION REACTION;
TRANSITION-METALS; ALKALINE; CATALYSTS; SUBSTRATE; OXIDATION
AB Anion exchange membrane (AEM)-based electrolysis of alkaline water using a transition metal electrocatalyst is supposed to be the effective route for next-generation pure green hydrogen production, but development of a suitable electrocatalyst is challenging. Herein, we report the development of a simple and scalable protocol to grow a highly aligned ultrathin iron(III) oxyhydroxide (lepidocrocite, gamma-FeOOH) nanosheet on nickel foam (gamma-FeOOH-NS-NF) at room temperature (RT) through controlled simultaneous oxidation and hydrolysis in the presence of hydrazine. During synthesis, hydrazine plays crucial multiple roles, one of which is the generation of enormous Fe vacancies (V-Fe). The synthesized gamma-FeOOH-NS-NF showed superior bifunctional water splitting activity because of its thin sheet microstructure and enormous cationic defect. Particularly at high current density, it showed an exceptionally low overpotential of 320 at eta(1000) and a Tafel slope of 29 for the OER, and 309 mV at eta(1000) and 65 mV dec(-1) for the HER in aqueous 1 M KOH solution. For overall water splitting, a 10 mA cm(-2) current density was observed at a low potential of 1.6 V. It showed 98% Faradaic efficiency and excellent stability for continuous operation over 100 h at 500 mA cm(-2) current density. More importantly, a membrane electrode assembly (MEA) having gamma-FeOOH-NS-NF in both

the anode and cathode in a prototype anion exchange membrane (AEM) electrolyzer (4 cm(2)) showed outstanding water splitting performance and stability. The experimental results evidenced that the ultrathin sheet microstructure grown on NF and the generated V-Fe are primarily responsible for the efficient water splitting. Thus, the scalable and robust synthetic technique, direct usability in an AEM electrolyzer, and the correspondingly high AEM activity and excellent electrode stability make it suitable as an industrial-scale AEM electrolyzer for green hydrogen production.
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FX Science and Engineering Research Board (SERB), India (CRG/2023/003385) and Council of Scientific and Industrial Research (CSIR), India (HCP 44).
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TI Evaluation of the Catalytic Effect of Metal Additives on the Performance of a Combined Battery and Electrolyzer System
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DT Article
DE Green Hydrogen; Hydrogenproduction; Electrolysis; Battolysers; Battery-Electrolyzers; Catalysts; Hydrogen evolutionreaction
ID LEAD-ACID-BATTERIES; HYDROGEN EVOLUTION; ELECTROCHEMICAL-BEHAVIOR; ENERGY-STORAGE
AB A low-cost method of green hydrogen production via the modification of a lead acid battery has been achieved, resulting in a hydrogen flow rate of 5.3 L min-1 from a 20-cell string. The electrochemical behavior and catalytic effect of various metal additives on the hydrogen evolution reaction (HER) was evaluated using cyclic voltammetry. Nickel, cobalt, antimony, manganese, and iron were investigated, with 66 ppm nickel achieving a 75% increase in hydrogen produced from a modified lead acid battery. Design of Experiments (DOE) employing a simple centroid design model to analyze the combined additive effects of nickel, cobalt, and antimony was performed to evaluate the effect on the HER. A combination of Ni:Co:Sb in the ratio 66:17:17 ppm achieved the greatest end voltage shift of the HER from -1.65 to -1.50 V; however, no increase in hydrogen yield was observed in comparison to 66 ppm of nickel when added to a full-scale cell. Gas chromatography using a thermal conductive detector and a sulfur chemiluminescence detector were used to measure the purity of hydrogen obtained from a string of 20 battery electrolyzer cells connected in series. 99% purity hydrogen gas was obtained from the battery electrolyzer cells, with H2S impurities below the limit of detection (0.221 ppm).
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TI Astonishing performance of zinc iron sulfide with MoS 2 composite in allium-shaped structure for comprehensive alkaline water splitting
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DT Article
DE Electrochemical water splitting; Non-noble metals; HER; OER; Electrocatalyst
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AB Electrochemical water splitting offers a promising avenue for producing clean hydrogen fuel, essential for a sustainable energy landscape. A highly efficient catalyst, featuring a one-dimensional structure, has been synthesized by combining zinc iron sulfide with molybdenum disulfide (ZFSMS) on a nickel foam substrate. This synthesis method utilizes a simple yet effective hydrothermal approach tailored for efficient water splitting. By carefully engineering the interface between zinc iron sulfide and molybdenum disulfide, the electronic conductivity of the catalyst is significantly boosted, enhancing its catalytic performance. The resulting hybrid, ZFSMS, exhibits remarkable electrocatalytic efficiency with minimal overpotentials. Specifically, overpotentials of 130 mV and 220 mV are recorded for the oxygen evolution reaction at 20 mA cm-2 and 50 mA cm-2, respectively. Moreover, for the hydrogen evolution reaction, overpotentials of 145 mV and 257 mV are observed at 10 mA cm-2 and 40 mA cm-2, respectively, in a 1.0 M potassium hydroxide solution. Notably, the ZFSMSbased electrolyzer operates at a low voltage of 1.5 V at 10 mA cm-2, underscoring its efficiency in facilitating electrochemical hydrogen generation. This catalyst good candidate for advancing green hydrogen production, contributing to the progress of sustainable and clean hydrogen fuel production methods.
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TI Fe-Based Materials for Electrocatalytic Water Splitting: A Mini Review
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DE Fe-based MOFs; Electrocatalysis; Homo and heterogenous electrocatalysts; Oxygen Evolution Reaction (OER); Hydrogen Evolution Reaction (HER); Overall water splitting (OWS)
ID METAL-ORGANIC FRAMEWORKS; OXYGEN EVOLUTION REACTION; DINUCLEAR IRON COMPLEX; HYDROGEN EVOLUTION; INTRINSIC ACTIVITY; OXIDATION CATALYSIS; EVOLVING CATALYST; RECENT PROGRESS; GRAPHENE OXIDE; EFFICIENT
AB In the last few years, the development of effective electrocatalysts hold fascinating importance towards scalable green hydrogen (H2) and oxygen (O2) production has become an appealing area of research. A good number of iron-based catalysts have been designed and synthesized which can mediate water splitting under mild conditions with minimum energy requirements. In this review, recent progress on iron-based electrocatalysts focusing on Oxygen Evolution Reaction (OER), Hydrogen Evolution Reaction (HER), and Overall Water Splitting (OWS) are summarized. Tactical designing, targeted synthesis with electronic tuning, efficiency as well as durability are discussed here. The review is comprehensive and our target is to promote the development of highly efficient economical catalysts, to make their way from the laboratory to market by replacing noble metal-based electrocatalysts.

This review systematically summarizes and highlights the recent developments in Fe-based heterogeneous and homogeneous electrocatalysts toward water splitting. The benefits and drawbacks of MOFs and molecular electrocatalysts are discussed. Our target is to endorse the Fe-based electrocatalysts, to make their way from laboratory to market by replacing noble metal-based catalysts. image
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TC 2
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U2 40
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AU Ta, XMC
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Nguyen, HT
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TI Optimizing Surface Composition and Structure of FeWO₄
Photoanodes for Enhanced Water Photooxidation
SO ADVANCED MATERIALS TECHNOLOGIES
LA English
DT Article
DE flame spray pyrolysis; iron tungstate (FeWO4); PEC water splitting
ID MOTT-SCHOTTKY ANALYSIS; OXYGEN-EVOLUTION; OPTICAL-PROPERTIES;
THIN-FILMS; HYDROGEN; IRON; OXIDATION; PHOTOELECTRODES; NANOSTRUCTURES;
STABILITY
AB Photoelectrochemical water splitting is a promising approach to produce green hydrogen using solar energy. A primary bottleneck remains the lack of efficient photoanodes to catalyze the sluggish water photooxidation reaction. Engineering photoabsorbers with a

narrow bandgap and suitable band edge can boost the photoelectrochemical performance. Herein, nanostructured iron tungstate (FeWO4) photoanodes are engineered directly on a fluorine doped tin oxide glass substrate via a scalable and ultra-fast flame synthesis route in 13 seconds. Physiochemical, optoelectronic, and electrochemical properties of these photoanodes are systematically investigated. The key roles of charge transport, transfer, and dissolution of W and Fe ions from the FeWO4 matrix within long-term performance are revealed. Optimal FeWO4 photoanode with a bandgap of 1.82 eV and a FeOOH/NiOOH co-catalyst coating shows an improved water photooxidation performance, reaching a photocurrent density of 0.23 mA cm(-2) at 1.4 V versus reversible hydrogen electrode in 1 m potassium hydroxide. It further demonstrates relatively good photostability, maintaining approximate to 96% of photocurrent density after 1-hour continuous photooxidation, albeit some trace of Fe, W and Ni elements dissolution. Insights on the photooxidation performance of nanostructured FeWO4 provide promising directions for the engineering of small band-gap catalysts for a variety of photoelectrochemical applications.
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NR 86
TC 4
Z9 4
U1 6
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JI Adv. Mater. Technol.
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WC Materials Science, Multidisciplinary
WE Science Citation Index Expanded (SCI-EXPANDED)
SC Materials Science
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AU Zhang, JY
Zeng, Y
Xiao, TY
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AF Zhang, Jiayi
Zeng, Yu
Xiao, Tanyang
Tian, Song
Jiang, Jing
TI Aerophobic/Hydrophilic Nickel-Iron Sulfide Nanoarrays for Energy-Saving Hydrogen Production from Seawater Splitting Assisted by Sulfion Oxidation Reaction
SO INORGANIC CHEMISTRY
LA English
DT Article
ID CATALYST; NI
AB Electrolysis of infinite seawater is a promising and sustainable approach for clean hydrogen production. However, it remains a big challenge to accomplish corrosion-resistant and chlorine-free seawater electrolysis at low power input. Herein, the bimetallic nickel-iron sulfide-based electrocatalytic nanoarrays are constructed by a facile hydrothermal sulfidation of redox-etched iron foam (IF), which manifests an effective and reliable strategy for the sulfion oxidation reaction (SOR) to assist alkaline seawater electrolysis for the achievement of energy-saving hydrogen production and value-added sulfion upcycling. The resulting NiFeS x /FeNi3/IF required 0.353 and 0.415 V vs RHE for SOR at current densities of 50 and 100 mA cm(-2), which are considerably lower than the theoretical potential of the oxygen evolution reaction (OER, 1.23 V vs RHE). In situ spectroscopy analysis demonstrated efficient sulfion oxidation on the surface of NiFeS x /FeNi3/IF. Furthermore, the NiFeS x /FeNi3/IF-assembled electrolyzer delivered a greatly reduced cell voltage of 0.92 V at 50 mA cm(-2) and maintains excellent durability for 30 h, achieving high Faradaic efficiency for both hydrogen production and sulfion degradation. In addition, under natural sunlight (660.4 W m(-2)), only a 0.947 V voltage of the solar panel smoothly powers the SOR-coupled seawater electrolysis for green hydrogen production and economic sulfur recovery.

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WC Chemistry, Inorganic & Nuclear
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AU Cartagena, S
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AF Cartagena, Santiago
   Calderon, Jorge A.
TI Corrosion of non-noble metal-based catalysts during oxygen evolution
   reaction under on/off operation
SO CORROSION SCIENCE
LA English
DT Article
DE Oxygen evolution reaction; Nickel corrosion; Nickel-based catalysts;
   Anodic dissolution; Alkaline water electrolysis
ID ALKALINE WATER ELECTROLYSIS; FE-P ALLOY; HYDROGEN EVOLUTION; IN-SITU;
   ELECTROCHEMICAL EVOLUTION; POLARIZATION TIME; OXIDE ELECTRODES;
   STAINLESS-STEELS; SURFACE OXIDES; NICKEL-OXIDE
AB Green-hydrogen generation has become a focus for research due to its promising future as an energy vector. In this regard, one topic that has not been explored in depth, is the corrosion of catalytic layers under on/off operation in alkaline media during oxygen evolution reaction (OER) on the anode. Here, we studied the corrosion of, and changes to, the catalytic layer on stainless steel (SS) electrodes under different surface treatments. The results showed that there was formation of a passive and catalytic layer of NiOOH during the anodic polarization concomitantly with iron dissolution.
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WC Materials Science, Multidisciplinary; Metallurgy & Metallurgical
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SC Materials Science; Metallurgy & Metallurgical Engineering
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PT J
AU Fondjo, LOM
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Yonti, Cedrik Ngnintedem
Kouotou, Patrick Mountapmbeme
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TI Nanoarchitectonics with Fe-doping on the optical and electrocatalytic
properties of ZnO prepared by the malonate coprecipitation route:
Application in the hydrogen evolution reaction
SO JOURNAL OF ALLOYS AND COMPOUNDS
LA English
DT Article
DE Malonate-based precursors; Coprecipitation; Fe-doped zinc oxide; Optical
properties; Hydrogen evolution reaction
ID ELECTRODES; ALKALINE
AB Producing green hydrogen through water electrolysis in alkaline media using a suitable, eco-friendly, and inexpensive electrocatalyst is an effective approach to address the current energy problem. Transition metal oxides like ZnO are promising alternatives to noble metal-based electrocatalysts. However, their electrocatalytic properties are less reported due to their low performance. Doping is a proven strategy to enhance the functional properties of metal oxides, and the effectiveness of doping strongly depends on the synthesis route. In this work, Fe-doped ZnO (FexZn(1-x)O, x Zn (1-x) O, x = 0, 0.06, 0.07, 0.11) was successfully synthesized via the pyrolysis of Fe-doped Zn malonate precursors obtained by the coprecipitation method. Results from a set of instrumental techniques revealed that the main phase formed is ZnO nanoparticles, with iron substituting zinc in the structure. UV-Visible diffuse reflectance results demonstrated that the optical band gap gradually decreases from 3.09 eV to 2.52 eV upon increases of iron content. The optimal amount of iron in ZnO exhibited an overpotential of 448 mV at 10 mA cm-- 2 (lower than that of pure ZnO and Fe2O3) 2 O 3) and a small Tafel slope of 70 mV dec-1.- 1 . The observed enhancement in electrocatalytic performance can be attributed to the generation of more active sites due to the optimal amount of iron in the matrix of the ZnO parent structure.
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NR 26
TC 0
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AF Krishnamurthy, Palani
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   Rahaman, Mostafizur
TI Iron-Doped Nickel Hydroxide Nanosheets as Efficient Electrocatalysts in
   Electrochemical Water Splitting
SO CATALYSTS
LA English
DT Article
DE iron doping; nickel hydroxide; oxygen evolution reaction; hydrogen
   evolution reaction; low overpotential
ID OXYGEN EVOLUTION; NI(OH)(2) NANOSHEETS; HIGHLY EFFICIENT; GRAPHENE
   OXIDE; NI FOAM; BETA-NI(OH)(2); CATALYST; ELECTRODES; REDUCTION; ARRAY
AB The development of non-noble-metal-based electrocatalysts for water electrolysis is essential to produce sustainable green hydrogen. Highly active and stable non-noble-metal-based electrocatalysts are greatly needed for the replacement of the benchmark electrocatalysts of iridium, ruthenium, and platinum oxides. Herein, we synthesized non-noble-metal-based, Fe-doped, & beta;-Ni(OH)(2) interconnected hierarchical nanosheets on nickel foam via a conventional hydrothermal reaction. Iron doping significantly modified the electronic structure of & beta;-Ni(OH)(2) due to the electron transfer of iron to nickel hydroxide. Fe-doped & beta;-Ni(OH)(2) was investigated both as a cathode and anode electrode for hydrogen and oxygen evolution reactions (OERs and HERs). It facilitated significant improvements in electrochemical performance due to its huge intrinsic active sites and high electrical conductivity. As a result, the electrocatalytic activity of Fe-doped Ni(OH)(2) exhibited a lesser overpotential of 189 and 112 mV at a current density of 10 mA cm(-2) and a Tafel slope of 85 and 89 mV dec(-1) for the OER and HER, respectively. The Fe-doped & beta;-Ni(OH)(2) displayed excellent durability for 48 h and a cell voltage of 1.61 V @ 10 mA cm(-2). This work demonstrates that Fe-doped & beta;-Ni(OH)(2) is an efficient electrocatalyst with superior electrocatalytic performance towards overall water splitting that can be useful at the industrial scale.
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NR 66
TC 13
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AF Yu, Xiaorui
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   Li, Jing
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TI Ion exchange synthesis of Fe-doped clustered CoP nanowires as superior
   electrocatalyst for hydrogen evolution reaction
SO INTERNATIONAL JOURNAL OF HYDROGEN ENERGY
LA English
DT Article
DE CoFeP; Electrocatalyst; Hydrogen evolution reaction Nanostructure
ID HIGHLY EFFICIENT ELECTROCATALYST; NICKEL-COBALT PHOSPHIDE; ARRAYS;
   NANOSTRUCTURES; PERFORMANCE; NANOARRAYS; NANOSHEETS; CATALYSTS
AB Green hydrogen production from electrochemical water splitting currently suffers from the key issues of high energy consumption and cost. Herein, we demonstrated the synthesis of highly efficient and stable clustered CoP nanowires electrocatalysts on nickel foam. Moreover, an ion exchange strategy was proposed to precisely control the doping content of iron to further modify the intrinsic electrochemical activity of CoP nanowires. The introduction of iron effectively alters the surface atomic configuration and electronic structure of CoP and increases the active sites, thus accelerating the overall reaction rate and enhancing the catalytic performance. It has been demonstrated that the CoFeP-30-30/NF electrode exhibits platinum-like catalytic activity with only an overpotential of 29.8 mV at 10 mA.cm(-2) and outstanding stability toward hydrogen evolution reaction. The synthetic strategy of CoFeP/NF electrode proposed in this work will significantly promote

the development of highly efficient transition metal phosphides electrocatalysts with lower overpotential and better stability.
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NR 58
TC 13
Z9 14
U1 7
U2 42
PU PERGAMON-ELSEVIER SCIENCE LTD
PI OXFORD
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   An, Q
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   An, Qi
   Zhang, Yang

Yue, Qu
Liu, Chongbo
Li, Xiaoqin
Li, Bing
Qiu, Lu
Xiao, Dan
Zhao, Qian
TI Surface <i>in situ</i> modulation of carbon nanotube-supported Fe-Ni compounds <i>via</i> electrochemical reduction to enhance the catalytic performance for the oxygen evolution reaction
SO INORGANIC CHEMISTRY FRONTIERS
LA English
DT Article
ID IRON
AB Exploring efficient strategies to enhance the catalytic performance for the oxygen evolution reaction (OER) is crucial for the rapid development of green hydrogen production based on water electrolysis. Here, a simple and extensible in situ electrochemical reduction method is proposed to improve the OER catalytic performance. A carbon nanotube-supported iron-nickel organometallic compound (Fe-Ni@CNT) and the corresponding R-Fe-Ni@CNT with further electrochemical reduction modulation serve as the pre-catalysts to obtain O-Fe-Ni@CNT and RO-Fe-Ni@CNT catalysts during the OER process, respectively. The characterization results show that the electrochemical reduction modulation can adjust the redox properties of the active species and the in situ transformation process to induce the formation of a greater abundance of Ni3+ (efficient OER active sites). Hence, the RO-Fe-Ni@CNT catalyst displays significantly enhanced OER catalytic activity and stability compared to the O-Fe-Ni@CNT catalyst. This work reveals the unique role of electrochemical reduction modulation in OER catalytic performance, providing more opportunities for the design of efficient catalysts.
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OI Li, Xiaoqin/0009-0001-8478-7490
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NR 62
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PA THOMAS GRAHAM HOUSE, SCIENCE PARK, MILTON RD, CAMBRIDGE CB4 0WF, CAMBS, ENGLAND
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AF Meshesha, Mikiyas Mekete
Chanda, Debabrata
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TI Efficient green hydrogen production through metal-organic framework-derived Ni and Co mediated iron selenide hexagonal nanorods and wireless coupled with photovoltaics for urea and alkaline water electrolysis
SO APPLIED CATALYSIS B-ENVIRONMENT AND ENERGY
LA English
DT Article
DE Bifunctional catalyst; Electrocatalyst; Water splitting; Urea electrolysis; Photovoltaics-electrochemical; AEMWE
ID OXYGEN EVOLUTION; ELECTROCATALYSTS; NANOSHEETS; CARBON; PHOTOCATALYST; PERFORMANCE
AB Metal-organic framework (MOF)-based catalysts are gaining attention due to their tunable properties. In this study, we synthesized MOF based Ni and Co doped iron selenide (NiCoFeSe) hexagonal nanorods electrocatalyst. This NiCoFeSe catalyst exhibited outstanding performance in the hydrogen evolution reaction (HER), oxygen evolution reaction (OER), and urea oxidation reaction (UOR) with impressively low overpotentials of 220, 275 mV for HER, 230, 330 mV for OER, and 210, 300 mV for UOR at current densities of 50 and 100 mAcm(-2), respectively. Additionally, we fabricate a wireless flexible and rigid photovoltaic-electrochemical device utilizing NiCoFeSe as both the anode and cathode, achieving an impressive solar-to-hydrogen efficiency of 11.1%. Furthermore, we developed an anion exchange membrane water electrolyzer with NiCoFeSe as anode and cathode, achieving a current density of 1.07 Acm (-2) at 1.85 V, along with a cell efficiency of 69.67% and an energy consumption of 47.85 kWh to produce 1 kg of hydrogen.
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PT J
AU Jung, SY
Lee, J
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Kim, T
Han, H
Jeong, YK
AF Jung, Sun Young
Lee, Jieon
Aydin, Kubra
Jang, Jinuk
Ahn, Chisung
Kim, Taesung
Han, Hyuksu
Jeong, Young Kyu
TI Transition metal sulfide and nickel-iron layered double hydroxide nanohybrids for promising alkaline seawater oxidations
SO APPLIED SURFACE SCIENCE
LA English
DT Article
DE Direct seawater electrolysis; Oxygen evolution reaction; Chloride corrosion; Electrocatalysts; Layered double hydroxide; Transition metal sulfide
ID OXYGEN EVOLUTION; ELECTROCATALYSIS; HYDROGEN
AB Direct seawater electrolysis is of great significance to produce green hydrogen using sustainable resources which can be applicable for water-scarce regions. Herein, a nanohybrid consisted of transition metal sulfide and layered double hydroxide is designed with aims to modify unfavorable surface electronic state of nickel-iron LDH (NF-LDH) for seawater oxidation. Specifically, Mo-doped NiS2 is deposited onto the self-standing two dimentional NF-LDH nanosheets, (Ni,Mo)S2//NF-LDH 300, using an e-beam evaporator. Physical deposition technique. The designed (Ni, Mo)S2//NF-LDH 300 catalyst proves a superior catalytic activity and stability for seawater oxidation under alkaline electrolyte. The deposited transition sulfide layer induces an improved charge transfer as well as reaction kinetics for the (Ni, Mo)S2//NF-LDH 300. Further, adsorptions of chloride anions at the surface is substantially suppressed due to the deposited transition metal sulfide effectively preventing chloride corrosions. The (Ni, Mo)S2//NF-

LDH 300 demonstrates practical level of performance for alkaline seawater oxidation, shedding lights on our catalyst design strategy for direct seawater electrolysis.
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C3 Konkuk University; Korea Institute of Industrial Technology (KITECH); Sungkyunkwan University (SKKU); Sungkyunkwan University (SKKU); Korea Institute of Industrial Technology (KITECH); Sungkyunkwan University (SKKU); Sungkyunkwan University (SKKU); Sungkyunkwan University (SKKU); Sungkyunkwan University (SKKU)
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U2 54
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PA RADARWEG 29, 1043 NX AMSTERDAM, NETHERLANDS
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J9 APPL SURF SCI
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PT J
AU Agarwalla, US
AF Agarwalla, Uday Sankar
TI Catalytic oxyfunctionalization of saturated hydrocarbons by non-heme
   oxo-bridged diiron(III) complexes: role of acetic acid on oxidation
   reaction
SO TRANSITION METAL CHEMISTRY
LA English
DT Article
ID ALKANE FUNCTIONALIZATION; BIOMIMETIC OXIDATION; DIOXYGEN ACTIVATION;
   CRYSTAL-STRUCTURE; ACTIVE-SITE; IRON; LIGAND; MONONUCLEAR; CENTERS
AB Oxo-bridged diiron(III) complexes [Fe2O(L-1)(2)(H2O)(2)](ClO4)(4)(1) and [Fe2O(L-2)(2)(H2O)(2)](ClO4)(4)(2), where L(1)and L(2)are tetradentateN-donorN,N '-bis(2-pyridylmethyl)-1,2-cyclohexanediamine andN,N '-bis(2-pyridylmethyl)ethane-1,2-diamine respectively, have been isolated as synthetic models of non-heme iron oxygenases and characterized by physicochemical and spectroscopic methods. Both the complexes have been studied as catalysts for the oxyfunctionalization of saturated hydrocarbons using green hydrogen peroxide (H2O2) as oxidant under mild conditions. The selectivity (A/K) and

regioselectivity (3 degrees/2 degrees) in oxidative C-H functionalization of alkanes suggests the involvement of metal-based intermediate in the oxygenation reaction. The catalytic efficiency is found to be strongly dependent on the presence of acetic acid. Remarkable increase in conversion and selectivity favoring the formation of alcohols in the oxidation of cyclohexane and cyclooctane and exclusive hydroxylation of adamantane with drastic enhancement of regioselectivity has been achieved by the addition of acetic acid in the presence of H2O2.
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NR 41
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PT J
AU Birat, JP
AF Birat, Jean-Pierre
TI Net-Zero transition in the steel sector: beyond the simple emphasis on
   hydrogen, did we miss anything?☆
SO MATERIAUX & TECHNIQUES
LA English
DT Article
DE Net-Zero transition; steel; hydrogen; epistemic shock; addiction to
   fossil fuel; addiction to rare metals
AB There is an explosion of publications and of various announcements regarding the use of hydrogen in the steel sector as a way to arrive at Net-Zero steel production - particularly in Europe. Most of them describe process technologies on the one hand and commitment to implement them quickly in the steel sector in the form of roadmaps and agendas, on the other hand. The most popular process technology is H-2 Direct Reduction (H-2-DR) in a shaft furnace. Available technical literature, as abundant as it may be, is still fairly incomplete in making the pathway to Net-Zero explicit and credible. This paper tries to identify important issues which are not openly discussed nor analyzed in the literature, yet. Process-wise, open questions in technical papers are: (1) what are the best-fitted iron ores for H-2-DR, (2) what downstream furnace, after H-2-DR, can accommodate various raw materials, (3) how and how much carbon ought to be fed into the process, (4) what is the best design for the shaft, (5) should it be designed for both natural gas and H-2 operations, or simply for H-2, (6) how should the progress of R&D be organized from pilot plants up to full-scale FOAK plants and then to a broad dissemination of the technology, (7) what kind of refractories should be implemented in the various new reactors being imagined, etc. Cost issues are also widely open, as a function of green hydrogen, green electricity and carbon prices. How is hydrogen fed to the steel mill and what exactly is the connection to renewable electricity? Is the infrastructure that this calls for planned in sufficiently details? What is still missing is a full value chain picture and planning from mining to steel mills, including electricity and hydrogen grids. Two years after our last review paper on hydrogen, the overall picture has changed significantly. Countries beyond Europe, including China, have come up with roadmaps and plans to become net-zero by 2050, plus or minus 10 years. However, they do not rely as much on H-2 alone, as Europe seems to be doing. What is most likely is that several process routes will develop in parallel, including, beyond H-2-DR, Blast Furnace ironmaking and NG Direct Reduction with CCS, electrolysis of iron ore and scrap-based production in EAFs fed with green electricity, which would single-handedly support the largest part of production by the end of the century; as more and more scrap is to become available and be actually used. There is also a question for historians. The

influence of Climate Change on Steel has been discussed continuously for more than 30 years. Why has the commitment to practical answers only solidified recently?
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AU Villemur, J
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   Gordo, Elena
TI Fabrication and Coating of Porous Ti6Al4V Structures for Application in
   PEM Fuel Cell and Electrolyzer Technologies
SO MATERIALS
LA English
DT Article
DE Ti64; porous; titanium nitride; corrosion; interfacial contact
   resistance; PEM
ID TITANIUM BIPOLAR PLATES; TIN-COATED TITANIUM; STAINLESS-STEEL;
   PERFORMANCE; PARAMETERS; HYDROGEN
AB The production of green hydrogen through proton exchange membrane water electrolysis (PEMWE) is a promising technology for industry decarbonization, outperforming alkaline water electrolysis (AWE). However, PEMWE requires significant investment, which can be mitigated through material and design advancements. Components like bipolar porous plates (BPPs) and porous transport films (PTFs) contribute substantially to costs and performance. BPPs necessitate properties like corrosion resistance, electrical conductivity, and mechanical integrity. Titanium, commonly used for BPPs, forms a passivating oxide layer, reducing efficiency. Effective coatings are crucial to address this issue, requiring conductivity and improved corrosion resistance. In this study, porous Ti64 structures were fabricated via powder technology, treating them with thermochemical nitriding. The resulting structures with controlled porosity exhibited enhanced corrosion resistance and electrical conductivity. Analysis through scanning electron microscopy (FE-SEM), X-ray diffraction (XRD), grazing incidence XRD and X-ray photoelectron spectroscopy (XPS) confirmed the effectiveness of the coating, meeting performance requirements for BPPs.
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TI Nano-composites of NiFe-LDH/VSe 2 heterostructures for effective water
splitting electrocatalyst
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LA English
DT Article
DE Oxygen Evolution Reaction; Hydrogen Evolution Reaction;
Electrocatalysts; Overpotential; Current density; Tafel slope
ID HIGHLY EFFICIENT; BIFUNCTIONAL ELECTROCATALYSTS; VSE2 NANOSHEETS; LDH;
EVOLUTION; ALKALINE; HYDROXIDE; OXIDATION; KINETICS; OER
AB In the realm of sustainable and environmentally friendly "green-hydrogen"fuel demand, water electrolysis stands as a pathway of hope for the extraction of renewable hydrogen. However, the durability and efficiency of electrocatalysts have been a major challenge in this process, owing to factors like the high costs of noble catalysts (Pt, Ir, Ru, etc.) and their limited stability. Layered Nickel -iron double hydroxides (NiFeLDH) have shown potential as low-cost and efficient electrocatalysts because of their suitable electronic configuration and distinguished orbital confinement. However, their durability In the realm of sustainable and environmentally friendly "green-hydrogen"fuel demand, water electrolysis stands as a pathway of hope for the extraction of renewable hydrogen. However, the durability and efficiency of electrocatalysts have been a major challenge in this process, owing to factors like the high costs of noble catalysts (Pt, Ir, Ru, etc.) and their limited stability. Layered Nickel -iron double hydroxides (NiFe-LDH) have shown potential as lowcost and efficient electrocatalysts because of their suitable electronic configuration and distinguished orbital confinement. However, their performance and durability in corrosive alkaline water at high current density remain limited. In this regard, one can make the nano -composites of this NiFe-LDH with high electronic conductivity materials and layered structures like VSe 2 . With this motivation, this work presents a novel electrocatalyst, NiFe-LDH, supported with VSe 2 nanosheets (VSe 2 /NiFe - LDH), designed to address these challenges and enhance water splitting efficiency. Experimental results demonstrate that the heterostructure synergistically reduces charge transfer resistance, increases exposure of active sites, and enhances oxygen gas evolution ability. Consequently, the VSe 2 /NiFe - LDH electrocatalyst demonstrated superior sustainability, maintaining an elevated current density (500 mA cm -2) for over 50 h of continuous electrolysis without noticeable degradation. This research opens up new possibilities and shows that nano-compositing can be a good option for achieving efficient and durable electrocatalysts in alkaline water splitting, thereby contributing to sustainable hydrogen production.
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AU Afshan, G
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AF Afshan, Gul
Karim, Suhana
Kharwar, Yashwant Pratap
Aziz, Tarik
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TI Green H₂ Generation from Seawater Deploying a Bifunctional
Hetero-Interfaced CoS₂-CoFe-Layered Double Hydroxide in an
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DE bifunctional electrocatalyst; functional electrolyzer; green hydrogen;
heterostructured materials; seawater splitting

ID HIGHLY EFFICIENT; EVOLUTION; OXYGEN; CATALYSTS; ELECTROCATALYSTS;
CHLORINE; LDH

AB This work illustrates the practicality and economic benefits of employing a hetero-interfaced electrocatalyst (CoS2@CoFe-LDH), containing cobalt sulphide and iron-cobalt double-layer hydroxide for large-scale hydrogen generation. Here, the rational synthesis and detailed characterization of the CoS2@CoFe-LDH material to unravel its unique heterostructure are essayed. The CoS2@CoFe-LDH operates as a bifunctional electrocatalyst to trigger both the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER) in alkaline seawater (pH 14.0) while showcasing low overpotential requirement for HER (311 mV) and OER (450 mV) at 100 mA cm(-)(2) current density. The identical CoS2@CoFe-LDH on either electrode in an H-cell setup results in simultaneous H-2 and O-2 production from seawater with a approximate to 98% Faradaic efficiency with an applied potential of 1.96V@100 mA cm(-)(2). Next, this CoS2@CoFe-LDH catalyst is deployed on both sides of a membrane electrode assembly in a one-stack electrolyzer, which retains the intrinsic bifunctional reactivity of the catalyst to generate H-2 and O-2 in tandem from alkaline seawater with an impeccable energy efficiency (50 kWh kg(-1)-of-H-2). This electrolyzer assembly can be directly linked with a Si-solar cell to produce truly green hydrogen with a solar-to-hydrogen generation efficiency of 15.88%, highlighting the potential of this converting seawater to hydrogen under solar irradiation.

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FU Indian Institute of Technology Bombay (IITB); DST
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U1 28
U2 31
PU WILEY-V C H VERLAG GMBH
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PA POSTFACH 101161, 69451 WEINHEIM, GERMANY

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JI Small
PD FEB
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WE Science Citation Index Expanded (SCI-EXPANDED)
SC Chemistry; Science & Technology - Other Topics; Materials Science;
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PT J
AU Park, J
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AF Park, Jinkyu
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TI Recent advances in amorphous electrocatalysts for oxygen evolution
reaction
SO FRONTIERS IN CHEMISTRY
LA English
DT Review
DE amorphous electrocatalysts; oxygen evolution reaction; water splitting;
electrolysis; amorphous material
ID WATER OXIDATION; COBALT; OXIDE; IRON; DEPOSITION; FILMS; FE; NI; CO
AB Oxygen evolution reaction (OER) has attracted great attention as an important half-reaction in the electrochemical splitting of water for green hydrogen production. However, the inadequacy of highly efficient and stable electrocatalysts has impeded the development of this technology. Amorphous materials with long-range disordered structures have exhibited superior electrocatalytic performance compared to their crystalline counterparts due to more active sites and higher structural flexibility. This review summarizes the preparation methods of amorphous materials involving oxides, hydroxide, phosphides, sulfides, and their composites, and introduces the recent progress of amorphous OER electrocatalysts in acidic and alkaline media. Finally, the existing challenges and future perspectives for amorphous electrocatalysts for OER are discussed. Therefore, we believe that this review will guide designing amorphous OER electrocatalysts with high performance for future energy applications.
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AF Chen, Shan
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Bu, Junfei
Yue, Qin
TI Reevesite with Ordered Intralayer Atomic Arrangement as an Optimized Nickel-Iron Oxygen Evolution Electrocatalyst
SO CHEMELECTROCHEM
LA English
DT Article
DE oxygen evolution reaction; reevesite; ordered intralayer; superstructures; layered double hydroxides
AB Green hydrogen production through electrocatalytic water splitting relies on inexpensive and highly efficient electrocatalysts. Ni-Fe layered double hydroxide (LDH) is considered as one of the most promising non-precious metal electrocatalysts for the oxygen evolution reaction (OER). Previous research identified the Fe octahedral site surrounded by [NiO6] octahedrons as a highly active and stable site for OER; however, an optimized electrocatalyst material in such a structure is still missing. Herein, reevesite hierarchical nanostructure supported on Ni foam (Reevesite/NF) is constructed to enable the optimal structure toward the OER. Such Reevesite/NF electrocatalysts with a unique ordered intralayer structure are capable of achieving a high current density (300 mA cm(-2)) at a low overpotential of only 283 mV, while the durability of the Reevesite/NF is equally outstanding, offering a promising non-precious metal OER catalyst toward high-efficiency water splitting.
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U2 34
PU WILEY-V C H VERLAG GMBH
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JI ChemElectroChem
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WC Electrochemistry
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SC Electrochemistry
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TI Effect of Electrodeposited Nickel Coatings on the High Temperature
   Degradation and Electrical Performance of Steel SOEC Interconnects
SO HIGH TEMPERATURE CORROSION OF MATERIALS
LA English
DT Article
DE Solid oxide electrolyzer cell; Green hydrogen; Coating;
   Electrodeposition; Oxidation; ASR
ID CHROMIUM VAPORIZATION; STAINLESS-STEEL; OXIDE; ALLOYS
AB The performance of solid oxide electrolyzer cells (SOEC) can be improved through the development of coatings applied to the surface of ferritic steel interconnects in view of mitigating chromium evaporation and reducing the growth rate of low conductive oxides in oxidizing environments. This work investigated the oxidation and area specific resistance (ASR) of two electrodeposited nickel coatings on preoxidized and non-preoxidized AISI 441 ferritic stainless steel substrates. The nickel coating effectively restricted the outward diffusion of chromium after 100 h of exposure at 700 degrees C in air but led to nickel/iron interdiffusion between the substrate and coating forming an iron-nickel-rich spinel on the surface, with NiO underneath and Cr2O3 at the coating-substrate interface and at the coating grain boundaries. The application of a LSM ((La0.80Sr0.20)0.95MnO3-x) coating on top of the Ni electrodeposited coatings resulted in the same type of oxides but the oxidation kinetics were slower. Interdiffusion continued with the exposure at 700 degrees C for 2400 h resulting in the growth of a thick iron-rich oxide layer on top of Cr2O3, steadily raising the interconnect ASR to 25 m Omega cm2. The addition of a preoxidation step before the electrodeposit of nickel helped to limit iron-nickel interdiffusion, leading to the formation of a thicker NiO layer on a Cr2O3 layer between substrate and coating. While the ASR was higher than without preoxidation at the beginning of the test, it stabilized at about 33 m Omega cm2 after 1750 h. Despite displaying a higher electrical resistance, the coatings effectively limited the outward chromium diffusion throughout exposure compared to the bare substrate.
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NR 27
TC 0
Z9 0
U1 7
U2 7
PU SPRINGER
PI NEW YORK
PA ONE NEW YORK PLAZA, SUITE 4600, NEW YORK, NY, UNITED STATES
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J9 HIGH TEMP CORR MATER
JI High Temp. Corr. Mater.
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WC Metallurgy & Metallurgical Engineering
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PT J
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BinSabt, M
Ahmed, AM
Mohamed, F
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BinSabt, Mohammad
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Mohamed, Fatma
TI Recycling Rusty Iron with Natural Zeolite Heulandite to Create a Unique Nanocatalyst for Green Hydrogen Production
SO NANOMATERIALS
LA English
DT Article
DE rusted iron; Fe2O3; zeolite nanocomposite; water splitting; hydrogen production; photocatalyst
ID PHOTOCATALYTIC ACTIVITY; THIN-FILMS; AQUEOUS-SOLUTION; METHYL-ORANGE; ALPHA-FE2O3; DEGRADATION; ZNO; DYE; ADSORBENTS; PARTICLES
AB Corrosion-induced iron rust causes severe danger, pollution, and economic problems. In this work, nanopowders of Fe_2O_3 and Fe_2O_3/zeolite are synthesized for the first time using rusted iron waste and natural zeolite heulandite by chemical precipitation. The chemical composition, nanomorphologies, structural parameters, and optical behaviors are investigated using different techniques. The Fe_2O_3/zeolite nanocomposite showed smaller sizes and greater light absorption capability in visible light than Fe_2O_3 nanopowder. The XRD pattern shows crystalline hematite (alpha-Fe_2O_3) with a rhombohedral structure. The crystallite sizes for the plane (104) of the Fe_2O_3 and Fe_2O_3/zeolite are 64.84 and 56.53 nm, respectively. The Fe_2O_3 and Fe_2O_3/zeolite have indirect bandgap values of 1.87 and

1.91 eV and direct bandgap values of 2.04 and 2.07 eV, respectively. Fe2O3 and Fe2O3/zeolite nanophotocatalysts are used for solar photoelectrochemical (PEC) hydrogen production. The Fe2O3/zeolite exhibits a PEC catalytic hydrogen production rate of 154.45 mmol/g.h @ 1 V in 0.9 M KOH solution, which is the highest value yet for Fe2O3-based photocatalysts. The photocurrent density of Fe2O3/zeolite is almost two times that of Fe2O3 catalyst, and the IPCE (incident photon-to-current conversion efficiency) reached ~27.34%@307 nm and 1 V. The electrochemical surface area (ECSA) values for Fe2O3 and Fe2O3/zeolite photocatalysts were 7.414 and 21.236 m(2)/g, respectively. The rate of hydrogen production for Fe2O3/zeolite was 154.44 mmol h(-1)/g. This nanophotocatalyst has a very low PEC corrosion rate of 7.6 pm/year; it can retain ~97% of its initial performance. Therefore, the present research can be applied industrially as a cost-effective technique to address two issues at once by producing solar hydrogen fuel and recycling the rusted iron wires.
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OI Ahmed, Ashour/0000-0002-1971-341X; BinSabt, Mohammad/0000-0003-4057-233X
NR 0
TC 9
Z9 9
U1 4
U2 51
PU MDPI
PI BASEL
PA MDPI AG, Grosspeteranlage 5, CH-4052 BASEL, SWITZERLAND
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JI Nanomaterials
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Chicardi, E

Sepúlveda, R
AF Damizia, M.
Lloreda-Jurado, P. J.
De Filippis, P.
de Caprariis, B.
Chicardi, E.
Sepulveda, R.
TI Green hydrogen production using doped Fe2O3 foams
SO INTERNATIONAL JOURNAL OF HYDROGEN ENERGY
LA English
DT Article
DE Pure hydrogen; Chemical looping; PEM fuel cell; Fe2O3 foams; Freeze-casting
ID OXYGEN CARRIERS; IRON-OXIDE; GAS; EVOLUTION; ETHANOL; CATALYST; STORAGE; ENERGY
AB Hydrogen is the ideal energy vector to reduce our fossil-fuels dependency and diminish the climate change consequence. However, current production is still methane based. It is possible to produce hydrogen using bioethanol from the alcoholic fermentation of organic waste by chemical looping processes, but unfortunately current redox systems generate hydrogen with significant traces of CO. In the case of proton exchange membrane fuel cells (PEMFC), hydrogen must be highly purified to produce electricity. Here, high porosity inter-connected Fe2O3 foams doped with 2 wt% Al2O3 were manufactured by the freeze-casting method, obtaining around 5.1 mmol H2$g?1 sample of highly pure hydrogen (<10 ppm of CO) consuming only 3.42 mmol of ethanol on each redox cycles, with no deactivation. This result shows the possibility of using an abundant and inexpensive raw material as the iron oxide to scale-up the direct pure H2 production and facilitates its use in the automotive sector.
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RI Lloreda-Jurado, Pedro Javier/AAP-3049-2021; De+Filippis, Paolo/AAE-2253-2022; Sepulveda Ferrer, Ranier Enrique/S-6622-2017
OI Lloreda Jurado, Pedro Javier/0000-0002-9139-9605; Sepulveda Ferrer, Ranier Enrique/0000-0002-7195-8131; Damizia, Martina/0000-0002-6953-8971; de Caprariis, Benedetta/0000-0002-4331-9869; De Filippis, Paolo/0000-0001-7107-3790
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NR 53
TC 7
Z9 7
U1 4
U2 10
PU PERGAMON-ELSEVIER SCIENCE LTD
PI OXFORD
PA THE BOULEVARD, LANGFORD LANE, KIDLINGTON, OXFORD OX5 1GB, ENGLAND
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WC Chemistry, Physical; Electrochemistry; Energy & Fuels
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AU Yousaf, M
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AF Yousaf, Maryam
   Ahmad, Muhammad
   Batool, Aisha
   Zhao, Zhi-Ping
TI Highly-stable, bifunctional, binder-free & stand-alone photoelectrode
   (Fe_xNi_{1-x}O@a-CC) for natural waters splitting into
   hydrogen
SO INTERNATIONAL JOURNAL OF HYDROGEN ENERGY
LA English
DT Article
DE Iron doped nickel oxide; Oxygen evolution reaction; Hydrogen evolution
   reaction; Carbon cloth; Photoelectrochemical water splitting
ID OXYGEN-EVOLUTION; EFFICIENT; ELECTROCATALYSTS; OXIDE; NANOSHEETS;
   CATALYST; CARBON
AB Photoelectrochemical (PEC) water splitting is a promising approach to boost green
hydrogen production. Herein, we prepared novel binder-free photoelectrode by direct
growth of iron doped nickel oxide catalyst over activated carbon cloth (FexNi1-xO@a-CC)
having band gap energy of 2.2 eV for overall water splitting. FexNi1-xO@a-CC
photoelectrode had shown remarkable lower potential of only 1.36 V for oxygen evolution
reaction (OER) to reach 10 mA cm(-2) current density using very low photonic intensity of
8.36 x 10(-4) E/L.s. For the first time, we also reported electrical efficiency required
for PEC water splitting for 1 m(3) of water that is equal to 0.09 kWh/m(3). FexNi1-xO@a-
CC photoelectrode also exhibits low potentials of 1.44 V (OER) and -0.210 V (HER) at 10
mA cm(-2) to split sea water. Our results confirmed that designing FexNi1-xO@a-CC
photoelectrode would be an innovative step to widen green energy conversion applications
using natural waters (both sea and fresh water). (C) 2022 Hydrogen Energy Publications
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Z9 12
U1 3
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PI OXFORD
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   Cuenya, BR
AF Davis, Earl Matthew
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   Cuenya, Beatriz Roldan
TI Facet Dependence of the Oxygen Evolution Reaction on
   Co₃O₄, CoFe₂O₄, and
   Fe₃O₄ Epitaxial Film Electrocatalysts
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DT Article
ID THIN-FILMS; COBALT OXIDE; GAMMA-FEOOH; OXYHYDROXIDE; OXIDATION; GROWTH;
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AB The main obstacle for the electrocatalytic production of "green hydrogen" is finding suitable electrocatalysts which operate highly efficiently over extended periods of time. The topic of this study is the oxygen evolution reaction (OER), one of the half-reactions of water splitting. It is complex and has intricate kinetics, which impairs the reaction efficiency. Transition metal oxides have shown potential as electrocatalysts for this reaction, but much remains unknown about the atomic scale processes. We have investigated structure-composition-reactivity correlations for Co3O4, CoFe2O4, and Fe3O4 epitaxial thin-film electrocatalysts exposing either the (001) or (111) surface facets. We found that for Co3O4, the (001) facet is more reactive, while for the other oxides, the (111) facet is more active. A Tafel-like evaluation reveals systematically smaller "Tafel" slopes for the (001) facets. Furthermore, the slopes are smaller for the iron-containing films. Additionally, we found that the oxyhydroxide skin layer which forms under OER reaction conditions is thicker on the cobalt oxides than on the other oxides, which we attribute to either a different density of surface defects or to iron hindering the growth of the skin layers. All studied skin layers were thinner than 1 nm.
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TI Effect of the interfacial electronic coupling of nickel-iron sulfide nanosheets with layer Ti3C2 MXenes as efficient bifunctional electrocatalysts for anion-exchange membrane water electrolysis
SO APPLIED CATALYSIS B-ENVIRONMENT AND ENERGY
LA English
DT Article
DE NiFeS@Ti 3 C 2 MXene catalysts; Interfacial coupling; Gas diffusion electrode; AEMWE
ID MOS2 ULTRATHIN NANOSHEETS; TOTAL-ENERGY CALCULATIONS; HYDROGEN EVOLUTION; NIFE-LDH; SULFUR; DEFECT; OXIDE; FOAM; HETEROSTRUCTURES; NANOHYBRID
AB In this study, nickel-iron sulfide (NiFeS) nanosheets were immobilized on Ti3C2 MXene-decorated nickel foam (Ti3C2 MXene/NF) by hydrothermal reaction (NiFeS@Ti3C2 MXene/NF). The morphology of NiFeS and in-teractions with Ti3C2 MXene resulted in electronic coupling that optimized the adsorption energies of water, protons, and oxygen atom for the HER (180 mV@20 mA cm-2) and OER (290 mV@20 mA cm-2). The NiFeS@Ti3C2 MXene/NF catalyst showed good water splitting performance in an alkaline membrane water electrolyzer, yielding a current density (j) of 401 mA cm-2 at 1.85 V with 67.65 % cell efficiency, performance comparable to Pt/C||RuO2 cells. From a commercial point of view, our electrolyzers are the best because of their low loading of catalysts (ca. 1.25 mg cm-2) and low operating temperatures (50 degrees C), resulting in low capital and operating costs. Our findings will aid the development of commercial green hydrogen production and offers an alternative to PEMWE.
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TC 55
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TI Bimetallic Fe/Ni-BTC MOF decorated MXene hybrid for improved oxidation of water
SO DIAMOND AND RELATED MATERIALS
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DT Article
DE MXene; MOF; Composites; Electrocatalytic OER; Iron/nickel BTC
ID METAL-ORGANIC FRAMEWORKS; OXYGEN-EVOLUTION; HYDROGEN-PRODUCTION; NICKEL FOAM; THIN-FILMS; ELECTROCATALYSTS; EFFICIENT; NANOSHEETS; CATALYSTS
AB Electrochemical production of green hydrogen via water-splitting is an emerging technology to generate a substitute source of energy. However, due to the slow kinetics of oxygen evolution reaction (OER), high cost, lesser availability and easy oxidation of noble metal-based electrocatalysts led the explorers to find an efficient and low-cost electrocatalysts. In the current communication, we have developed a synthesis strategy for the preparation of hybrid electrocatalyst composed of bimetallic (iron, nickel) based metal organic framework (FeNiBTC MOF) and MXene (Ti3C2Tx) via solvothermal reaction. Thanks to the ultrathin heterostructure with high electrical conductivity of MXene, with abundant active sites of FeNiBTC MOF, the as-prepared hybrid electrocatalyst FeNiBTC@MXene, leads the high efficiency OER in an alkaline environment. FeNiBTC MOF was impeccably decorated on the surfaces of MXene nanosheets with different FeNiBTC to MXene ratios and was characterized via pXRD, FESEM/EDS, XPS and BET. The optimized hybrid structured catalyst (FeNiBTC@Mx-3) revealed the best performance for OER with a low overpotential of 210 mV vs. RHE at a current density of 10 mA/cm2 and a Tafel plot value of 38.4 mV/dec and stable up to 1000th CV cycles.
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NR 50
TC 7
Z9 8
U1 24
U2 30
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PT J
AU Trinca, A
   Vilardi, G
   Verdone, N
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TI Towards carbon neutrality: The ammonia approach to green steel
SO ENERGY CONVERSION AND MANAGEMENT
LA English
DT Article
DE Hydrogen carrier; CO 2 emissions; Clean energy; Ammonia cracking; DRI;
   Decarbonization
ID MIDREX SHAFT FURNACE; DIRECT REDUCTION; HYDROGEN; SIMULATION; GAS;
   INJECTION
AB The steel sector accounts for 7 % of global greenhouse gas emissions, making its decarbonization a critical challenge. The use of green hydrogen in the direct reduction process enables a significant reduction in CO2 emissions, reaching levels as low as 29 kgCO2/tSTEEL. However, one of the major challenges lies in the temporal and geographical mismatch between steel and hydrogen production. This issue is particularly pressing for the survival of steel supply chains in regions where green hydrogen production costs are expected to remain high. In such cases, transporting hydrogen from areas with more competitive production costs becomes essential. The transportation costs associated with hydrogen present an additional hurdle, driving the search for alternative solutions. Among these, ammonia has emerged as a viable option as a hydrogen carrier. This study uses an Aspen Plus process simulation model to analyze the complete steel production cycle, including ammonia cracking and the production of steel from direct reduced iron. It evaluates the impact of ammonia usage on the process and its overall efficiency. Two main scenarios are analyzed: direct injection of ammonia into the reduction furnace and external ammonia cracking. Production costs are calculated based on the transportation distances of hydrogen and ammonia. In a scenario where hydrogen is produced on-site, with an energy cost of 50 $/MWh and a hydrogen production cost of 5 $/kg, the final steel production cost amounts to 816 $/tSTEEL. However, these costs increase significantly with transportation distances. Using ammonia in these scenarios, despite its higher energy consumption, offers economic savings of up to 11 % for transportation distances of 5000 km. Looking ahead, with hydrogen production costs expected to drop to 2 $/kg, these savings could rise to 20 %.
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NR 89
TC 0
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PT J
AU Röper, K
Kunz, N
Gast, L
AF Roeper, Katja
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TI Renewable hydrogen in industrial production: A bibliometric analysis of
current and future applications
SO INTERNATIONAL JOURNAL OF HYDROGEN ENERGY
LA English
DT Article
DE Renewable hydrogen; Green hydrogen; Industrial production; Hydrogen gap;
Industrial ecology; GHG mitigation
ID FUEL; AMMONIA; CHAIN
AB Renewable hydrogen is widely considered a key technology to achieve net zero emissions in industrial production processes. This paper presents a structured bibliometric analysis, examining current and future applications of hydrogen as feedstock and fuel across industries, quantifying demand for different industrial processes, and identifying greenhouse gas emissions reduction potential against the context of current fossil-based practices. The findings highlight significant focus on hydrogen as feedstock for steel, ammonia, and methanol production and its use in high-to medium-temperature processes, and a general emphasis on techno-economic and technological evaluations of hydrogen applications across industries. However, gaps exist in research on hydrogen use in sectors like cement, glass, waste, pulp and paper, ceramics, and aluminum. Additionally, the analysis reveals limited attention in the identified literature to hydrogen supply chain efficiencies, including conversion and transportation losses, as well as geopolitical and raw material challenges. The analysis underscores the need for comprehensive and transparent data to align hydrogen use with decarbonization goals, optimize resource allocation, and inform policy and investment decisions for strategic deployment of renewable hydrogen.
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Grzebielec, Andrzej
Shuhayeu, Pavel
TI Overview of the e-Fuels Market, Projects, and the State of the Art of Production Facilities
SO ENERGIES
LA English
DT Review
DE e-fuel; Fischer-Tropsch; e-methanol; hydrogen
ID FISCHER-TROPSCH SYNTHESIS; TECHNOLOGY; CO2; TRENDS

AB E-fuels, or synthetic fuels produced from green hydrogen and captured CO2, are a promising solution for achieving climate neutrality by replacing fossil fuels in transportation and industry. They help reduce greenhouse gas emissions and efficiently utilize renewable energy surpluses. This study aims to assess the current state and future potential of e-fuel production technologies, focusing on their scalability and market integration. A comprehensive literature review and market trend analysis, including modeling based on historical data and growth forecasts, were used to estimate market penetration. Results indicate that e-fuels could reach a 10% market share within the next 5 years, potentially reaching 30% in 20 years, particularly in aviation, maritime transport, and the steel industry. Ongoing projects expected to be completed this decade may cover about 20% of the global liquid fuel demand for transportation. However, challenges such as high costs, scalability, and recent project terminations due to funding shortages highlight the need for substantial investment, regulatory support, and innovation. Global collaboration and policy alignment are essential for the successful development and integration of e-fuels as a critical pathway to decarbonization.
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FU Polish National Center for Research and Development within the LIDER XIV program; Warsaw University of Technology within the Excellence Initiative: Research University [CPR-IDUB/55/Z01/2024]; [LIDER14/0086/2023]
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J9 ENERGIES
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IS 3
AR 552
DI 10.3390/en18030552
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WC Energy & Fuels
WE Science Citation Index Expanded (SCI-EXPANDED)
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TI Engineering Multilevel Collaborative Catalytic Interfaces with
   Multifunctional Iron Sites Enabling High-Performance Real Seawater
   Splitting
SO ACS NANO
LA English
DT Article
DE seawater splitting; electrocatalyst; bifunctional water splitting;
   non-noble metal; porous material
ID HYDROGEN EVOLUTION; ELECTROCATALYSTS; PHOSPHIDES; ARRAYS
AB Given the abundant reserves of seawater and the scarcity of freshwater, real seawater electrolysis is a more economically appealing technology for hydrogen production relative to orthodox freshwater electrolysis. However, this technology is greatly precluded by the undesirable chlorine oxidation reaction and severe chloride corrosion at the anode, further restricting the catalytic efficiency of overall seawater splitting. Herein, a feasible strategy by engineering multifunctional collaborative catalytic interfaces is reported to develop porous metal nitride/phosphide heterostructure arrays anchoring on conductive Ni2P surfaces with affluent iron sites. Collaborative catalytic interfaces among iron phosphide, bimetallic nitride, and porous Ni2P supports play a positive role in improving water adsorption/dissociation and hydrogen adsorption behaviors of active Fe sites evidenced by theoretical calculations for hydrogen evolution reactions, and enhancing oxygenated species adsorption and nitrate-rich passivating layers resistant to chloride corrosion for oxygen evolution reaction, thus cooperatively propelling high-

performance bifunctional seawater splitting. The resultant material Fe2P/Ni1.5Co1.5N/Ni2P performs excellently as a self-standing bifunctional catalyst for alkaline seawater splitting. It requires extremely low cell voltages of 1.624 and 1.742 V to afford current densities of 100 and 500 mA/cm2 in 1 M KOH seawater electrolytes, respectively, along with superior long-term stability, outperforming nearly all the ever-reported non-noble bifunctional electrocatalysts and benchmark Pt/IrO2 coupled electrodes for freshwater/seawater electrolysis. This work presents an effective strategy for greatly enhancing the catalytic efficiency of non-noble catalysts toward green hydrogen production from seawater electrolysis.
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FU National Science Foundation of China [52172197]; Youth 1000 Talent Program of China, Science and Technology Innovation Platform [2019RS1032]; Major Projects "Takes the Lead" of Natural Science Foundation; Undergraduate Scientific Research Innovation Project of Hunan Province [2021JC0008, 2022213]; Hunan Normal University [22CSZ011, 22CSZ010, 22CSY156]
FX This project was supported by the funds from National Science Foundation of China (No. 52172197) , the Youth 1000 Talent Program of China, Science and Technology Innovation Platform (No. 2019RS1032) , Major Projects "Takes the Lead" of Natural Science Foundation and Undergraduate Scientific Research Innovation Project of Hunan Province (No.2021JC0008 and 2022213) , and Hunan Normal University (No. 22CSZ011, No. 22CSZ010 and No. 22CSY156).
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PU AMER CHEMICAL SOC
PI WASHINGTON
PA 1155 16TH ST, NW, WASHINGTON, DC 20036 USA
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J9 ACS NANO
JI ACS Nano
PD JAN 3
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BP 1681
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WC Chemistry, Multidisciplinary; Chemistry, Physical; Nanoscience &
   Nanotechnology; Materials Science, Multidisciplinary
WE Science Citation Index Expanded (SCI-EXPANDED)
SC Chemistry; Science & Technology - Other Topics; Materials Science
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PT J
AU de Araujo, DM
   Segundo, IDB
   Cardozo, JC
   Santos, JEL
   Nascimento, JHO

Gondim, AD
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   Martínez-Huitle, CA
AF de Araujo, Danyelle M.
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   Cardozo, Jussara C.
   Santos, Jose Eudes L.
   Nascimento, Jose H. O.
   Gondim, Amanda D.
   dos Santos, Elisama V.
   Martinez-Huitle, Carlos A.
TI Produced water electrolysis with simultaneous green H2 generation: From
   wastewater to the future of the energetic industry
SO FUEL
LA English
DT Article
DE Circular economy; Green hydrogen; Produced water; PEM cell;
   Integrated-hybrid approach; Diamond electrode
ID REMOVING PETROLEUM-HYDROCARBONS; CATHODIC HYDROGEN-PRODUCTION;
   ELECTROCHEMICAL TECHNOLOGY; SIMULTANEOUS OXIDATION; METHYL RED; DOPED
   SNO2; 2,4-DICHLOROPHENOXYACETATE; BDD
AB The dual-purpose treatment of effluents with simultaneous green hydrogen (H2) generation represents an optimal synergy, addressing environmental concerns through effective pollution control while harnessing valuable clean energy resources, thereby promoting sustainable and eco-friendly industrial practices. In this way, produced waters (PW) stemming from industrial processes like oil and gas extraction, possess varying chemical compositions, elevated salinity, temperature fluctuations, and diverse contaminant profiles. Recognizing and addressing these characteristics, it is vital for implementing effective and environmentally responsible treatment and final disposal. Thus, a proton-exchange membrane cell (PEM) featuring a boron-doped diamond (BDD) anode (15 cm2) and a 316-Ni-Fe-based stainless steel mesh as the cathode (18.2 cm2), energized by a solar source of energy through a photovoltaic (PV), was used as an integrated-hybrid approch to guarantee the decontamination of the effluent at the anodic compartment, while produces green H2 at the cathodic one, both with a volume of 0.04 L. The electrolysis was performed by applying approximately 7, 13 and 26 mA cm-2 for up to 600 min. The study demonstrates that anodic oxidation achieves almost total mineralization of organics in various tested scenarios. Higher current densities are found to optimize green H2 generation, yielding a theoretical value of 1.27 L of dry H2 per 0.5 L of produced water (PW) treated over 10 h with favorable current efficiency (specifically 18.6 mA cm-2). While the assay duration focused on H2 production linearity, practical application should consider regulatory discharge limits and raw effluent characteristics. Despite membrane fouling, H2 production remained unaffected. Overall, PW treatment and simultaneous green H2 generation emerge as a promising solution, mitigating cost barriers associated with industrial effluents while promoting carbon-neutral energy, cleaner industries, decarbonized transportation, and resilient energy solutions.
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RI CARDOZO, JUSSARA/LZG-0598-2025; Gondim, Amanda/AAI-9806-2021; Barbosa
   Segundo, Inalmar/LOS-4838-2024; nascimento, jose/AAG-7423-2020

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FU Conselho Nacional de Desenvolvimento Cientifico e Tecnologico (CNPq, Brazil) [408110/2022-8, 317075/2023- 3, 315879/2021-1]; Fundacao de Amparo a Pesquisa do Estado de Sao Paulo (Brazil) [FAPESP 2014/50945-4, 2019/13113-4]; CNPq [116925/2022-1, 152760/2022-1, 351605/2022-3, 350643/2023-7]
FX Financial support from Conselho Nacional de Desenvolvimento Cientifico e Tecnologico (CNPq, Brazil) (408110/2022-8, 317075/2023- 3, 315879/2021-1), and from Fundacao de Amparo a Pesquisa do Estado de Sao Paulo (Brazil), FAPESP 2014/50945-4 and 2019/13113-4, are gratefully acknowledged. Araujo, D.M, Barbosa Segundo, I.D., Cardozo, J.C., and Santos, J.E.L acknowledge the postdoctoral fellowships awarded by CNPq (116925/2022-1, 152760/2022-1, 351605/2022-3, 350643/2023-7 respectively) .
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NR 45
TC 4

Z9 4
U1 13
U2 15
PU ELSEVIER SCI LTD
PI London
PA 125 London Wall, London, ENGLAND
SN 0016-2361
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J9 FUEL
JI Fuel
PD OCT 1
PY 2024
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AR 132369
DI 10.1016/j.fuel.2024.132369
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WC Energy & Fuels; Engineering, Chemical
WE Science Citation Index Expanded (SCI-EXPANDED)
SC Energy & Fuels; Engineering
GA XY1N0
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PT J
AU Astesiano, D
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AF Astesiano, Davide
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   Malfa, Enrico
   Wuppermann, Christian
TI Flexible hydrogen heating technologies, with low environmental impact☆
SO MATERIAUX & TECHNIQUES
LA English
DT Review
DE CO2 emission reduction; hydrogen; combustion systems; heating and
   treatment furnaces
AB Several roadmaps worldwide identify the decarbonization as one of the main pathways to transform the steel industry into a climate-neutral sector by 2050. New technologies and processes based on the massive use of renewable electricity, green hydrogen, and their combination, will play a fundamental role in this transformation. Aside this decarbonization pathway, the steel sector suffers from a strong inertia due to its characteristics of being very capital intensive, operating in a highly competitive global market and being characterized by an investment cycle between 20 and 30 years. In such scenario, the Tenova "Hydrogen Ready" combustion technology (which identifies a burner family able to work with any natural gas/hydrogen mixture up to 100% H-2 without hardware modifications) represents a solution able to support the steelmakers through the current energy transition scenario and, at the same time, to ensure their investments for the future. This paper continues a previous work on the Tenova "SmartBurner" technology and shows the application of the "Hydrogen Ready" concept to three additional burner families, covering a wider range of downstream processes: Tenova TRKSX (flameless self-recuperative burner for heat treatment furnaces), Tenova TRGX (regenerative flameless burner for reheating furnaces), and the Tenova THSQ burners (flameless combustion system for batch annealing furnaces, heat treatment furnaces and other special heat treatment application). All these burners show NOx emissions well below the next envisioned limits (80 mg/Nm(3) at 5% of O-2 with furnace at 1250 & DEG;C) with all the NG/H-2 mixtures, as well as with 100% H-2. These results confirm the viability of the "Hydrogen Ready" approach, and the effectiveness of the flameless technology in controlling the NOx formation. The first industrial applications of these concepts are also presented.

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RI Astesiano, Davide/IUN-0030-2023
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U2 1
PU EDP SCIENCES S A
PI LES ULIS CEDEX A
PA 17, AVE DU HOGGAR, PA COURTABOEUF, BP 112, F-91944 LES ULIS CEDEX A, FRANCE
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J9 MATER TECHNIQUE-FR
JI Mater. Tech.
PD JUL 18
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DI 10.1051/mattech/2023018
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WC Materials Science, Multidisciplinary
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SC Materials Science
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PT J
AU Demnitz, M
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   van der Schaaf, J
   de Groot, MT
AF Demnitz, Maximilian
   Lamas, Yuran Martins
   Barros, Rodrigo Lira Garcia
   den Bouter, Anouk de Leeuw
   van der Schaaf, John
   de Groot, Matheus Theodorus
TI Effect of iron addition to the electrolyte on alkaline water
   electrolysis performance
SO ISCIENCE
LA English
DT Article
ID HYDROGEN EVOLUTION; NICKEL; ELECTROCATALYSTS; HYDROXIDES; MEMBRANE;
   CATHODES; CATALYST; BEHAVIOR; FE
AB Improvement of alkaline water electrolysis is a key enabler for quickly scaling up green hydrogen produc-tion. Fe is omnipresent within most industrial alkaline water electrolyzers and its effect on electrolyzer performance needs to be assessed. We conducted three-electrode and flow cell experiments with electro-lyte Fe and Ni electrodes. Three-electrode cell experiments show that Fe ([Fe] = 6-357 mM; ICP-OES) promotes HER and OER by lowering both overpotentials by at least 100 mV at high current densities (T = 35 degrees C-91 degrees C). The overpotential of a zero-gap flow cell was decreased by 200 mV when increasing the Fe concentration ([Fe] = 13-549 mM, T = 21 degrees C-75 degrees C). HER benefits from the formation of Fe dendrite layers (SEM/EDX, XPS), which prevent NiHx formation and increase the overall active area. The OER ben-efits from the formation of mixed Ni/Fe oxyhydroxides leading to better catalytic activity and Tafel slope reduction.
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   experimental work performed by the TU/e DBL students and the help from
   the technicians of the Sustainable Process Engineering group.
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NR 50
TC 18
Z9 18
U1 13
U2 35
PU CELL PRESS
PI CAMBRIDGE
PA 50 HAMPSHIRE ST, FLOOR 5, CAMBRIDGE, MA 02139 USA
EI 2589-0042
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JI iScience
PD JAN 19
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WC Multidisciplinary Sciences
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SC Science & Technology - Other Topics
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ER

PT J
AU Qi, Y
   Zhang, FX
AF Qi, Yu
   Zhang, Fuxiang
TI Recent Advances in Redox-Based Z-Scheme Overall Water Splitting under
   Visible Light Irradiation
SO JOURNAL OF PHYSICAL CHEMISTRY LETTERS
LA English
DT Review
ID DRIVEN Z-SCHEME; PHOTOCATALYTIC Z-SCHEME; HYDROGEN EVOLUTION;
   HETEROGENEOUS PHOTOCATALYSIS; 2-STEP PHOTOEXCITATION; ELECTRON MEDIATOR;
   H-2; O-2; HETEROSTRUCTURE; SYSTEM
AB Photocatalytic overall water splitting (OWS) using suspended particulate photocatalysts to produce green hydrogen has inspired continuous interest due to its low cost for easy large-scale application. The two-step photoexcitation system (Z-scheme) mimicking natural photosynthesis was proposed to efficiently use visible light for realization of efficient conversion of solar irradiation. In this Perspective, we will introduce recent advances in redox-based Z-scheme OWS systems, including iodine-based, iron-based, metal complex-based, and other special ion redox couples. The advantages and challenges of each couple and the factors affecting the Z-scheme OWS efficiency are discussed in detail. Finally, the challenges and feasible solutions for the achievement of highly efficient Z-scheme OWS are then outlined. This Perspective provides guidance on how to construct a Z-scheme OWS system and enhance photocatalytic performance.
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TI Fe species-decorated nickel selenides on Ni foam (FNS/NF) for efficient overall water splitting
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LA English
DT Article
DE Oxygen evolution reaction; Hydrogen evolution reaction; Overall water splitting; Nickel selenide; Iron oxyhydroxide; Metal foam
ID OXYGEN EVOLUTION REACTION; HYDROGEN; ELECTROCATALYSTS; PERFORMANCE; DESIGN
AB For industrial-scale green hydrogen production by water electrolysis, the catalyst used should exhibit the following characteristics: low cost, ease of use, high electrochemical activity, and good stability. In this study, we prepare a Pt replacement catalyst that can be used as an effective catalyst for both the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) as well as exhibits excellent stability. FeOOH-decorated nickel selenide on a Ni foam (FNS/NF), synthesized by decorating FeOOH on a NiSe/NF prepared by reacting an NF with a Se precursor under a hydrothermal condition, exhibited superior electrocatalytic activities in OER and HER. Furthermore, the (FNS/NF-5)||(FNS/NF-5) full-cell requires only 1.599 V to obtain 10 mA cm-2, demonstrating the utmost overall water splitting performance with convenience in a simple cell configuration.

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TI Surface phosphorization for the enhanced photoelectrochemical
performance of an Fe₂O₃/Si photocathode
SO NANOSCALE
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DT Article
ID HYDROGEN EVOLUTION REACTION; WATER OXIDATION; PHOTOANODES; EFFICIENT;
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AB Transition metal phosphates (TMPs) are regarded as efficient co-catalysts for photoanodes, but they are rarely applied in hydrogen production reactions. In this work, iron phosphate (FePi), a co-catalyst for hydrogen production, is introduced onto the Fe2O3 surface by facile surface phosphorization under low-temperature conditions. The surface FePi leads to a shift of the onset potential by +201 mV and an increase in the photocurrent density by more than 10 mA cm(-2) at 0 V-RHE for the Fe2O3/p-Si photocathode in a strong alkaline electrolyte. The role of FePi stems from the smaller transfer resistance, efficient photogenerated carrier separation and electron injection, and preferable H* adsorption energy, as suggested by Kelvin probe force microscopy and

density functional theory (DFT) calculation. The surface phosphorization presents a facile and attractive strategy for the treatment of transition metal oxide catalyzed photocathodes for green hydrogen production.
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TI Substitutional effects in TiFe for hydrogen storage: a comprehensive
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ID NANOCRYSTALLINE INTERMETALLIC COMPOUND; IGNITION COMBUSTION SYNTHESIS;
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AB The search for suitable materials for solid-state stationary storage of green hydrogen is pushing the implementation of efficient renewable energy systems. This involves rational design and modification of cheap alloys for effective storage in mild conditions of temperature and pressure. Among many intermetallic compounds described in the literature, TiFe-based systems have recently regained vivid interest as materials for practical applications since they are low-cost and they can be tuned to match required pressure and operation conditions. This work aims to provide a comprehensive review of publications involving chemical substitution in TiFe-based compounds for guiding compound design and materials selection in current and future hydrogen storage applications. Mono- and multi-substituted compounds modify TiFe thermodynamics and are beneficial for many hydrogenation properties. They will be reviewed and deeply discussed, with a focus on manganese substitution.
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PA THOMAS GRAHAM HOUSE, SCIENCE PARK, MILTON RD, CAMBRIDGE CB4 0WF, CAMBS, ENGLAND
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AU Li, T
Chen, JH
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Zhong, Shujie
Feng, Wei
TI FeNi-Based Aerogels Containing FeNi₃ Nanoclusters Embedded
with a Crystalline-Amorphous Heterojunction as High-Efficiency Oxygen
Evolution Catalysts
SO MOLECULES
LA English
DT Article
DE nanoclusters embedded; crystalline-amorphous heterojunction; FeNi-based;
amorphous aerogels
ID BIFUNCTIONAL ELECTROCATALYSTS; IRON; FILMS; GRAPHENE; NICKEL; OXIDES; NI
AB In green hydrogen production via water electrolysis, catalysts with multiscale nanostructures synthesized by compositing micro-heterojunctions and nanoporous structures exhibit excellent electrocatalytic oxygen evolution reaction (OER) performance. Moreover, they are the most promising non-noble metal catalysts. Herein, FeNi-based aerogels with a three-dimensional nanoporous structure and amorphous matrix embedded with FeNi3 nanoclusters were synthesized via wet chemical reduction coprecipitation. The FeNi3 nanoclusters and the FeNi-based amorphous matrix formed a crystalline-amorphous heterojunction. These aerogels exhibited excellent OER performance and electrocatalytic stability in alkaline electrolytes. In 1 mol/L of KOH electrolyte, the as-synthesized aerogel exhibited an overpotential of 262 mV at a current density of 20 mA cm-2 with a Tafel slope of only 46 mV dec-1. It also demonstrated excellent stability during a 12 h chronopotentiometry test.
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PA ST ALBAN-ANLAGE 66, CH-4052 BASEL, SWITZERLAND
EI 1420-3049
J9 MOLECULES
JI Molecules
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VL 29
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AR 5429
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PG 12
WC Biochemistry & Molecular Biology; Chemistry, Multidisciplinary
WE Science Citation Index Expanded (SCI-EXPANDED)
SC Biochemistry & Molecular Biology; Chemistry
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PT J
AU Singhvi, M
   Kim, BS
AF Singhvi, Mamata
   Kim, Beom Soo
TI Green hydrogen production through consolidated bioprocessing of
   lignocellulosic biomass using nanobiotechnology approach
SO BIORESOURCE TECHNOLOGY
LA English
DT Article
DE Biohydrogen; Lignocellulosic biomass; Consolidated bioprocessing;
   Clostridium cellulovorans; Hydrogenase; Cerium iron oxide nanoparticles
ID BIOHYDROGEN PRODUCTION; WHEAT-STRAW; NANOPARTICLES; PRETREATMENT;
   SACCHARIFICATION; DELIGNIFICATION; FERMENTATION; OPTIMIZATION;
   ENHANCEMENT
AB The main objective of this study was to develop a sustainable process for hydrogen production by implementing nanotechnology in combination with consolidated bioprocessing (CBP) approach from lignocellulosic biomass (LCB). Peroxidase mimicking CeFe3O4 nanoparticles (NPs, 4.0 g/L) were applied for degradation of lignin from raw corn cob (CC) biomass for generation of cellulose-hemicellulose fractions amenable towards Clostridium cellulovorans during fermentation process. NP-treated biomass exhibited 43.26 % lignin removal from raw CC which was further employed for hydrogen fermentation by C. cellulovorans through CBP method. The strain yielded maximum 78.45 mL of cumulative hydrogen with hydrogen production rate of 1.55 mL/h using NP -treated CC. To the best of our knowledge, this is the first study on enhanced hydrogen production using NP -treated CC biomass in single pot fermentation which can prove to be a simpler, easier, and more economical process.
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FX The authors acknowledge the financial support of the National Research
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PU ELSEVIER SCI LTD
PI London
PA 125 London Wall, London, ENGLAND
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J9 BIORESOURCE TECHNOL
JI Bioresour. Technol.
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WC Agricultural Engineering; Biotechnology & Applied Microbiology; Energy & Fuels
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SC Agriculture; Biotechnology & Applied Microbiology; Energy & Fuels
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AU Tüysüz, H
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TI Alkaline Water Electrolysis for Green Hydrogen Production
SO ACCOUNTS OF CHEMICAL RESEARCH
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DT Review
ID OXYGEN EVOLUTION REACTION; METAL-OXIDES; ELECTROCATALYSTS; CATALYSIS; CATHODES; BEHAVIOR; DIOXIDE; TRENDS
AB The global energy landscape is undergoing significant change. Hydrogen is seen as the energy carrier of the future and will be a key element in the development of more

sustainable industry and society. However, hydrogen is currently produced mainly from fossil fuels, and this needs to change. Alkaline water electrolysis with advanced technology has the most significant potential for this transition to produce large-scale green hydrogen by utilizing renewable energy. The assembly of industrial electrolyzer plants is more complex on a larger scale, but it follows a basic working principle, which involves two half-cells of anode and cathode sites where the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) occur. Out of the two reactions, the OER is more challenging both thermodynamically and kinetically. Besides having access to renewable electricity, developing durable and abundant electrocatalysts for the OER remains a challenge in large-scale alkaline water electrolysis. Among different physicochemical properties, the electrocatalyst surface and its interaction with water and reaction intermediates, as well as formed molecular hydrogen and oxygen, play an essential role in the catalytic performance and the reaction mechanism. In particular, the binding strengths between the catalyst surface and intermediates determine the rate-limiting step and electrocatalytic performance. This Account gives some insights into the status of the hydrogen economy and basic principles of alkaline water electrolysis by covering its fundamentals as well as industrial developments. Further, the HER and OER reaction mechanisms of alkaline water electrolysis and selected electrocatalyst progress for both half-reactions are briefly discussed. The Adsorbate Evolution Mechanism and the Lattice Oxygen Mechanism for the OER are explained with specific references. This Account also deliberates on the author's selected contributions to the development of transition metal-based electrocatalysts for alkaline water electrolysis with an emphasis on OER. The focus is particularly given to the enhancement of intrinsic activity, the role of e(g)-filling, phase segregation, and defect structure of cobalt-based electrocatalysts for OER. Structural modification and phase transformation of the cobalt oxide electrocatalyst under working conditions are further deliberated. In addition, the creation of new active surface species and the activation of cobalt- and nickel-based electrocatalysts through iron uptake from the alkaline electrolyte are discussed. In the end, this Account provides a brief overview of challenges related to large-scale production and utilization of green hydrogen.
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TI Facile synthesis of Fe2.96Cr0.03Ni0.01O4@Ag core-shell nanoparticles and its efficient applications in green hydrogen generation and in removing hazardous dyes
SO SURFACES AND INTERFACES
LA English
DT Article
DE FeCrNiO@Ag CS-NPs; Dyes removal; H2 generation; 4-Nitrophenol; Powder synthesis; Cathodic deposition
ID CATALYTIC-REDUCTION; THERMAL-DECOMPOSITION; NI; HYDROLYSIS; POWDERS; BLUE; CU
AB A unique class of materials with nanostructures known as core-shell nanoparticles (CS-NPs) has drawn more attention recently because of its intriguing characteristics and wide range of uses in drug delivery, biology, materials chemistry, photocatalysis, catalysis, sensors, and other electronic device applications. One advantage of the approach was that it was easy to use, safe, affordable, and controlled. The CS-NPs of Fe2.96Cr0.03Ni0.01O4@Ag were successfully synthesized via electrolytic cathodic deposition of FeCrNi alloy thin film on a steel substrate and then annealed at 800 degrees C for two hours, resulting in a FeCrNiO powder that is converted easily to FeCrNiO@Ag CS-NPs using aqueous Ag-NPs. The XRD patterns of both FeCrNiO and FeCrNiO@Ag CS-NPs show the formation of a mixture of iron oxide (Fe2O3) and magnetite oxide (Fe2.96Cr0.03Ni0.01O4) with an average grain size of 38.36 nm and 30.18 nm, respectively. The synthesized FeCrNiO@Ag CS-NPs exhibit excellent applications in catalytic efficiency during the production of hydrogen from NaBH4 hydrolysis in addition to the reduction of the nitro group of 4NP to 4AP. In another successful application, the data show that using FeCrNiO@Ag, the dyes' total reduction occurred at 0.42 min for Remazol red (RR), 1.16 min for Methyl orange (MO), 0.83 min for Congo red (CR), and 1 min for Methylene blue (MB). The kinetics investigation was conducted and proved that the reduction reactions of the dyes followed a pseudo-first-order model. This data shows that our catalytic system performs well when compared to the other catalytic systems for dye reduction, and FeCrNiO@Ag CS-NPs is a favorable material for organic dye reduction. Therefore, the CS-NPs exhibit promise efficiency towards important applications in industrial catalysis and dye reduction, as evidenced by their stability and recyclability.
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TI Interfacial Acid-Like Microenvironment and Orbital Modulating Strategy
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SO SMALL STRUCTURES
LA English
DT Article
DE electrocoagulations; high-salinity wastewater; hydrogen evolution
   reaction catalysts; hydrogen productions; wastewater treatments
ID ELECTROLYTIC HYDROGEN; WATER; ELECTROCATALYSTS; OXIDATION; OXYGEN;
   METAL; OXIDE; HYDROXIDE; CATALYSTS; WO3
AB Electrochemical high-salinity wastewater splitting is a promising technology for green hydrogen (H2) production. However, the kinetics of hydrogen evolution reaction (HER) in neutral media is slow, and the high theoretical potential of oxygen evolution reaction leads to large energy losses. Herein, an iron-based electrocoagulation-coupled hydrogen production integrated system (IEHPS) is constructed, which is realized by coupling low-potential anodic iron oxidation reaction with cathodic HER. The non-noble metal HxWO3-Ni catalyst is synthesized by fabricating a proton sponge HxWO3 to achieve an interfacial acid-like microenvironment and doping it with Ni heteroatom to modulate the 4d orbital of

W, thereby weakening the adsorption strength of the W site toward hydrogen. Consequently, the HxWO3 Ni demonstrates remarkable performance characteristics, boasting a mere 131 mV overpotential at 10 mA cm-2 and Tafel slope of 44 mV dec- in neutral media. Operating at an applied voltage of 1.5 V, the IEHPS exhibits a high hydrogen production rate of 235 mL g-1 min-1 in seawater. It achieves nearly complete removal of contaminants like rhodamine B and heavy metal ions within a rapid 8-20 min, with an energy consumption of only 3.7 kWh Nm-3. This study provides a promising pathway for efficient and energy-saving production of high-purity hydrogen and effective treatment of high-salinity wastewater.

The HxWO3-Ni catalyst is synthesized by constructing an interfacial acid microenvironment and introducing Ni heteroatom. Then, the anodic iron oxidation reaction and cathodic hydrogen evolution reaction are coupled to construct the iron-based electrocoagulation-coupled hydrogen production system (IEHPS), which achieves efficient ecofriendly H2 while purifying wastewater/seawater simultaneously.image (c) 2024 WILEY-VCH GmbH
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NR 60
TC 0
Z9 0
U1 23
U2 23
PU WILEY
PI HOBOKEN
PA 111 RIVER ST, HOBOKEN 07030-5774, NJ USA
EI 2688-4062
J9 SMALL STRUCT
JI Small Struct.
PD FEB
PY 2025
VL 6
IS 2
DI 10.1002/sstr.202400398
EA OCT 2024
PG 11
WC Chemistry, Physical; Nanoscience & Nanotechnology; Materials Science,
Multidisciplinary
WE Science Citation Index Expanded (SCI-EXPANDED)
SC Chemistry; Science & Technology - Other Topics; Materials Science

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OA gold
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PT J
AU Liu, YH
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   Yuan, YJ
   Huang, HS
   Ma, XG
   Li, XQ
   Jin, ZY
AF Liu, Yunhua
   Mao, Jianfei
   Yuan, Yujie
   Huang, Hongsheng
   Ma, Xianguo
   Li, Xiaoqin
   Jin, Zhaoyu
TI Accelerating corrosion of iron foam enables a bifunctional catalyst for
   overall water splitting
SO MATERIALS CHEMISTRY FRONTIERS
LA English
DT Article
ID OXYGEN EVOLUTION REACTION; OXIDE; NANOARRAYS; EFFICIENT
AB To facilitate the green hydrogen economy, it is essential to establish an economical, secure, and large-scale method for producing highly efficient electrocatalysts capable of facilitating overall water splitting. Herein, we demonstrate a facile approach by growing nickel-iron nanoparticles and layered double hydroxide (LDH) nanosheet composites in situ on a Fe-foam substrate via ammonium chloride-assisted corrosion at room temperature. This method does not require electrical input, high temperature, or a tedious synthesis procedure. The obtained catalyst exhibits high catalytic activity for the oxygen evolution reaction (OER) and the hydrogen evolution reaction (HER), providing a high current density of 500 mA cm-2 at an overpotential of 270 mV for the OER and 183 mV for the HER. In addition, the catalyst that serves as both the cathode and anode for overall water splitting also exhibits satisfactory performance with a low cell voltage of 1.55 V at 10 mA cm-2 with high stability at different current densities from 10 to 300 mA cm-2 for 70 h. Our findings underline a highly efficient and scalable strategy for the large-scale preparation of bifunctional electrocatalysts for alkaline water electrolysis.
   A bifunctional NiFe nanoparticle-modified layered double hydroxide nanosheet electrocatalyst was fabricated using a facile NH4Cl-assisted corrosion strategy at room temperature for highly efficient overall water splitting.
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RI Li, Xiaoqin/W-3020-2019; Jin, Zhaoyu/N-4237-2016; liu,
   yunhua/A-8334-2017; Yuan, yujie/HCI-8220-2022
OI Jin, Zhaoyu/0000-0003-0840-3931; Li, Xiaoqin/0009-0001-8478-7490
FU This work was supported by the Natural Science Foundation of Guizhou
   Province (QiankeheJichu-ZK [2021] Yiban050), High-Level Scientific
   Research Founding Project of Guizhou Institute of Technology
   (XJGC20190961), Key Laboratory of Energy Chemistry in Guizh
FX This work was supported by the Natural Science Foundation of Guizhou
   Province (QiankeheJichu-ZK [2021] Yiban050), High-Level Scientific
   Research Founding Project of Guizhou Institute of Technology

(XJGC20190961), Key Laboratory of Energy Chemistry in Guizhou universities (Qian Jiao Ji [2022]035), and Top Talent Project of Guizhou Provincial Department of Education (Guizhou Education Technology [2022]084).
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NR 59
TC 5
Z9 5

U1 10
U2 39
PU ROYAL SOC CHEMISTRY
PI CAMBRIDGE
PA THOMAS GRAHAM HOUSE, SCIENCE PARK, MILTON RD, CAMBRIDGE CB4 0WF, CAMBS,
   ENGLAND
EI 2052-1537
J9 MATER CHEM FRONT
JI Mat. Chem. Front.
PD NOV 6
PY 2023
VL 7
IS 22
BP 5858
EP 5867
DI 10.1039/d3qm00567d
EA SEP 2023
PG 10
WC Chemistry, Multidisciplinary; Materials Science, Multidisciplinary
WE Science Citation Index Expanded (SCI-EXPANDED)
SC Chemistry; Materials Science
GA W5SR2
UT WOS:001071091700001
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PT C
AU Bi, SH
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   Xue, MZ
   Zhang, CM
AF Bi, Songhu
   Geng, Zhen
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   Zhang, Cunman
BE Sun, H
   Pei, W
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   Yu, H
   You, S
TI Porous Heterogeneous Sulfide Nickel/Nickel Iron Alloy Catalysts for
   Oxygen Evolution Reaction of Alkaline Water Electrolysis at High Current
   Density
SO PROCEEDINGS OF THE 10TH HYDROGEN TECHNOLOGY CONVENTION, VOL 1, WHTC 2023
SE Springer Proceedings in Physics
LA English
DT Proceedings Paper
CT 10th Hydrogen Technology Convention (WHTC)
CY MAY 22-26, 2023
CL Foshan, PEOPLES R CHINA
DE Alkaline water electrolysis; Oxygen evolution reaction; Porous
   heterogeneous catalyst; High current density
ID HYDROGEN-PRODUCTION; EFFICIENT
AB Alkaline water electrolysis is the important pathway for the green hydrogen
production, where oxygen evolution reaction (OER) is the rate-limiting step due to the
sluggish reaction kinetics. Transition metal heterogeneous catalyst is the kind of
important OER catalyst for alkaline water electrolysis due to its good performance, low
price and environmental friendliness. In this work, the porous sulfide nickel@nickel iron
alloy catalyst (i.e. NM/NS@Ni3Fe) is prepared by the designed high-temperature
vulcanization and multi-step electrodeposition method. The NM/NS@Ni3Fe catalyst exhibits
an outstanding OER performance in an alkaline environment, with a low potential of 1.53 V
at high current density of 1000 mA cm(-2) and a low Tafel slope of 89 mV dec(-1). The
excellent OER performance is attributed to the unique electronic structure of Ni3S2/Ni3Fe
heterogeneous interface and the catalyst layer with porous structure. The results

indicate that Ni3S2 provides good electronic conductivity and the low electronegativity S atoms increase the formation of oxygen vacancies, which effectively improves the OER performance. In addition, the hydrophilic and porous structure of the electrode facilitates bubbles release and electrolyte flow at high current density. It provides the guidance for the design of porous heterogeneous OER catalysts with good-performance.
C1 [Bi, Songhu; Geng, Zhen; Jin, Liming; Xue, Mingzhe; Zhang, Cunman] Tongji Univ, Clean Energy Automot Engn Ctr, Sch Automot Studies, Shanghai 201804, Peoples R China.
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RI Jin, Liming/V-4771-2018; Geng, Zhen/AAX-1367-2021
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NR 11
TC 0
Z9 0
U1 6
U2 6
PU SPRINGER-VERLAG SINGAPORE PTE LTD
PI SINGAPORE
PA 152 BEACH ROAD, #21-01/04 GATEWAY EAST, SINGAPORE, 189721, SINGAPORE
SN 0930-8989
EI 1867-4941
BN 978-981-99-8633-0; 978-981-99-8631-6; 978-981-99-8630-9
J9 SPRINGER PROC PHYS
PY 2024
VL 393
BP 116
EP 121
DI 10.1007/978-981-99-8631-6_13
PG 6
WC Chemistry, Applied; Electrochemistry; Energy & Fuels
WE Conference Proceedings Citation Index - Science (CPCI-S)
SC Chemistry; Electrochemistry; Energy & Fuels
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PT J
AU Li, T
Ling, S
Zhong, SJ
Chen, JH
Li, ML
Sun, Y
AF Li, T.
Ling, S.
Zhong, S. J.
Chen, J. H.
Li, M. L.
Sun, Y.
TI In situ synthesis of FeNi₃/(Fe,Ni)₉S₈/Ni₄S<sub>3<
/sub>/C nanorods and enhanceent of oxygen evolution reaction properties

SO DIGEST JOURNAL OF NANOMATERIALS AND BIOSTRUCTURES
LA English
DT Article
DE Nanorods; FeNi3; OER; Synergy enhancement
ID NANOPARTICLES; NANOSHEETS; HYDROGEN
AB NiFe-based nanomaterials have emerged as highly promising catalysts to replace platinum, ruthenium and iridium for oxygen evolution reaction (OER), in "green hydrogen" production process through water splitting. Using iron (2+) sulfate and nickel acetate as the raw materials, with the molar ratio of Ni acetate to iron (2+) sulfate controlled at 8:5, the concentration of metal-ion was 0.6 mol/L, and precursor fibers rich in Ni2+, Fe2+, and SO42- were prepared using electrospinning technology, with polyvinyl alcohol acting as the colloid. Subsequently, composite nanorods rich in the elements of Ni, Fe, S, and C were successfully obtained at a heat treatment temperature of 1000 degrees C in an Ar gas atmosphere. The results demonstrate that the nanorod samples possessed a surface diameter of similar to 200 nm, and the main phases of the nanorods after heat treatment at 1000 degrees C included FeNi3 alloy, (Fe,Ni)(9)S-8, Ni4S3, and amorphous C. Electrochemical performance tests conducted in a 1.0 mol/L KOH solution exhibited excellent oxygen evolution reaction properties of the catalysts prepared using FeNi3/(Fe,Ni)(9)S-8/Ni4S3/C nanorods as the materials. The overpotential was about 258.6 mV of the catalyst material at 10 mA.cm(-2).
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FU Sichuan Science and Technology Program [2023YFG0229]
FX <BOLD>Acknowledgments</BOLD> This research work was funded by the
Sichuan Science and Technology Program (2023YFG0229) .
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NR 44
TC 0
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U1 3
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PU VIRTUAL CO PHYSICS SRL
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J9 DIG J NANOMATER BIOS
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DI 10.15251/DJNB.2024.193.1333
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WC Nanoscience & Nanotechnology; Materials Science, Multidisciplinary
WE Science Citation Index Expanded (SCI-EXPANDED)
SC Science & Technology - Other Topics; Materials Science
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PT J
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Yu, FQ
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Wu, Yuanhang
Yu, Hongliang
Hang, Congshu
Tang, Wangshu
Yang, Yijie
Chen, Hongyi
Li, Hui
Yu, Faquan
TI Three-dimensional pine-tree-like bimetallic sulfide with maximally
exposed active sites by secondary structural restructuring for efficient
electrocatalytic OER
SO INTERNATIONAL JOURNAL OF HYDROGEN ENERGY
LA English
DT Article
DE Hydrogen energy; Iron -cobalt sulfide; Pine -tree -like structure;
Structural restructuring; Electrocatalysts; OER
ID WATER; DESIGN; NANOPARTICLES; NANORODS; IRON

AB Developing efficient, low-cost and bifunctional catalysts with predominant durability for the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER) is an extraordinary challenge in the preparation of green hydrogen energy by electrochemical water splitting. Three-dimensional (3D) transition metal compounds have become a research hotspot as OER electrocatalysts, which can replace noble metal oxides such as RuO2 and IrO2 to reduce application costs. Herein, we synthesized a novel three-dimensional pine-tree-like bimetallic sulfide arrays on nickel foam (FeCoS/NF) using various optimization strategies such as morphology optimization, in situ growth and introduction of heterogeneous structures. The as-synthesized FeCoS/NF electrocatalyst only requires relatively low overpotential of 156 mV to achieve a current density of 20 mA cm(-2) for OER, with a Tafel slope of only 37 mV dec(-1). It also has a small charge transfer resistance, an electrochemical surface area and good electrochemical stability in alkaline electrolytes. The excellent performance of FeCoS/NF can be attributed to the synergistic effect and amorphous phase of FeCoS as well as the well-defined pine-tree-like array architecture with a large surface area, abundant active sites, and sufficient gas and electrolyte diffusion channels.
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NR 52
TC 2
Z9 3
U1 11
U2 11
PU PERGAMON-ELSEVIER SCIENCE LTD
PI OXFORD
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EI 1879-3487
J9 INT J HYDROGEN ENERG
JI Int. J. Hydrog. Energy
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VL 79
BP 1418
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DI 10.1016/j.ijhydene.2024.07.111
EA JUL 2024
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WC Chemistry, Physical; Electrochemistry; Energy & Fuels
WE Science Citation Index Expanded (SCI-EXPANDED)
SC Chemistry; Electrochemistry; Energy & Fuels
GA YW9E8
UT WOS:001271632500001
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ER

PT J
AU Dong, JT
Yu, C
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Huang, HL
Han, YN
Wei, QB
Qiu, JS
AF Dong, Junting
Yu, Chang
Wang, Hui
Chen, Lin
Huang, Hongling

Han, Yingnan
Wei, Qianbing
Qiu, Jieshan
TI A robust & weak-nucleophilicity electrocatalyst with an inert response for chlorine ion oxidation in large-current seawater electrolysis
SO JOURNAL OF ENERGY CHEMISTRY
LA English
DT Article
DE Nickel-iron hydroxide electrocatalysts; Highly selective seawater electrolysis; Weak nucleophilicity; Oxygen evolution reaction; Hydrogen
ID EVOLUTION REACTION; OPPORTUNITIES; CATALYSTS
AB Seawater splitting into hydrogen, a promising technology, is seriously limited by the durability and tol-erance of electrocatalysts for chlorine ions in seawater at large current densities due to chloride oxidation and corrosion. Here, we present a robust and weak-nucleophilicity nickel-iron hydroxide electrocatalyst with excellent selectivity for oxygen evolution and an inert response for chlorine ion oxidation which are key and highly desired for efficient seawater electrolysis. Such a weak-nucleophilicity electrocatalyst can well match with strong-nucleophilicity OH- compared with the weak-nucleophilicity Cl-, resultantly, the oxidation of OH- in electrolyte can be more easily achieved relative to chlorine ion oxidation, confirmed by ethylenediaminetetraacetic acid disodium probing test. Further, no strongly corrosive hypochlorite is produced when the operating voltage reaches about 2.1 V vs. RHE, a potential that is far beyond the ther-modynamic potential of chlorine ion oxidation. This concept and approach to reasonably designing weak-nucleophilicity electrocatalysts that can greatly avoid chlorine ion oxidation under alkaline seawater environments can push forward the seawater electrolysis technology and also accelerate the develop-ment of green hydrogen technique.
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FU National Natural Science Foundation of China (NSFC) [22078052]; Fundamental Research Funds for the Central Universities [DUT22ZD207, DUT22LAB612]
FX This work was partly supported by the National Natural Science Foundation of China (NSFC, No. 22078052) , and the Fundamental Research Funds for the Central Universities (DUT22ZD207, DUT22LAB612) .
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NR 39
TC 13
Z9 13
U1 11
U2 27
PU ELSEVIER
PI AMSTERDAM
PA RADARWEG 29, 1043 NX AMSTERDAM, NETHERLANDS
SN 2095-4956
J9 J ENERGY CHEM
JI J. Energy Chem.
PD MAR
PY 2024
VL 90
BP 486
EP 495
DI 10.1016/j.jechem.2023.11.001
EA DEC 2023
PG 10
WC Chemistry, Applied; Chemistry, Physical; Energy & Fuels; Engineering,
   Chemical
WE Science Citation Index Expanded (SCI-EXPANDED)
SC Chemistry; Energy & Fuels; Engineering
GA GA3W5
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PT J
AU Liu, ZW
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   Kong, QX
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AF Liu, Zhenwei
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TI One-Step Electrosynthesis of Bifunctional NiCu Nanosheets on Iron Foam
for Remarkably Enhanced Alkaline Water Splitting
SO SUSTAINABILITY
LA English
DT Article
DE bifunctional electrocatalysts; water splitting; spend cupronickel;
soluble anode; electrosynthesis
ID CUPRONICKEL ALLOY; EFFICIENT; ELECTROCATALYSTS; CATALYST
AB Electrocatalytic water splitting for hydrogen production driven by renewable electricity offers a promising way of achieving energy sustainability, but the design of highly efficient and cost-effective electrocatalysts is regarded as a bottleneck. Herein, a bifunctional microflowers NiCu is successfully deposited on an iron foam (IF) electrode via one-step electrolysis of spend cupronickel (SCN). Unexpectedly, the designed IF-supported NiCu (NiCu/IF) electrocatalysts exhibit excellent catalytic performance for oxygen evolution reactions (OER) and hydrogen evolution reactions (HER) in 1 M KOH. Only 98 and 267 mV are required to drive a current density of 10 mA cm(-2) for HER and OER, respectively. Importantly, the self-supported NiCu/IF electrode requires a low cell voltage of 1.57 V to achieve 10 mA cm(-2)of alkaline overall water splitting with extremely high stability. With the introduction of a glycerol oxidation reaction (GOR), the HER performance is further remarkably enhanced with an extremely low cell voltage of 1.29 V at 10 mA cem(-2), highlighting an attractive energy-efficient hydrogen production coupled with biomass conversion process. This study reports a novel synthesis strategy for low-cost and high-performance Ni-based nanostructure catalysts using SCN as precursors, which is of vital significance for green hydrogen production and waste recycling.
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OI Wang, Qiang/0000-0002-5037-2086
FU The authors gratefully acknowledge the financial support provided by the
National Natural Science Foundation of China (No. 22262017).; National
Natural Science Foundation of China; [22262017]
FX The authors gratefully acknowledge the financial support provided by the
National Natural Science Foundation of China (No. 22262017).
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AU Seuferling, TE
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AF Seuferling, Tess E.
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TI Carbonate-Derived Multi-Metal Catalysts for Electrochemical
   Water-Splitting at High Current Densities
SO ACS SUSTAINABLE CHEMISTRY & ENGINEERING
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DT Article
DE hydrogen evolution; oxygen evolution; electrocatalyst; overpotential;
   electrolyzer
ID OXYGEN EVOLUTION REACTION; RAY PHOTOELECTRON-SPECTROSCOPY; LAYERED
   DOUBLE HYDROXIDE; IRON; OXIDES; ELECTROCATALYSTS; XPS; ELECTROLYSIS;
   ELECTRODES; INSIGHTS
AB The renewable production of green hydrogen powered by water electrolysis will be an important step in the electrification of the chemical industry. However, to make water-splitting more sustainable and practical, earth-abundant catalysts need to be developed, which can both be synthesized using the principles of green chemistry and have high performance specifically at high hydrogen production rates. In this work, we report four main findings to help contribute toward this goal. First, we report a "green" synthesis method for producing a mixed-metal oxide catalyst that uses only water as the solvent and no harsh oxidizing or reducing agents. Second, we show that this synthesis method can enable an amorphous nickel-iron oxide/(oxy)hydroxide catalyst with a 1:1 Fe/Ni ratio. This increased iron content further improves the performance over the conventional 1:4 Fe/Ni ratio. Third, we show that these catalysts can be easily deposited on a 3D porous Ni-foam electrode and achieve current densities up to 1 A cm(-2) and an overpotential of 245 mV at 100 mA cm(-2) for oxygen evolution reaction (OER) and an overpotential of 422 mV at 100 mA cm(-2) for hydrogen evolution reaction (HER). Finally, we show that combining both HER and OER catalysts, synthesized with our method, in a flow-through water electrolyzer achieves an overpotential of 140 mV at 100 mA cm(-2) at 80 degrees C. In addition, this electrolyzer can achieve 76% efficiency at 1 A cm(-2) and 70% efficiency at 2 A cm(-2).
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   Kuroki, Hidenori
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   Tamaki, Takanori
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TI High-Performing Anion Exchange Membrane Water Electrolysis Using
   Self-Supported Metal Phosphide Anode Catalysts and an Ether-Free
   Aromatic Polyelectrolyte
SO ACS SUSTAINABLE CHEMISTRY & ENGINEERING
LA English
DT Article
DE anion exchange membrane water electrolysis; green hydrogen; oxygen
   evolution reaction; self-supported catalysts; metal phosphide; Nickel
   Foam
ID OXYGEN-EVOLUTION; NICKEL FOAM; BIFUNCTIONAL ELECTROCATALYSTS; HYDROGEN;
   ALKALINE; EFFICIENT; SPECTROSCOPY; DEGRADATION; REDUCTION; BACKBONE
AB Anion exchange membrane water electrolysis (AEMWE) is going through a critical transition phase from the laboratory scale to scale-up prospects owing to the development of highly durable ether-free aromatic anion exchange membranes. The next important step is processing competent nonprecious metal catalysts as scalable electrodes. Here, we fabricated an iron-integrated self-supported nickel phosphide (Ni2P-Fe/NF) catalyst for the sluggish oxygen evolution reaction (OER). It was demonstrated that this catalyst could work as a high-performing anode electrode in an AEMWE system when combined with a durable ether-free aromatic polyelectrolyte. The noble metal-free Ni2P-Fe/NF electrode, developed employing a simple and scalable strategy demonstrated higher performance as an anode electrode in water electrolysis with a cell voltage of 1.73 V for 1 A/cm(2) with an excellent energy conversion efficiency (86%) in 1 M KOH and the MEA is also found to be stable for 24 h at 200 mA/cm(2). Electrochemical and spectroscopic investigations over the Ni2P-Fe/NF metal electrode surface during and post-OER disclosed the beneficial synergistic interaction of the metal species, leading to lattice alterations, formation of oxy-hydroxide active species, and improved electron charge transfer as crucial factors responsible for the excellent performance and stability. This work involves scalable processing of catalyst structures over a nickel foam surface, insights into the thickness variation of the substrate for catalyst processing, and identifying the OER characteristics under water electrolysis conditions, which are significant in the

application direction of applying noble metal-free electrodes for green hydrogen generation in AEMWE.

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FU New Energy and Industrial Technology Development Organization (NEDO), Japan [JPNP14021]
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TI Effect of B-site Al substitution on hydrogen production of
La_{0.4}Sr_{0.6}Mn_{1-x}Al_x (x1/40.4,
0.5 and 0.6) perovskite oxides
SO INTERNATIONAL JOURNAL OF HYDROGEN ENERGY
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DE Perovskite oxide; Pechini method; Hydrogen production; Thermochemical water splitting
ID LANTHANUM MANGANITE PEROVSKITES; WATER-SPLITTING CYCLE; SOLAR THERMOCHEMICAL PRODUCTION; OXYGEN-EXCHANGE MATERIALS; REDOX REACTIONS; GREEN HYDROGEN; IRON-OXIDE; CO2; FUEL; ECONOMY
AB Thermochemical water splitting using perovskite oxides as redox materials is one of the important way to use solar energy to produce green hydrogen. Thus, it is hence important to discover new materials that can be used for this purpose. In this regard, we focused on Al-substituted La0.4Sr0.6Mn1-xAlxO3 (x = 0.4, 0.5 and 0.6) perovskite oxides, namely as La0.4Sr0.6Mn0.6Al0.4 (LSMA4664), La0.4Sr0.6Mn0.5Al0.5 (LSMA4655), and La0.4Sr0.6Mn0.4Al0.6 (LSMA4646) which have been successfully synthesized. Herein, synthesized LSMA4664, LSMA4655, and LSMA4646 were subjected to three consecutive thermochemical cycles in order to determine their oxygen capacity, hydrogen capacity, re-oxidation capability and structural stability following three cycles. Thermochemical cycles were carried out at 1400 degrees C for reduction and 800 degrees C for the oxidation reaction. LSMA4646 exhibited the highest O2 production capacity with 275 mmol/g among the other perovskites employed in the study. Moreover, LSMA4646 has also the highest H2 production, 144 mmol/g, with 90% of re oxidation capability by the end of three thermochemical water splitting cycles. On the other hand, LSMA4664 has the lowest H2 production and only kept approximately onethird of its hydrogen production capacity by the end of cycles. Thus, the current study provides insight that the increase in the Al-substitution enhances both oxygen and hydrogen production capacity. Besides, increasing the Al amount increases the structural stability during the redox reactions, the re-oxidation capability was also increased from 38% to 89% after thermochemical cycles. (C) 2021 Published by Elsevier Ltd on behalf of Hydrogen Energy Publications LLC.
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AU Limarev, IP
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TI In a search of the single-atom electrocatalysts for hydrogen production:
   The first sulfur-free mono- and diphenanthrenyl-terminated iron and
   cobalt(II) clathrochelates versus their thioanalogs
SO PROCESS SAFETY AND ENVIRONMENTAL PROTECTION
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DT Article
DE Green chemistry; Green hydrogen production; Clathrochelates; Hydrogen
   evolution reaction; Single-atom catalysts; Polymer electrolyte membrane
   (PEM) water; electrolysis
ID CAGE COMPLEXES; IMMOBILIZATION; RUTHENIUM; ENERGY
AB This paper reports on green chemistry approaches to the molecular design and synthesis of cheap, efficient and eco-friendly electrocatalysts of the hydrogen evolution reaction (HER). The title clathrochelates (including first those do not containing sulfur derivatives as "catalytic poisons") were prepared using nucleophilic substitution of their chloroclathrochelate precursors and characterized by analytical, spectral and XRD methods. These complexes showed the HER 2 H+/H2 electrocatalytic activity in the solutions. They form the Langmuir monolayers and possess a high physisorption on activated carbon (AC, up to 0.55 mmol center dot g-1) and reduced graphene oxide (RGO, up to 0.33 mmol center dot g-1). Contrary that on carbon paper (CP) is very low. Therefore, AC- or RGO-containing clathrochelate-immobilized components are suitable for preparation of hybrid CP-based cathodes, allowing to substantially increase a surface concentration of electrocatalytically active centers up to 0.5 mu mol center dot m-2. Cyclic voltammetry data suggest that the electrochemically generated cobalt(I) complexes, as the catalytically active intermediates, are stable and most prospective candidates for electrocatalytic hydrogen production. Clathrochelate-based single-atom catalysts were prepared in accordance with basic principles of green chemistry. They are derivatives of abundant and cheap 3d-biometals and low-toxic alpha-dioximes and possess an extremely high atomic utilization efficiency matching the "economy of atoms" principle. Nowadays,

the carbon-supported metallic platinum is used as HER catalyst. The reserves of this noble and expensive metal on the Earth are limited and its replacement by such cheap and abundant HER materials will accelerate the development and implementation of green hydrogen-producing technologies. The recommendations on chemical structures of optimal molecular electrocatalysts were evaluated.
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RI Kottsov, Sergei/AAM-8410-2020; Dorovatovskii, Pavel/F-7723-2014; Teplonogova, Maria/B-7113-2018; Ivanov, Vladimir/H-4407-2011; Limarev, Ilya/ABC-7705-2021; Sterligov, Grigorii/GSE-2211-2022; Grigoriev, Sergey/A-1655-2014
OI Grigoriev, Sergey/0000-0002-5043-7409
FU Russian Science Foundation [24-13-00230]; IGIC RAS state assignment; Ministry of Science and Higher Education [FSWF-2023-0014]
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AU Fisher, OJ
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TI Techno-economic analysis and process simulation of alkoxylated
   surfactant production in a circular carbon economy framework
SO DIGITAL CHEMICAL ENGINEERING
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DT Article
DE Circular economy; Circular carbon economy; Techno-economic analysis
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   Surfactant
ID LIFE-CYCLE ASSESSMENT; FISCHER-TROPSCH; PERFORMANCE; CATALYSTS;
   HYDROGEN; CAPTURE; NETWORK; SYSTEMS; DESIGN; GREEN
AB Successfully transitioning to a net-zero and circular carbon economy requires adopting innovative technologies and business models to capture CO2 and convert it into valuable chemicals and materials. Given the high economic costs and limited funding available for this transition, robust economic modelling of potential circular carbon pathways is essential to identify economically viable routes. This study introduces a novel technoeconomic analysis (TEA) of producing alcohol ethoxylate (AE7), a valuable surfactant, from industrial flue gas. Traditionally, AE7 is produced by reacting fatty alcohols with ethylene oxide derived from fossil or bio-based sources. This research explores a method using CO2 captured from steel industry flue gas to produce AE7, addressing a notable gap in the literature. It evaluates a thermo-catalytic pathway involving Fischer-Tropsch (FT) synthesis with syngas generated by the reverse-water gas-shift reaction, where CO2 reacts with H2. CO2 conversion rates range around 3% across processing capacities of 25 kt/a, 100 kt/a, and 1000 kt/a. The study finds that the CO2 mass fraction concentration in the process emission is 2.47 x 10-5, compared to 0.13 in the incoming flue gas, highlighting the system's positive environmental impact. A radial basis function neural network was built to forecast the long-term average price of fossil-based and bio-based surfactants to benchmark the results against. Economic analysis reveals that the cost of green hydrogen significantly impacts the minimum selling price (MSP), making cost parity with existing fossil-based surfactants challenging. The lowest MSP of $8.77/kg remains above the long-term forecasted price of $3.75/kg for fossil-based C12-14 AE7. However, Monte Carlo simulations show a 21% probability of achieving a positive net present value (NPV) compared to leading bio-based surfactant alternatives. Sensitivity analyses identify capital costs, the price of low-carbon hydrogen (LCOH), and diesel prices as the most influential factors affecting the MSP. Continued advancements in FischerTropsch catalyst technologies, reductions in green hydrogen costs and growing consumer demand for environmentally friendly products could significantly enhance the economic feasibility of this sustainable approach, paving the way for broader adoption and contributing to a circular carbon economy.
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PI London
PA 125 London Wall, London, ENGLAND
SN 2772-5081
J9 DIGIT CHEM ENG
JI Digit. Chem. Eng.
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PY 2024
VL 13
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WC Engineering, Chemical
WE Emerging Sources Citation Index (ESCI)
SC Engineering
GA O6E3D
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OA gold
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AF Chen, Xinran
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Asefa, Tewodros
TI Sulfur-bridged iron-polyphthalocyanine on Cu_{<i>x</i>}O/copper foam: efficient and durable electrocatalyst for overall water splitting
SO SUSTAINABLE ENERGY & FUELS
LA English
DT Article
ID OXYGEN REDUCTION; RAMAN-SPECTROSCOPY; COBALT; PERFORMANCE; OXIDATION; CATALYST; PHTHALOCYANINES; NANOSHEETS; SULFIDE
AB Overall water splitting is a promising route to produce green hydrogen in a sustainable manner. However, its practical large-scale use critically requires efficient, sustainable and easy-to-operate catalysts that can drive both the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER) in the same electrolyte. In this report, we present a facile synthesis of one such electrocatalyst that is composed of amorphous sulfur-bridged iron polyphthalocyanine (FeSPPc) grown in situ on CuxO-coated Cu foam. The material is denoted as FeSPPc/CuxO/CF, where x indicates the non-stoichiometric hybrid valence states of Cu, including its +1 and +2 oxidation states. The as-generated material has unique catalytic sites, large electrochemically active surface area, and high electrical conductivity. It electrocatalyzes the HER in N-2-saturated KOH electrolyte (1 M) with a current density of 10 mA cm(-2) at an overpotential of only 38 mV. It also electrocatalyzes the OER in O-2-saturated KOH solution (1 M) with 10 mA cm(-2) at an overpotential of 350 mV. The material is stable while catalyzing both reactions as well. Importantly, a water electrolyzer assembled using FeSPPc/CuxO/CF as both cathode and anode electrodes in the same alkaline electrolyte requires only 1.48 V to drive the reaction with 10 mA cm(-2) while remaining stable.
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NR 48
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U2 48
PU ROYAL SOC CHEMISTRY
PI CAMBRIDGE
PA THOMAS GRAHAM HOUSE, SCIENCE PARK, MILTON RD, CAMBRIDGE CB4 0WF, CAMBS,
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SN 2398-4902
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JI Sustain. Energ. Fuels
PD NOV 23
PY 2021
VL 5
IS 23
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EP 5993
DI 10.1039/d1se01167g
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PG 9
WC Chemistry, Physical; Energy & Fuels; Materials Science,
   Multidisciplinary
WE Science Citation Index Expanded (SCI-EXPANDED)
SC Chemistry; Energy & Fuels; Materials Science
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AU Duan, DH
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AF Duan, Donghong
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Wang, Yunfang
TI Electrodeposition of cobalt-iron bimetal phosphide on Ni foam as a bifunctional electrocatalyst for efficient overall water splitting
SO JOURNAL OF COLLOID AND INTERFACE SCIENCE
LA English
DT Article
DE Electrodeposition; Cobalt-iron phosphide; Water splitting; Oxygen evolution reaction; Hydrogen evolution reaction
ID HYDROGEN EVOLUTION REACTION; HIGHLY EFFICIENT; METAL PHOSPHIDE; NANOSHEET ARRAYS; OXYGEN; COP; DESIGN; FEP
AB To solve environmental pollution and energy crisis, it is essential to design an efficient, economical, and stable bifunctional electrocatalyst for water splitting to produce renewable energy sources H2 and O-2. In this study, low-crystallinity and microspherical CoFe-P/NF catalyst synthesized by potentiostat electrodeposition on a foam nickel substrate had an excellent hydrogen evolution reaction (HER), oxygen evolution reaction (OER), and water splitting performance. In 1 M KOH solution, the CoFe-P/NF required the overpotentials of 45 mV for HER and 287 mV for OER in order to create a current density of 10 mA cm(-2). Furthermore, the Tafel slope for HER and OER was measured as 35.4 and 43.2 mV dec(-1), respectively. Serving as the bifunctional catalysts, the CoFe-P/NF electrode couple displays a low voltage of only 1.58 V at 10 mA cm(-2) with an excellent long-term stability. Such remarkably properties of the CoFe-P/NF are attributed to the crystalline-amorphous phase structure, the synergistic effect of Co, Fe and P, and rapid separation of bubbles from the electrode surface. In summary, this study provides a new method for developing cost-effective catalyst towards green hydrogen production via water splitting. (c) 2022 Elsevier Inc. All rights reserved.
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J9 J COLLOID INTERF SCI
JI J. Colloid Interface Sci.
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AU Bi, SH
   Geng, Z
   Wang, YW
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AF Bi, Songhu
   Geng, Zhen
   Wang, Yuwei
   Gao, Zijian
   Jin, Liming
   Xue, Mingzhe
   Zhang, Cunman
TI Multi-Stage Porous Nickel-Iron Oxide Electrode for High Current Alkaline
   Water Electrolysis
SO ADVANCED FUNCTIONAL MATERIALS
LA English
DT Article
DE alkaline water electrolysis; bubbles removal; lattice Boltzmann
   simulation; oxygen evolution reaction; porous electrodes
ID OXYGEN EVOLUTION REACTION; NI CATALYSTS; OXIDATION; ELECTROCATALYST;
   EFFICIENCY; BUBBLES
AB Alkaline water electrolysis (AWE) is the promising technical pathway of large-scale green hydrogen production. The sluggish oxygen evolution reaction seriously hampers the water decomposition reaction kinetics for AWE, especially at high current density above 500 mA cm(-2). It is closely related with bubbles removal dynamic performance of porous electrodes. In this study, the multi-stage porous nickel-iron oxide electrode is prepared by a two-step electro-deposition method. The electrode shows good oxygen evolution reaction performance at high current densitiy of 1000 mA cm(-2), which is attributed to both the good electro-catalytic performance of NiFeOx with nano-cone structure and good bubbles removal performance of porous Ni interlayer with the curved pore channels. Bubbles motion inside the pore channels is deeply analyzed by Lattice Boltzmann simulation of gas-liquid two-phase flows, combining with the experiments. The results indicate that bubbles motion speed is faster in curved pore channels than that in straight pore channels due to the role of bubble buoyancy. It illuminates the effects of pore channel curvature on bubbles motion for porous electrodes prepared by electro-deposition. It provides the possibility of designing porous electrodes with both good electro-catalytic performance and good bubbles removal performance by the electro-deposition method, from the view of industrial applications.
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AU Dristy, SA
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TI Manganese doped NiBP: A promising electrocatalyst for sustainable
   hydrogen production at high-current-density (HCD)
SO INTERNATIONAL JOURNAL OF HYDROGEN ENERGY
LA English
DT Article
DE Mn-doping; Cost-effective; Hydrogen generation; Stability; High current
ID EFFICIENT ELECTROCATALYST; NANOSHEETS; IRON; FOAM
AB Exploring non-precious metal-based electrocatalysts with superior electrocatalytic performance and stability can be crucial for green hydrogen generation to achieve carbon neutrality and address energy demands. Herein, Mndoped NiBP microsphere electrocatalyst is synthesized by combining hydrothermal and electrochemical deposition. The Mn/NiBP microsphere exhibits low overpotentials of 62 and 250 mV for hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) at 50 mA/cm2 in 1 M KOH. The Mn/NiBP (-) || Mn/NiBP (+) demonstrates a low cell voltage of 3.07 V at 2000 mA/cm2 in 1 M KOH, suppressing the benchmark Pt/C (-) || RuO2 (+). Further, the Pt/C (-) || Mn/NiBP (+) hybrid system exhibits an ultra-low cell voltage of 2.82 Vat 2000 mA/cm2 in 1 M KOH, indicating electrocatalytic robustness and strong anti-corrosion resistance of Mn/NiBP microspheres. Mn doping on NiBP microspheres accelerates charge transfer and enhances electrocatalytic activity, making it a cost-effective electrocatalyst candidate for industrial applications.
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NR 86
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AU Pham, TM
   Plevova, M
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Francke, R
AF Pham, Trang Minh
Plevova, Michaela
Bartling, Stephan
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Springer, Armin
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Francke, Robert
TI Oxygen-deficient annealing boosts performance of CoNiFe oxide electrocatalyst in oxygen evolution reaction
SO JOURNAL OF CATALYSIS
LA English
DT Article
DE Alkaline water electrolysis; Oxygen evolution reaction; Electrocatalyst; Cobalt; Nickel; Iron; Oxygen vacancy
ID WATER OXIDATION; GREEN HYDROGEN; ALKALINE; OXYHYDROXIDE; ELECTROLYZER; EFFICIENCY; VACANCIES; CATALYST; NICO2O4; COBALT
AB Mixed oxides of transition metals have emerged as promising catalysts for the oxygen evolution (OER) reaction in alkaline water electrolysis. Since OER is significantly slower than hydrogen evolution, developing stable and easily accessible materials that effectively promote OER is one of the keys to improving overall efficiency. In this context, we present a promising method for preparing Co-Ni-Fe oxides which is based on a straightforward sol-gel procedure. Key to success is a thermal treatment under oxygen-deficient atmosphere, which renders superior electrocatalytic properties compared to a treatment under reductive and aerobic conditions, respectively. Attractive performance characteristics are thereby obtained, e.g., a n10 value of 291 mV and a Tafel slope of 32 mV dec- 1. The impact of the annealing conditions on the material properties has been elaborated using cyclic voltammetry, impedance spectroscopy, and structural analyses. Stability and strong performance under practical conditions were confirmed in long-term studies using an AEM electrolyzer.
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TI Highly efficient and robust nickel-iron bifunctional catalyst coupling
selective methanol oxidation and freshwater/seawater hydrogen
evolution<i> via</i> CO-free pathway
SO CHEMICAL ENGINEERING JOURNAL
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DT Article
DE Nickel-iron catalyst; Selective oxidation of methanol; Hydrogen

evolution; Electrochemical water; seawater splitting; CO-free pathway
ID WATER; ELECTROCATALYSTS; NANOSHEETS; CARBON; HETEROSTRUCTURE; CONVERSION; CRYSTALS; NANORODS
AB The production of green hydrogen by water electrolysis is often kinetically limited by the sluggish oxygen evolution reaction (OER) at the anode. Here, we prepared a bifunctional nickel foam supported NiFe2O4 spinel catalyst (i.e. NiFe2O4/NF) that is capable of facilitating the coupling of hydrogen evolution reaction (HER) with selective methanol oxidation reaction (SMOR) in seawater to produce formate via a CO-free pathway. At a cell potential of 2.0 V, the NiFe2O4/NF||NiFe2O4/NF catalyzed HER-SMOR system produces remarkably high current density (>800 mA cm-2) with high Faradaic efficiencies (FE) at both electrodes (>96 % for HER and >95 % for SMOR to formate). The NiFe2O4/NF||NiFe2O4/NF HER-SMOR system also exhibits excellent stability over 48 h of continuous operation. With H2 being the only gaseous product, the HER-SMOR electrolysis system could operate in the absence of a membrane. Furthermore, the NiFe2O4/NF||NiFe2O4/NF electrodes are sufficiently robust for continuously catalyzing HER-SMOR in seawater electrolysis, showing no sign of deactivation or chlorine oxidation reactions over 6 h of continuous operation at a high current density of 700 mA cm-2. Mechanistic investigation and DFT calculations reveal that SMOR proceeds via a CO-free pathway, with Ni and Fe as the active sites for methanol and OH activation, respectively.
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TI Highly Efficient and Stable Saline Water Electrolysis Enabled by Self-Supported Nickel-Iron Phosphosulfide Nanotubes With Heterointerfaces and Under-Coordinated Metal Active Sites
SO ADVANCED FUNCTIONAL MATERIALS
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DT Article
DE electronic structure modulations; hydrogen evolution; saline water electrolyses; self-supported NiFeSP electrodes; urea oxidation
ID HYDROGEN EVOLUTION; OXYGEN EVOLUTION; BIFUNCTIONAL ELECTROCATALYST; PERFORMANCE; ELECTROOXIDATION; NANOSHEET; CATALYSTS; PYRITE; UREA
AB Direct seawater electrolysis is proposed as a potential low-cost approach to green hydrogen production, taking advantage of the vastly available seawater and large-scale offshore renewable energy being deployed. However, developing efficient, earth-abundant electrocatalysts that can survive under harsh corrosive conditions for a long time is still a significant technical challenge. Herein, the fabrication of a self-supported nickel-iron phosphosulfide (NiFeSP) nanotube array electrode through a two-step sulfurization/phosphorization approach is reported. The as-obtained NiFeSP nanotubes comprise abundant NiFeS/NiFeP heterointerfaces and under-coordinated metal sites, exhibiting outstanding activity and durability for the hydrogen and oxygen evolution reactions (HER and OER) in simulated alkaline-seawater solution (KOH + NaCl), with an overpotential of 380 (HER) and 260 mV (OER) at 500 mA cm(-2) and outstanding durability of 1000 h. Theoretical calculations support the observed outstanding performance, showing that the heterointerface and under-coordinated metal sites synergistically lower the energy barrier of the rate-determining step reactions. The NiFeSP electrode also shows good catalytic performance for the urea oxidation reaction (UOR). By coupling UOR with HER, the bifunctional NiFeSP electrode pair can efficiently catalyze the overall urea-mediated alkaline-saline water electrolysis at 500 mA cm(-2) under 1.938 V for 1000 h without notable performance degradation.
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TC 62
Z9 63
U1 25
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PU WILEY-V C H VERLAG GMBH
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J9 ADV FUNCT MATER
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WC Chemistry, Multidisciplinary; Chemistry, Physical; Nanoscience &
   Nanotechnology; Materials Science, Multidisciplinary; Physics, Applied;
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WE Science Citation Index Expanded (SCI-EXPANDED)
SC Chemistry; Science & Technology - Other Topics; Materials Science;
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AU Ahmed, HE
   Rashed, AE
   El-Khouly, ME
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AF Ahmed, Hany E.
   Rashed, Ahmed E.
   El-Khouly, Mohamed E.
   Albolkany, Mohamed K.
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TI Green approach for sustainable production of paraffin fuel from
   CO₂ hydrogenation on Fe-MOF catalyst
SO JOURNAL OF ENVIRONMENTAL CHEMICAL ENGINEERING
LA English
DT Article
DE Carbon dioxide hydrogenation; Paraffin fuel; Natural gas; Kerosene;
   Iron-based catalyst; Metal-organic frameworks
ID METAL-ORGANIC FRAMEWORKS; FISCHER-TROPSCH SYNTHESIS; CONVERSION;
   NANOPARTICLES; TEMPERATURE; PERFORMANCE; METHANATION; MIL-100(FE);
   PHOTOCATALYST; DEGRADATION
AB With increasing global fuel demand, circular carbon economy and related carbon-neutral fuels are a cleaner way to reduce CO2 emissions significantly. Our work involves utilizing green hydrogen formed by water electrolysis and CO(2)to produce paraffin hydrocarbon (up to C-16) using a well-distributed and small particle size (similar to 3 nm) iron-based metal-organic framework (Fe-MOF) catalyst. The MIL-100(Fe) MOF precursor was synthesized with a green, cost-efficient, large-scale, and facile room temperature method. The highest CO2 conversion (44.1 %) and low CO selectivity (7.5 %) was attained at 340 C and 30 bar. The paraffin hydrocarbon product (99 %, yielding 40.3 %) is composed mainly of natural gas (C-1-C-4) (90 %) and liquid fuel (10 %) in the gasoline range (C-5-C-12). However, adjusting conditions at 300 C and 10 bar directed the liquid fuel to the kerosene range C-5-C-16 (11 %). The catalyst's capacity to function as an industrial catalyst was proved after more than 120 h on a continuous stream without sintering or deactivation. Compared to reference catalyst and earlier work, the unpromoted FeMOF-derived catalyst shows excellent potential for CO2 mitigation and production of combined gas and liquid alkane fuel.
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TC 6
Z9 7
U1 20
U2 49
PU ELSEVIER SCI LTD
PI London
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SN 2213-2929
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PT J
AU Tan, YH
   Yang, HT
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   Hu, JC
   Tian, GC
   Yu, XH
AF Tan, Yuhua
   Yang, Haitao
   Cheng, Jiaxin
   Hu, Jiacheng
   Tian, Guocai
   Yu, Xiaohua
TI Preparation of hydrogen from metals and water without CO₂
   emissions
SO INTERNATIONAL JOURNAL OF HYDROGEN ENERGY
LA English
DT Review
DE Hydrogen production; Metal energy; Metal -water reactions; Water
   cracking; Low carbon
ID AL-BASED MATERIALS; MG-BASED MATERIALS; FUEL PRODUCTION; GENERATION;
   ALUMINUM; HYDROLYSIS; IRON; POWER; OXIDATION; CARBON
AB Considering the high calorific value and low-carbon characteristics of hydrogen energy, it will play an important role in replacing fossil energy sources. The production of hydrogen from renewable energy sources for electricity generation and electrolysis of water is an important process to obtain green hydrogen compared with classic low-carbon hydrogen production methods. However, the challenges in this process include the high cost of liquefied hydrogen and the difficulty of storing hydrogen on a large scale. In this paper, we propose a new route for hydrogen storage in metals, namely, electricity generation from renewable energy sources, electrolysis to obtain metals, and subsequent hydrogen production from metals and water. Metal monomers facilitate large-scale and long-term storage and transportation, and metals can be used as large-scale hydrogen storage carriers in the future. In this technical route, the reaction between metal and water for hydrogen production is an important link. In this paper, we systematically summarize the
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OI Tan, Yuhua/0009-0008-5072-9103; Tian, Guocai/0000-0002-0913-6903
FU National Natural Science Foundation of China; Yunnan Ten Thousand
   Talents Plan Young & Elite Talents Project; [51504231]; [51774158];

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   Juneja, G
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AF Saptal, Vitthal B.
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TI B(C₆F₅)₃: a robust catalyst for the
   activation of CO₂ and dimethylamine borane for the
   <i>N</i>-formylation reactions
SO NEW JOURNAL OF CHEMISTRY
LA English
DT Article
ID FRUSTRATED LEWIS PAIRS; DEFINED IRON CATALYST; CARBON-DIOXIDE;
   AMMONIA-BORANE; PROPARGYL REARRANGEMENT; TRANSFER HYDROGENATIONS;
   FORMIC-ACID; AMINES; CYCLIZATION; EFFICIENT
AB In this work, B(C6F5)(3) is utilized as an organocatalyst for the transition-metal-free N-formylation of amines using carbon dioxide (CO2) as a C1 source and dimethylamine borane (Me2NH center dot BH3) as a green hydrogen transfer source at 80 degrees C. Most reported works utilize silane and hydrogen for the N-formylation reactions using CO2 which have thus far been limited by low atom economy, high cost or the use of harsh reaction conditions. This catalytic protocol affords a broad range of formylated products in moderate to excellent yields under mild reaction conditions with a high TON and TOF. The bulky boron (B(C6F5)(3)) catalyst reacts with amines and forms a Frustrated Lewis Pair (FLP) and activates CO2 and Me2NH center dot BH3 molecules. Additionally, this boron catalyst shows high catalytic activity for the cyclization of o-phenylenediamines using CO2 and Me2NH center dot BH3 to synthesize benzimidazoles.
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TI Decoupled supercapacitive electrolyzer for membrane-free water splitting
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ID HYDROGEN-PRODUCTION; OXYGEN EVOLUTION; HIGH-PERFORMANCE;
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AB Green hydrogen production via water splitting is vital for decarbonization of hard-to-abate industries. Its integration with renewable energy sources remains to be a challenge, due to the susceptibility to hazardous gas mixture during electrolysis. Here, we report a hybrid membrane-free cell based on earth-abundant materials for decoupled hydrogen production in either acidic or alkaline medium. The design combines the electrocatalytic reactions of an electrolyzer with a capacitive storage mechanism, leading to spatial/temporal separation of hydrogen and oxygen gases. An energy efficiency of 69% lower heating value (48 kWh/kg) at 10 mA/cm(2) (5 cm-by-5 cm cell) was achieved using cobalt-iron phosphide bifunctional catalyst with 99% faradaic efficiency at 100 mA/cm(2). Stable operation over 20 hours in alkaline medium shows no apparent electrode degradation. Moreover, the cell voltage breakdown reveals that substantial improvements can be achieved by tunning the activity of the bifunctional catalyst and improving the electrodes conductivity. The cell design offers increased flexibility and robustness for hydrogen production.
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Jin, Zhaoyu
TI Understanding the Atomic and Defective Interface Effect on Ruthenium Clusters for the Hydrogen Evolution Reaction
SO ACS CATALYSIS
LA English

DT Article
DE electrocatalysis; single-atomic site; substrate effect; vacancy defect;
   hydrogen evolution reaction
ID DENSITY-FUNCTIONAL THEORY; UNDERPOTENTIAL DEPOSITION; OXYGEN; ENERGY;
   ELECTROCATALYSTS; NANOPARTICLES; EFFICIENT; CATALYST
AB Water electrolysis powered by renewable electric energy is a promising technology for green hydrogen production without carbon emissions, while highly efficient and cost-effective electrocatalysts with long durability are urgently needed. Here, we demonstrate oxygen-coordinated single-atom iron sites (Fe-O-4) decorated carbon nanotubes with abundant vacancies as the substrate for stabilizing Ru clusters (CNT-V-Fe-Ru). The catalyst shows high performance for the hydrogen evolution reaction (HER) in both acidic and alkaline media, respectively. The HER kinetics analysis demonstrates that the defective substrate with single-atomic sites could significantly improve the intrinsic activity of Ru species. Theoretical calculations also support the superior HER behavior of CNT-V-Fe-Ru with fundamental insights into metal-substrate interactions. The present study highlights a unique feature of single-atom catalysts for serving as advanced supporting materials, which offers tremendous opportunities to adequately regulate electronic structures of metal-substrate interfaces at the atomic level.
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TI Insight into the Co/Fe intrinsically assembled structure in
   cobalt-iron-layered double hydroxides on catalytic oxygen evolution
   reaction
SO MATERIALS TODAY ENERGY
LA English
DT Article
DE Electrocatalysis; CoFe-LDHs; Intrinsic structure engineering; Oxygen
   vacancy; Electron structure modulation; Oxygen evolution reaction
ID TOTAL-ENERGY CALCULATIONS; HIGHLY EFFICIENT; COFE-LDH; COOOH
AB Green hydrogen production via water electrolysis is crucial to the strategic path toward carbon neutrality. Therefore, exploration of efficient and low-cost electrocatalysts for oxygen evolution reaction (OER) is essential due to the sluggish OER kinetics, where cobalt-iron-layered double hydroxides (CoFe-LDHs) represent a class of promising OER catalysts. Herein, a systematic study gives insights into the Co/Fe intrinsically assembled structures in CoFe-LDHs on their catalytic performances in OER, representing a new route for rational design of catalysts. Theoretical calculations suggest that the electron structure at exposed active sites can be modulated by varying the Co/Fe assembled structure and introducing oxygen vacancy. The structural characterizations of the as-synthesized CoFe-LDHs with varied Co/Fe assembled structures indicate that Co1Fe3-LDHs-Vo induces the suitable distortion in the octahedral unit structure of [CoO6] with a shorter cobalt-oxygen bonding distance and hence leads to the favorable Co active sites exposed for the formation of oxygenated intermediates. Consequently, the Co1Fe3-LDHs-Vo exhibits the unprecedented OER activity with an overpotential of 253 mV at 50 mA/cm2 and Tafel value of 26.8 mV/ dec. The overall water splitting is driven by a voltage of 1.47 V at 10 mA/cm2 in 1.0 M KOH electrolyte.(c) 2023 Elsevier Ltd. All rights reserved.
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TI Improved biohydrogen evolution through calcium ferrite nanoparticles assisted dark fermentation
SO BIORESOURCE TECHNOLOGY
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DE Dark fermentation; Hydrogen yield; Calcium ferrite nanoparticles; Soluble metabolites; Microbial structure
ID HYDROGEN-PRODUCTION; SLUDGE; NANOTECHNOLOGY
AB Dark fermentation (DF) is a green hydrogen (H2) production process, but it is far below the theoretical H2 yield. In this study, calcium ferrite nanoparticles (CaFe2O4 NPs) were produced to augment H2 yield via DF. The highest H2 yield of 250.1 +/- 6.5 mL/g glucose was achieved at 100 mg/L CaFe2O4 NPs. Further increase in CaFe2O4 NPs above 100 mg/L, such as 600 mg/L, would slightly lower H-2 yield to 208.6 +/- 2.6 mL/g glucose. The CaFe2O4 NPs in DF system released calcium and iron ions, promoting granular sludge formation and DF microbial activity. Soluble metabolites revealed that butyric acid was raised by CaFe2O4 NPs, which indicated the improved metabolic pathway for more H-2. Microbial structure composition further illustrated that CaFe2O4 NPs could increase the abundance of dominant microbial populations, with the supremacy of Firmicutes up to 71.22 % in the bioH(2) evolution group augmented with 100 mg/L CaFe2O4 NPs.
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AF Khan, Abuzar
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TI Red mud as high-performance bifunctional electrocatalysts in alkaline
media
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LA English
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DE Red mud recycling; Laser annealing; Bifunctional electrocatalyst; Green
hydrogen production; Sustainability
ID HYDROGEN EVOLUTION; NICKEL FOAM; WATER; IRON; CATALYST
AB Red mud, an industrial byproduct containing metal oxides, is typically landfilled, posing environmental hazards like soil and water contamination. This study investigated the potential of red mud as a cost-effective bifunctional electrocatalyst for oxygen evolution reaction and hydrogen evolution reaction. Red mud samples from two different geographic locations were laser-annealed onto nickel foam substrates and their electrochemical activity was systematically evaluated and compared with benchmark electrocatalysts under alkaline conditions. The results showed that, sample RM2/NF demonstrated the lowest overpotential during oxygen evolution reaction at current densities of 10, 50, and 100 mA cm-2, followed by the sample, RM1/NF. Specifically RM1/NF required 310 mV to achieve a current density of 10 mA cm-2, outperforming RM2/NF and benchmark IrO2. For hydrogen evolution reaction, RM1/NF exhibited slightly higher activity than RM2/NF at lower overpotentials, needing only 125 mV to reach current density of 10 mA cm-2. Electrochemical impedance spectroscopy measurement indicated a lower charge transfer resistance for both electrodes. Chronoamperometric measurements showed that RM1/NF had limited stability during oxygen evolution reaction while RM2/NF

maintained superior stability during hydrogen evolution reaction over extended periods. The enhanced electrocatalytic performance of the RM2/NF electrode highlights the potential of red mud as an effective electrocatalyst, likely due to its rich elementalcomposition including iron, aluminum, titanium, and vanadium.

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NR 42
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An, BH
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TI Cation-induced interface electric field redistribution and molecular orbital coupling in Co-FeS/MoS₂for boosting electrocatalytic overall water splitting
SO CHEMICAL ENGINEERING JOURNAL
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DT Article
DE Bifunctional electrocatalyst; Electric field redistribution; Ion doping; Orbital coupling
ID BIFUNCTIONAL ELECTROCATALYSTS; CATALYST; SULFIDE; SHELL; IRON; NI
AB A green hydrogen economy requires efficient bifunctional electrocatalysts for simultaneous hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). In this study, a mild sulfuration strategy was used to create a Co-FeS/MoS2 catalyst from metal-organic frameworks (MOFs) on foam nickel. This catalyst exhibits exceptional activity in 1 M KOH, only requiring ultralow overpotentials of 63 mV and 230 mV to

achieve current densities of 10 mA cm(-2) and 100 mA cm(-2) for the HER and OER processes. Additionally, it achieves a low cell voltage of 1.45 V at 10 mA cm(-2), surpassing reported catalysts. DFT calculations and XPS tests show that Co introduction induces high-valence Fe active sites and facilitates interface electric field redistribution. Crystal orbital Hamilton population (COHP) calculations reveal d-p orbital hybridization, enhancing conductivity and charge transfer kinetics. This research sheds light on the catalytic impacts of metal cations on transition metal sulfides to design high efficient electrocatalysts.
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TI Interface oxygen vacancy enhanced alkaline hydrogen evolution activity
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LA English
DT Article
DE Hollow hexagonal rods; Heterojunctions; Oxygen vacancy; Optimized
electronic structure; Superior HER activity
ID N-DOPED CARBON; EFFICIENT; NANOTUBES; ELECTROCATALYSTS; HETEROJUNCTION;
COP
AB Electrocatalytic hydrogen evolution reaction (HER) is a promising way to develop the green hydrogen economy. Transition metal phosphides (TMPs) based hybrids are potential catalyst candidates for HER. Herein, hollow hexagonal rods (HHRs) of Co-Fe-P/CeO2 heterojunctions are fabricated using the metal-organic frameworks (MOFs) as the templates. The hollow frame provides abundant active sites and sufficient mass transfer, the interfacial synergistic effects and the oxygen vacancies at the interface could modulate the electronic structure, improve the water dissociation, and optimize the hydrogen adsorption free energy (delta G(H)*). As a result, the Co-FeP/CeO2 HHRs nanohybrids exhibit excellent HER performances, for which a current density of 10 mA cm(-2) can be obtained at an overpotential of only 69.7 mV in alkaline medium, together with good long-term durability. The results supply the novel platform and useful guidelines for design and construction of non-noble metal based composite electrocatalysts towards HER.
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TI Greenhouse Gas Emission Dynamics of Saudi Arabia: Potential of Hydrogen Fuel for Emission Footprint Reduction
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DE greenhouse gas emissions; hydrogen; renewable energy; Saudi Arabia
ID ENERGY; CHALLENGES; CAPTURE; STORAGE
AB The growth of population, gross domestic product (GDP), and urbanization have led to an increase in greenhouse gas (GHG) emissions in the Kingdom of Saudi Arabia (KSA). The leading GHG-emitting sectors are electricity generation, road transportation, cement, chemicals, refinery, iron, and steel. However, the KSA is working to lead the global energy sustainability campaign to reach net zero GHG emissions by 2060. In addition, the country is working to establish a framework for the circular carbon economy (CCE), in which hydrogen acts as a transversal facilitator. To cut down on greenhouse gas emissions, the Kingdom is also building several facilities, such as the NEOM green hydrogen project. The main objective of the article is to critically review the current GHG emission dynamics of the KSA, including major GHG emission driving forces and prominent emission sectors. Then, the role of hydrogen in GHG emission reduction will be explored. Finally, the researchers and decision makers will find the helpful discussions and recommendations in deciding on appropriate mitigation measures and technologies.
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SC Science & Technology - Other Topics; Environmental Sciences & Ecology
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TI Coupling Fe(II)/Fe(III) Redox Mediated SO₂ Conversion with
Hydrogen Production
SO ADVANCED FUNCTIONAL MATERIALS
LA English
DT Article
DE anodic electrooxidation; electrocatalysis; hydrogen production; iron
redox; sulfur dioxide

ID CATALYTIC-ACTIVITY; EVOLUTION; BIOMASS
AB Water electrolysis is recognized as a green hydrogen production technology, but the high voltage required for anodic oxygen evolution reaction restricts the practical application. In this work, a Fe(II)/Fe(III) redox mediated SO2 conversion is proposed to couple the cathodic hydrogen evolution reaction to achieve sulfur dioxide conversion and hydrogen production at low voltage. The onset potential of Fe(II) electrooxidation to Fe(III) is as low as 0.75 V-RHE (vs reversible hydrogen electrode). Ex situ ultraviolet spectroscopy (UV) spectrum and ion chromatography indicate that SO2 in electrolyte can reduce Fe(III) to Fe(II), completing the Fe(II)/Fe(III) redox cycle as well as the conversion of SO2 to sulfuric acid. The assembled flow cell electrolyzer requires a low operating voltage of 0.97 V at 10 mA cm(-2) and shows good performance under both acidic and neutral conditions. This work proposes an innovative energy saving and environment friendly strategy for simultaneous hydrogen production and sulfur dioxide capture based on low-cost catalyst materials.
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TI CoFe hydroxide towards CoP2-FeP4 heterojunction for efficient and
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DT Article
DE Self-corrosion mechanism; Heterointerface; Electron redistribution;
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ID INITIO MOLECULAR-DYNAMICS; HYDROGEN EVOLUTION; HIGHLY EFFICIENT;
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AB Electrochemical water splitting stands out as a promising avenue for green hydrogen production, yet its efficiency is fundamentally governed by the oxygen evolution reaction (OER). In this work, we investigated the growth mechanism of CoFe hydroxide formed by in situ self-corrosion of iron foam for the first time and the significant influence of dissolved oxygen in the immersion solution on this process. Based on this, the CoP2-FeP4/IF heterostructure catalytic electrode demonstrates exceptional OER activity in a 1 M KOH electrolyte, with an overpotential of only 253 +/- 4 mV (@10 mA cm-2), along with durability exceeding 1000 h. Density functional theory calculations indicate that constructing heterojunction interfaces promotes the redistribution of interface electrons, optimizing the free energy of adsorbed intermediate during the water oxidation process. This research highlights the importance of integrating self-corroding in-situ growth with interface engineering techniques to develop efficient water splitting materials.
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AB Water electrolysis for green hydrogen production is gaining tremendous attention in the quest towards sustainable energy sources. At the heart of water splitting technology are the electrocatalysts, which facilitate the two half-cell reactions, i.e., the hydrogen evolu-tion reaction (HER) and oxygen evolution reaction (OER), with the latter being the most thermodynamically uphill. Herein, we managed to fabricate Ni1-xFexO microflowers (mFs) with varying % of Fe doping (0 < x < 0.36) via an easy chemical bath deposition (CBD) method. The as-synthesized mFs drop-casted on graphene paper (GP) are then applied as electrocatalysts for OER. Compared to contrast catalysts, the electrocatalyst with xFe = 0.1 exhibits a lower overpotential of 297 mV at a current density of 10 mA cm-2, Tafel slope of 44 mV dec-1 and unprecedented turnover frequency of 4.6 s-1 at 300 mV. It is believed that this remarkable electrochemical performance mainly stems from the synergistic effects of
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DE Mirco Gas Turbine; Combustion; Hydrogen; Emissions
AB On the way to defossilization, green hydrogen is a promising way to substitute natural gas and oil in the gas turbine industry.
   In the scope of the H2mGT project, a micro gas turbine (mGT) burner with 100% hydrogen firing is developed and validated. The project is funded by the German BMWK and it is a collaboration between TUB and the manufacturer Euro-K GmbH. It consists of three phases: 1. Atmospheric pressure tests with a fused silica combustion chamber; 2. Atmospheric pressure tests with counterflow-cooled steel flame tube and secondary air injection; 3. Validation of the burner in the mGT at elevated pressure levels. The current study will present the results of Phase 2.
   The hydrogen burner used in the project is based on a swirl-stabilized burner of TUB and was scaled to 36 kW thermal power at atmospheric conditions. The burner design features a variable swirl intensity, additional axial momentum of air in the mixing tube, a movable central fuel lance and pilot nozzles at the front plate. Furthermore, the burners steel flame tube is exchangeable, which allows the evaluation of different dilution hole patterns and, thus, the variation of the ratio of primary and secondary air. The study presents temperature, pressure, and emission measurements. It is found that the flame can be operated over a large range of equivalence ratios and preheating temperatures up to 500 degrees C. As expected, the NOx emissions are mainly influenced by the local equivalence ratio, which can be controlled by the fuel mass flow or the dilution hole pattern in the flame tube. Furthermore, the results show a decrease of NOx when the power density is increased at constant equivalence ratios, and a rise of NOx during the fuel transition from natural gas to hydrogen. The results indicate certain differences to the findings of Phase 1.
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DE microgas turbine; combustion; hydrogen; emissions
ID GAS-TURBINE
AB On the way to defossilization, green hydrogen is a promising way to substitute natural gas (NG) and oil in the gas turbine industry. In the scope of the H2mGT project, a microgas turbine (mGT) burner with 100% hydrogen firing is developed and validated. The project is funded by the German BMWK, and it is a collaboration between Technische Universit & auml;t Berlin (TUB) and the manufacturer Euro-K GmbH. It consists of three phases: (1) atmospheric pressure tests with a fused silica combustion chamber; (2) atmospheric pressure tests with counterflow-cooled steel flame tube and secondary air injection; (3) validation of the burner in the mGT at elevated pressure levels. The current study will present the results of phase 2. The hydrogen burner used in the project is based on a swirl-stabilized burner of TUB and was scaled to 36 kW thermal power at atmospheric conditions. The burner design features a variable swirl intensity, additional axial momentum of air in the mixing tube, a movable central fuel lance, and pilot nozzles at the front plate. Furthermore, the steel flame tube is exchangeable, which allows the evaluation of different dilution hole patterns and, thus, the variation of the ratio of primary and secondary air. The study presents temperature, pressure, and emission measurements. It is found that the flame can be operated over a large range of equivalence ratios and preheating temperatures up to 500 degrees C. As expected, the NOx emissions are mainly influenced by the local equivalence ratio, which can be controlled by the fuel mass flow or the dilution hole pattern in the flame tube. Furthermore, the results show a decrease of NOx when the power density is increased at constant equivalence ratios, and a rise of NOx during the fuel transition from natural gas to hydrogen. The results indicate certain differences to the findings of phase 1.
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TI A comprehensive review on the role of hydrogen in renewable energy
   systems
SO INTERNATIONAL JOURNAL OF HYDROGEN ENERGY
LA English
DT Article
DE Hydrogen; Renewable energy; Energy storage; Sustainability
ID LIFE-CYCLE ASSESSMENT; MICROBIAL FUEL-CELL; ELECTRICITY-GENERATION;
   THERMOCHEMICAL CYCLE; BIOMASS GASIFICATION; DIRECT ELECTROLYSIS; WATER
   ELECTROLYSIS; LIQUID-HYDROGEN; STORAGE-SYSTEMS; GREEN HYDROGEN
AB Hydrogen is emerging as a critical player in transitioning to sustainable and renewable energy systems, serving roles in energy storage, grid balancing, and decarbonization. This paper explores various aspects of hydrogen, including its production through renewable-electricity-driven electrolysis, advanced storage techniques, and incorporation into current energy systems. It highlights primary electrolysis methods like PEM and alkaline, noting their improved efficiency and cost-effectiveness. Various hydrogen storage methods, such as physical, chemical, and advanced porous materials, are examined for their benefits and limitations. The review further explores hydrogen's integration into grid storage systems and microgrids to enhance energy reliability. It discusses hydrogen's application in fuel cells for electricity generation, focusing on technological advancements that improve efficiency and reduce costs. Additionally, the paper underscores hydrogen's crucial role in reducing CO2 emissions in industrial processes like steel production and its use in residential and commercial energy supply through combined heat and power systems. Economic aspects and supportive policies from regions are analyzed, highlighting the global efforts and policies supporting the potential hydrogen in renewable energy systems. This analysis emphasizes hydrogen's comprehensive role in enhancing renewable energy systems and achieving global sustainability objectives, providing a thorough review of recent progress and challenges.
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TI Kinetic Analysis of the Decomposition Reaction of CH₄ Injecting into Molten Slag
SO ISIJ INTERNATIONAL
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DT Article
DE decomposition of CH4; kinetic analysis; rate constant; molten slag; injecting of methane
ID PHASE-CHANGE MATERIAL; LATENT-HEAT STORAGE; WASTE HEAT; THERMOELECTRIC PROPERTIES; METHANE; SYSTEM; PCM; STEELWORKS; PARTICLES; MECHANISM
AB Utilization of heat of slag is key technology for the reduction of CO2 emission in steel industries. While hydrogen production is important for the society of aiming to the sustainable energy system, the green hydrogen must be produced for the actual CO2 reduction.

In the present study, methane gas was injected into a molten slag and hydrogen was produced through the thermal decomposition reaction.

CH4 = C + 2H(2)

Kinetic analysis was performed using an graphite crucible both with empty and slag.

The rate constants for the graphite crucible, k(G) and the slag, k(S), were obtained separately. The rate constants for graphite surface and slag surface, k(G) and k(S), respectively, are as follows:

k(G) / cm . s(-1) = 41.74 x exp(51 741/RT) +/- 0.05

k(S) / cm . s(-1) = 4.053 x 10(6) x exp(190 310/RT) +/- 0.05

Using the obtained rate constants, the increase of the area of reaction surface during the CH4 injection was estimated.

It was found that the slow soaking of the injecting lance could be utilized for the heat of molten slag. In addition, the slag shape can be a powder type through the injection of CH4.
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TI Hydrogen and Oxygen Evolution on Flexible Catalysts Based on Nickel-Iron Coatings
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DT Article

DE nickel; iron; morpholine borane; electroless metal plating; water splitting; hydrogen evolution; oxygen evolution
ID EFFICIENT; ELECTROCATALYSTS; PERFORMANCE; FOAM
AB The electrolysis of water is one of low-cost green hydrogen production technologies. The main challenge regarding this technology is designing and developing low-cost and high-activity catalysts. Herein, we present a strategy to fabricate flexible electrocatalysts based on nickel-iron (NiFe) alloy coatings. NiFe coatings were plated on the flexible copper-coated polyimide surface (Cu/PI) using the low-cost and straightforward electroless metal-plating method, with morpholine borane as a reducing agent. It was found that Ni90Fe10, Ni80Fe20, Ni60Fe40, and Ni30Fe70 coatings were deposited on the Cu/PI surface; then, the concentration of Fe2+ in the plating solution was 0.5, 1, 5, and 10 mM, respectively. The morphology, structure, and composition of NixFey/Cu/PI catalysts have been examined using scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), X-ray diffraction (XRD), and inductively coupled plasma-optical emission spectroscopy (ICP-OES), whereas their activity has been investigated for hydrogen evolution (HER) and oxygen evolution (OER) reactions in 1 M KOH using linear sweep voltammetry (LSVs). It was found that the Ni80Fe20/Cu/PI catalyst exhibited the lowest overpotential value of -202.7 mV for the HER, obtaining a current density of 10 mA cm-2 compared to Ni90Fe10/Cu/PI (-211.9 mV), Ni60Fe40/Cu/PI (-276.3 mV), Ni30Fe70/Cu/PI (-278.4 mV), and Ni (-303.4 mV). On the other hand, the lowest OER overpotential (344.7 mV) was observed for the Ni60Fe40/Cu/PI catalyst, obtaining a current density of 10 mA cm-2 compared to the Ni35Fe65 (369.9 mV), Ni80Fe20 (450.2 mV), and Ni90Fe10 (454.2 mV) coatings, and Ni (532.1 mV). The developed Ni60Fe40/Cu/PI catalyst exhibit a cell potential of 1.85 V at 10 mA cm-2. The obtained catalysts seem to be suitable flexible catalysts for HER and OER in alkaline media.
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TI Repurposing the current collector of a car battery module into a bifunctional electrode for overall electrochemical water splitting
SO SUSTAINABLE ENERGY & FUELS
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ID ACTIVE FE SITES; OXYGEN EVOLUTION; EFFICIENT ELECTROCATALYST; HYDROGEN EVOLUTION; CATHODIC CORROSION; HIGHLY EFFICIENT; NI-FOAM; CATALYST; SURFACE; NANOSHEETS
AB Renewable power-driven electrochemical water splitting is rapidly emerging as a viable approach for producing large scale green hydrogen which is free from greenhouse gas emissions. However, there is a continuous need to develop electrocatalysts that are abundant and can be generated with minimal impact on the environment. Here, we explore the possibility of repurposing the anode current collector from a Toyota Prius battery module as a bifunctional electrocatalyst that can be used for overall electrochemical water splitting under alkaline conditions. The Ni coated iron electrode was found to have ideal properties for both the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) while also demonstrating bifunctional behaviour for both reactions upon repetitive cycling. The repurposed material also outperformed a Ni electrode of comparable surface area for both the OER and HER and demonstrated activity that is comparable to chemically synthesised Fe/Ni materials. The key aspect for enabling this behaviour was found to be the emergence of iron into the nickel coating to create a stable mixed FeNi oxide layer upon potential cycling of the electrode. This also resulted in a bifunctional electrode material that could operate between HER and OER without a loss of activity. This work indicates that not only should the active materials used in rechargeable batteries be used for recycling but that the current collectors should also be considered as potentially highly valuable components.
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PU ROYAL SOC CHEMISTRY
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TI Recent Advances in the Mitigation of the Catalyst Deactivation of
CO₂ Hydrogenation to Light Olefins
SO CATALYSTS
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DE CO2 hydrogenation; light olefins; catalyst deactivation;
CO2-Fischer-Tropsch (CO2-FT); iron-based catalysts; methanol to olefins;
bifunctional composite catalysts; SAPO-34
ID HIGHLY SELECTIVE CONVERSION; FISCHER-TROPSCH SYNTHESIS; FE-BASED
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CO/TIO2 CATALYSTS; IRON; STABILITY; SAPO-34
AB The catalytic conversion of CO2 to value-added chemicals and fuels has been long regarded as a promising approach to the mitigation of CO2 emissions if green hydrogen is used. Light olefins, particularly ethylene and propylene, as building blocks for polymers and plastics, are currently produced primarily from CO2-generating fossil resources. The identification of highly efficient catalysts with selective pathways for light olefin production from CO2 is a high-reward goal, but it has serious technical challenges, such as low selectivity and catalyst deactivation. In this review, we first provide a brief

summary of the two dominant reaction pathways (CO2-Fischer-Tropsch and MeOH-mediated pathways), mechanistic insights, and catalytic materials for CO2 hydrogenation to light olefins. Then, we list the main deactivation mechanisms caused by carbon deposition, water formation, phase transformation and metal sintering/agglomeration. Finally, we detail the recent progress on catalyst development for enhanced olefin yields and catalyst stability by the following catalyst functionalities: (1) the promoter effect, (2) the support effect, (3) the bifunctional composite catalyst effect, and (4) the structure effect. The main focus of this review is to provide a useful resource for researchers to correlate catalyst deactivation and the recent research effort on catalyst development for enhanced olefin yields and catalyst stability.
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TI Integrating multiphasic CuS_x/FeS_x nanostructured
   electrocatalyst for enhanced oxygen and hydrogen evolution reactions in
   saline water splitting
SO JOURNAL OF ALLOYS AND COMPOUNDS
LA English
DT Article
DE Oxygen evolution reaction (OER); Hydrogen evolution reaction (HER);
   Transitional metal sulfides (TMSs); Copper sulfide; Iron Sulfide;
   Seawater
ID NICKEL FOAM; THIN-FILMS; IRON; NANOSHEETS; EFFICIENT; FABRICATION;
   SULFIDES; ALKALINE; CATALYST; XPS
AB This study employed an electrodeposition approach to synthesize multiphasic CuSx and FeSx on nickel foam (NF) for application in saline water splitting. This multiphasic electrocatalyst exhibits a cauliflower morphology and develops a porous fused-type morphology upon partial oxidation. The NF/CuSx/FeSx electrode with partial oxidation exhibits the lowest overpotential of 181 mV at 10 mA/cm(2) and a Tafel slope of 163 mV/decade for the oxygen evolution reaction (OER). The overpotential of 73 mV at 10 mA/cm(2) and a Tafel slope of 165 mV/decade were found for the hydrogen evolution reaction (HER). A charge transfer coefficient value of similar to 0.5 in OER and HER indicates that the rate-determining step depends on the surface adsorption of reaction species. The presence of an unpaired electron during partial oxidation can create additional active sites and reduce solution resistance (R-s). This can improve the interaction between reactants and intermediates, improving OER and HER performance. NF/CuSx/FeSx composites demonstrated robust stability using real seawater splitting over 80 hours in HER with negligible degradation. However, catalyst breakdown in OER after 10 hours due to prolonged exposure to higher potentials, resulting in oxidative corrosion. This study offers a multiphasic electrode design using the electrodeposition technique to produce green hydrogen energy through seawater splitting.
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PT J
AU Okur, O
   Lu, PS
AF Okur, Osman
   Lu, Pinar Sakoglu
TI Development of a green catalytic route to light olefins by
   Fischer-Tropsch synthesis with renewable hydrogen: Investigation of
   boron doped activated carbon supported iron catalyst
SO INTERNATIONAL JOURNAL OF HYDROGEN ENERGY
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DT Article
DE Green hydrogen; Boron doped activated carbon; Fischer-tropsch synthesis;
   Light olefins
ID NANOPARTICLES; PERFORMANCE; SODIUM; SYNGAS; CO2
AB Hydrogen economy will open the door to a low carbon future and Fischer-Tropsch Synthesis (FTS) is one of the sustainable and carbon neutral catalytic route to a variety of products such as light olefins, kerosene, gasoline etc. when CO and H2 come from catalytic reduction of air captured CO2 and water electrolysis using the surplus renewable electricity, respectively. The aim of this study is to discover the new catalysts towards the sustainable C2-C4 olefins. Activated carbon (AC) supported zinc titanates w/o boron doping have been prepared and investigated for olefins via FTS. AC was deliberately chosen due to its surface structure more prone to modifi-cation since boron (B) is known to increase the interaction between surface metal atoms and defects. The B-doped AC supported iron catalyst showed comparable catalytic stability as the original AC supported one. However, an only increase in light olefin selectivity was observed with B-doping treated at 800 C. On the other side, a higher CH4 and paraffin but

lower olefin and C5+ selectivity was obtained at the lower thermal treatments. B-doping appeared to improve the catalytic stability but not to bring the expected catalytic activity and selec-tivity. The strong interaction between the surface metal sites and boron is believed to cause the restricted for-mation of active sites that leads less CO conversions.
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TI Seed-assisted formation of NiFe anode catalysts for anion exchange
   membrane water electrolysis at industrial-scale current density
SO NATURE CATALYSIS
LA English
DT Article
ID HYDROGEN-PRODUCTION; EVOLUTION; STABILITY; ELECTROCATALYSTS;
   PERFORMANCE; EFFICIENCY; FILMS
AB Alkaline oxygen evolution reaction is critical for green hydrogen production from water electrolysis but encounters great challenges when operated at industry-required ampere-scale current densities, such as insufficient mass transfer, reduced catalytic activity and limited lifetimes. Here we develop a one-step seed-assisted heterogeneous nucleation method (25 degrees C, 24 h) for producing a nickel-iron-based electrocatalyst (CAPist-L1, where CAP refers to the centre of artificial photosynthesis) for robust oxygen evolution reaction at >= 1,000 mA cm(-2). Based on the insoluble nanoparticles in the heterogeneous nucleation system, a dense interlayer is formed that anchors the catalyst layer tightly on the substrate, ensuring stable long-term durability of 15,200 h (>21 months) in 1 M KOH at 1,000 mA cm(-2). When applying CAPist-L1 as the anode catalyst in practical anion exchange membrane water electrolysis, it delivers a high activity of 7,350 mA cm(-2) at 2.0 V and good stability at 1,000 mA cm(-2) for 1,500 h at 80 degrees C.
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TI Fe-Ni-F electrocatalyst for enhancing reaction kinetics of water oxidation
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DT Article
DE Fluoride; Oxygen evolution reaction; Fe-Ni-F; Reaction kinetics
ID OXYGEN EVOLUTION; EFFICIENT ELECTROCATALYST
AB Highly active and low-cost oxygen evolution reaction (OER) catalytic electrodes are extremely essential for exploration of green hydrogen via water splitting. Herein, an advanced Fe-Ni-F electrocatalyst is fabricated by a facile annealing strategy using ammonium fluoride, of which the structure feature is unveiled by XRD, FESEM, TEM, EDS, BET, and XPS measurements. The as-prepared Fe-Ni-F addresses a low overpotential of 277 mV and a small Tafel slope of 49 mV dec(-1) at a current density of 10 mA cm(-2), significantly outperforming other control samples as well as the state-of-the-art RuO2. The advanced nature of our Fe-Ni-F catalyst could also be further evidenced from the robust stability in KOH alkaline solution, showing as 5.41% degradation after 24 h continuous working. Upon analysis, it suggests that the decent catalytic activity should be attributed to the formed bimetallic (oxy)hydroxides because of the introduction of fluoride and the synergistic effect of iron and nickel towards oxygen generation. This work represents the potential of Fe- and/or Ni-based fluoride as efficient catalyst for low-energy consumption oxygen generation.
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RI Cao, Yulin/E-1787-2011; Wang, Chundong/HDN-4227-2022; Hu, Chao/O-8030-2015; Humayun, Muhammad/M-6632-2015
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AF Cao, Yihua
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   Zhang, Xin
TI Coupling effect and electronic modulation for synergistically enhanced
   overall alkaline water splitting on bifunctional Fe-doped CoBi/CoP
   nanoneedle arrays
SO JOURNAL OF COLLOID AND INTERFACE SCIENCE
LA English
DT Article
DE CoBi/CoP hybrid; Fe doping; Bifunctional electrocatalysts; Electron
   modulation; Synergistic effect
ID HYDROGEN EVOLUTION; OXYGEN EVOLUTION; ELECTROCATALYST; EFFICIENT;
   NANOSHEETS; CATALYST; FILM
AB Designing bifunctional electrocatalysts with high efficiency and low cost for water splitting is urgently required for the production of green hydrogen. Herein, a bifunctional iron-doped cobalt borate/cobalt phosphide hybrid supported on nickel foam (Fe-CoBi/CoP/NF) was fabricated via hydrothermal and phosphating process. Benefit from the unique nanoneedle architecture for faster mass transfer, the existence of borate on CoBi for accelerating proton transfer, the moderate adsorption of H* species on CoP, Fe doping and the synergistic effect between CoBi and CoP, Fe-CoBi/CoP/NF hybrid exhibits a low overpotential of 137 mV and 260 mV at 100 mA cm-2 for hydrogen evolution reaction (HER) and oxygen evolution reaction (OER), respectively. Moreover, Fe-CoBi/CoP/ NF||Fe-CoBi/CoP/NF also presents a low cell potential of 1.65 V@100 mA cm-2 for overall alkaline water splitting and excellent durability (128 h) without decay. This work provides a new insight into the design of bifunctional electrocatalysts simultaneously through the morphological engineering and heteroatomic doping.
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TI Magnetite<i>-Bacillus subtilis</i> synergy on the metabolic selection of
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DE Platform chemicals; Green Hydrogen; Bioelectronic circuit; Electron
   shuttle; Nanomaterials
ID EXTRACELLULAR ELECTRON-TRANSFER; DARK FERMENTATION; FOOD WASTE; IRON;
   NANOTECHNOLOGY
AB The study examines the role of magnetite (1-150 mg/L) at the interface of Bacillus subtilis-electrode under poisedcondition (-0.2 V) for product-formation and catalytic-conduct with the relative-gene-expression encoding lactate dehydrogenase (lctE), pyruvate dehydrogenase (pdhA), acetate kinase (ackA), pyruvate carboxylase (pycA), and NADH dehydrogenase (ndh). The magnetite load of 25 mg/L showed positive influence on acidogenesis resulting in H-2 production of 264.7 mol/mL and fatty acids synthesis of 3.6 g/L. Additionally, this condition showed higher succinic acid productivity (2.8 g/L) which correlates with the upregulated pycA gene and fumarate to succinate redox peak. With 10 mg/L loading, production of higher acetic acid (3.1 g/L) along with H2 (181.6 mol/mL) was depicted wherein upregulation of pdhA, ackA and ndh genes was observed. In absence of magnetite, lctE gene was upregulated which resulted higher lactate production. The findings suggest that the mutual-interactions between magnetite-active sites of specific enzymes enhances the biocatalytic activity triggering product-formation.
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NR 50
TC 10
Z9 10
U1 6
U2 18
PU ELSEVIER SCI LTD
PI London
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SN 0960-8524
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J9 BIORESOURCE TECHNOL
JI Bioresour. Technol.
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PT J
AU Komiya, H
Shinagawa, T
Takanabe, K
AF Komiya, Hiroki
Shinagawa, Tatsuya
Takanabe, Kazuhiro
TI Electrolyte Engineering for Oxygen Evolution Reaction Over Non-Noble Metal Electrodes Achieving High Current Density in the Presence of Chloride Ion
SO CHEMSUSCHEM
LA English
DT Article
DE electrocatalysis; electrochemistry; electrolytes; seawater; water splitting
ID MAGNETIC-PROPERTIES; MANGANESE OXIDE; WATER; COBALT; OXIDATION; IRON; CATALYST; SEAWATER; FILM; EFFICIENCY
AB Direct seawater electrolysis potentially simplifies the electrolysis process and leads to a decrease in the cost of green hydrogen production. However, impurities present in the seawater, especially chloride ions (Cl-), cause corrosion of the electrode material, and its oxidation competes with the anodic oxygen evolution reaction (OER). By carefully tuning electrode substrate and electrolyte solutions, the CoFeOxHy/Ti electrode with high double-layer capacitance actively and stably electro-catalyzed the OER in potassium borate solutions at pH 9.2 in the presence of 0.5 mol kg(-1) Cl-. The electrode possesses an active site motif composed of either a Co- or Fe-domain and benefits from an enlarged surface area. Selective OER was demonstrated in Cl--containing electrolyte solutions at an elevated reaction temperature, stably achieving 500 mA cm(-2) at a mere potential of 1.67 V vs. reversible hydrogen electrode (RHE) at 353 K for multiple on-off and long-term testing processes with a faradaic efficiency of unity toward the OER.
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FU JSPS KAKENHI [19KK0126]; Mohammed bin Salman Center for Future Science and Technology for Saudi-Japan Vision 2030 at The University of Tokyo [MbSC2030]
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NR 68
TC 18
Z9 18
U1 6
U2 95
PU WILEY-V C H VERLAG GMBH
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PA POSTFACH 101161, 69451 WEINHEIM, GERMANY
SN 1864-5631
EI 1864-564X
J9 CHEMSUSCHEM
JI ChemSusChem
PD OCT 10
PY 2022
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WC Chemistry, Multidisciplinary; Green & Sustainable Science & Technology
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AU Mohapatra, L
Rathour, A
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Kushwaha, AK
AF Mohapatra, Lokanath
Rathour, Ajay
Sonwane, Akshay Kumar
Samanta, Aniket
Dalapati, Goutam
Kushwaha, Ajay Kumar
TI Substrate and potential-driven surface morphology of bifunctional Ni-Fe electrode for efficient alkaline water electrolysis
SO JOURNAL OF ELECTROANALYTICAL CHEMISTRY
LA English
DT Article
DE Ni-Fe alloy; Oxygen evolution reaction; Hydrogen evolution reaction; Electrodeposition; Water electrolysis; Green hydrogen; Bifunctional catalyst
ID HYDROGEN EVOLUTION; FACILE SYNTHESIS; ALLOY; ELECTROCATALYST; NANOCUBES; CATALYSTS
AB Nickel-iron (Ni-Fe) alloy electrodes are synthesized using chronoamperometry. The influence of substrate type (copper, stainless steel, and nickel) and deposition potential on the structural, morphological, and electrocatalytic characteristics are systematically investigated. X-ray diffraction (XRD) analysis revealed the formation of a face-centered cubic (FCC) Ni-Fe alloy. Electrodeposition at higher potential (-1.45 V) forms well-defined nanoflakes, whereas electrodeposition at lower potential (-1.00 V) results aggregated Ni-Fe particles. The NiFe alloy electrodes having well-defined nanoflakes demonstrated superior electrocatalytic performance, exhibiting a overpotential of -168 mV vs. RHE for the hydrogen evolution reaction (HER) and 236 mV vs. RHE for the oxygen evolution reaction (OER), at current density of 10 mA/cm2. The enhanced electrocatalytic activity of the nanoflakes based Ni-Fe alloy is attributed due to their larger catalytic surface area, porous morphology and higher Fe concentration. The Ni-Fe alloy electrodes displayed bifunctional electrocatalytic behavior, making them highly suitable for both HER and OER processes.
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NR 46
TC 0
Z9 0
U1 16
U2 16
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PI LAUSANNE
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PD DEC 1

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WC Chemistry, Analytical; Electrochemistry
WE Science Citation Index Expanded (SCI-EXPANDED)
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PT J
AU Meng, XY
Wang, M
Zhang, YC
Li, ZH
Ding, XG
Zhang, WQ
Li, C
Li, Z
AF Meng, Xin-ying
Wang, Meng
Zhang, Yicong
Li, Zhihao
Ding, Xiaogang
Zhang, Weiquan
Li, Can
Li, Zhen
TI Superimposed OER and UOR performances by the interaction of each component in an Fe-Mn electrocatalyst
SO DALTON TRANSACTIONS
LA English
DT Article
ID LAYERED DOUBLE HYDROXIDE; OXYGEN EVOLUTION; HIGHLY-EFFICIENT; NICKEL FOAM; WATER; MODULATION; HYDROGEN; IRON; CRYSTALLINE; NANOSHEETS
AB The oxygen evolution reaction (OER) and alternative urea oxidation reaction (UOR) are both important half reactions correlated with hydrogen production. Transition metal based catalysts with double metal composition exhibit excellent electrocatalytic performance for the OER or UOR due to their synergetic effect and coupling of different active sites. However, the development of OER/UOR bifunctional electrocatalysts is unsatisfying and the role of each metallic active site in the OER and UOR is still unclear. Herein, we report a Fe-Mn based OER and UOR bifunctional catalyst through a simple one-step electrodeposition method. For the OER, the introduction of Mn improves the conductivity of the catalysts and fine-tunes the electron density of the Fe active sites. For the UOR, both Fe and Mn act as active sites and their coupling effect further improves the UOR activity. The catalyst with the optimal Mn/Fe ratio achieved an overpotential of 237 mV for the OER and a potential of 1.35 V for the UOR at 100 mA cm(-2). This study provides a simple synthesis protocol for constructing bifunctional catalysts for green hydrogen production.
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TI Interwoven N-doped carbon nanotubes with capped Ni-doped FeP as
   double-functional electrocatalysts for overall seawater electrolysis
SO SCIENCE CHINA-MATERIALS
LA English
DT Article
DE metal-organic frameworks; phosphide; carbon nanotubes; seawater
   electrolysis; bifunctional catalyst
ID METAL-ORGANIC FRAMEWORKS; OXYGEN EVOLUTION REACTION; HIGHLY EFFICIENT;
   HYDROGEN; NANOSHEETS; CATALYST; NANOPARTICLES; CONSTRUCTION; CO;
   PERFORMANCE
AB Seawater electrolysis technology powered by clean new energy is recognized as the most promising sustainable and green hydrogen preparation method. The extremely expensive and low reserve of commercially available noble metal electrocatalysts and the rapid inactivation of catalysts under complex ionic environments hamper their industrialization. Herein, a novel interwoven N-doped carbon nanotube (N-CNTs) structure capped with Ni-doped FeP nanoparticles (NFP@NC) is successfully developed by Ni-doped Fe cluster-catalyzed CNT growth process and the gas phosphating method. The unique interwoven nanotube network and strong interaction of Ni-doped FeP and N-CNTs provide fast mass transfer and gas bubble emission, as well as drastically enhanced stability. The NFP@NC presents an overpotential of 280 mV for the oxygen evolution reaction and 206 mV for the hydrogen evolution reaction at 10 mA cm(-2), lower than most reported iron-based catalysts. This research provides an effective way to construct interwoven CNT networks as high-performance bifunctional seawater electrolysis catalysts.
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TI Oxygen defect engineering on low-crystalline iron(iii) oxyhydroxide as a highly efficient electrocatalyst for water oxidation
SO INORGANIC CHEMISTRY FRONTIERS
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DT Article
ID EVOLUTION REACTION; NANOSHEETS; CATALYST; VACANCIES
AB Improving the water oxidation performance of non-precious nanoelectrocatalysts is the key to developing green hydrogen energy. Herein, we developed a simple method to synthesize FeOOH nanocatalysts with low crystallinity and oxygen vacancies (V-O). These catalysts demonstrate excellent electrocatalytic performance for water oxidation. The V-O-FeOOH catalyst exhibits an overpotential of 255 mV at 10 mA cm(-2) and maintains stability for more than 120 hours at a high current output (50 mA cm(-2)). DFT calculations show that the rate-determining step (RDS) of V-O-FeOOH and FeOOH is O* to OOH* (the Gibbs free energy (Delta G) of the RDS is 1.65 eV and 1.91 eV, respectively). This result indicates that V-O can effectively reduce the energy barrier from *O to *OOH of the OER process, thus improving the activity of the V-O-FeOOH nanocatalysts. Our focus was on utilizing one of the abundant metallic elements to fabricate defect-rich OER electrocatalysts with improved performance through a convenient one-step synthesis approach. This methodology shows great promise for the development of high-performance catalysts.
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AB Hydrogen is believed to be one of the essential clean secondary energy sources in the energy structure revolution of both industry and daily life. Driven by renewable electricity such as solar and wind power, water electrolysis for hydrogen production is deemed as one of the main processes of green hydrogen production in the future by both academia and industry. Transition metal chalcogenides (TMCs) are promising candidates to replace noble metals as earth-abundant electrocatalysts for water splitting. However, it remains challenging to further improve the electrocatalytic activity and long-term stability of TMCs, especially in a practical water electrolyzer. This Review summarizes the recent advances and the strategies of optimizing the electrocatalytic activities of TMCs toward water splitting as well as the latest investigations on the surface reconstructions of TMCs during water electrolysis. The performances of TMCs in practical electrocatalytic water splitting cells are particularly discussed. Finally, a concluding remark and perspective is provided, and we hope to inspire future works in this area, narrowing the gap between material design and practical application.
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TI Nickel foam supported Mn-doped NiFe-LDH nanosheet arrays as efficient bifunctional electrocatalysts for methanol oxidation and hydrogen evolution
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DT Article
DE Electrocatalysis; Methanol oxidation reaction; Formate; Hydrogen fuel; Bifunctional catalyst
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AB Electrochemical upgrading methanol into value-added formate at the anode in alkaline media enables the boosting production of hydrogen fuel at the cathode with saved energy. To achieve such a cost-effective and efficient electrocatalytic process, herein this work presents a Mn-doped nickel iron layered double hydroxides supported on nickel foam, derived from a simple hydrothermal synthesis. This developed electrocatalyst could act as an efficient bifunctional electrocatalyst for methanol-to-formate with a high faradaic efficiency of nearly 100 %, and for hydrogen evolution reaction, at an external potential of 1.5 V versus reversible hydrogen electrode. Additionally, a current density of 131.1 mA cm-2 with a decay of merely 12.2 % over 120 h continuous long-term testing was generated in co-electrocatalysis of water/methanol solution. Further density functional theoretical calculations were used to unravel the methanol-to-formate reaction mechanism arising from the doping of Fe and/or Mn. This work offers a good example of co-electrocatalysis to produce formate and green hydrogen fuel using a bifunctional electrocatalyst.
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TI Short-time potentiostatic assisted borate to induce the generation of
ultrathin NiFe LDH active phase for industrial-level water oxidation
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DT Article
DE NiFe-based; Oxygen evolution reaction; NiB4O7/Ni(Fe)OOH; Anion exchange
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ID ELECTROCATALYTIC OXYGEN EVOLUTION; IRON
AB Self-supported NiFe-based oxygen evolution reaction (OER) catalysts with high activity and durability are essential for the industrialization of green hydrogen. Herein, Boron-interfered NiFe LDH nanosheets (B-2-NiFe-(a-10)) with abundant wrinkle structure are prepared by introducing nonmetallic sources into the surface reconstruction of layered double hydroxide (NiFe LDH) through a novel short-time potential constant activation strategy. It enhances interactions with the electrolyte, decreases Arrhenius activation energy (Ea), accelerates efficient charge transfer and O-2 escape rate. The as-reconstructed B-2-NiFe-(a-10) exhibits outstanding alkaline OER activity with an ultralow overpotential of 290 mV at 100 mA cm(-2) and excellent durability (100 h). Additionally, density functional theory calculations further reveal that the interaction optimizes the adsorption of oxygenated intermediates (*OH ->*O), induces the center of the d-band toward the Fermi energy level, and lowers the dissociation barrier of H2O. Moreover, the anion-exchange membrane water electrolyzer (AEMWE) achieves a current density of 1 A cm(-2) at 1.97 V.

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U1 28
U2 46
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PA PO BOX 564, 1001 LAUSANNE, SWITZERLAND
SN 1385-8947
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J9 CHEM ENG J
JI Chem. Eng. J.
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WC Engineering, Environmental; Engineering, Chemical
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SC Engineering
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PT J
AU Deng, GX
Liao, YW
Lin, YK
Ding, L
Wang, HH
AF Deng, Guoxiong
Liao, Yiwen
Lin, Yakai
Ding, Li
Wang, Haihui
TI Engineering Robust Triazine Crosslinked and Pyridine Capped Anion Exchange Membrane for Advanced Water Electrolysis
SO ANGEWANDTE CHEMIE-INTERNATIONAL EDITION
LA English
DT Article
DE Anion exchange membrane; alkaline water electrolysis; non-precious metal catalysts
ID PIPERIDINIUM) MEMBRANES; HIGH-PERFORMANCE; POLYMER; OPERATION; IONOMERS; WORKING; CATIONS
AB Exploring high-performance anion exchange membranes (AEM) for water electrolyzers (AEMWEs) is significant for green hydrogen production. However, the current AEMWEs are restricted by the poor mechanical strength and low OH- conductivity of AEMs, leading to the low working stability and low current density. Here, we develop a robust AEM with polybiphenylpiperidium network by combining the crosslinking with triazine and the capping with pyridine for advanced AEMWEs. The AEM exhibits an excellent mechanical strength (79.4MPa), low swelling ratio (19.2%), persistent alkali stability (approximate to 5,000hours) and high OH- conductivity (247.2mScm(-1)) which achieves the state-of-the-art AEMs. Importantly, when applied in AEMWEs, the corresponding electrolyzer equipped with commercial nickel iron and nickel molybdenum catalysts obtained a current density of up to 3.0 Acm(-2) at 2V and could be stably operated similar to 430h at a high current density of 1.6Acm(-2), which exceeds the most of AEMWEs. Our results suggest that triazine crosslinking and pyridine capping can effectively improve the overall performance of the AEMWEs.

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OI Ding, Li/0000-0002-2393-1188; Wang, Haihui/0000-0002-2917-4739
FU Nation Natural Science Foundation of China [22138005, 22141001, 22378226, 22422809]; Young Elite Scientists Sponsorship Program by BAST
FX We gratefully acknowledge the funding from the Nation Natural Science Foundation of China (22138005, 22141001, 22378226, and 22422809), Young Elite Scientists Sponsorship Program by BAST.
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NR 54
TC 2
Z9 2
U1 59
U2 72
PU WILEY-V C H VERLAG GMBH
PI WEINHEIM
PA POSTFACH 101161, 69451 WEINHEIM, GERMANY
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JI Angew. Chem.-Int. Edit.
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WC Chemistry, Multidisciplinary
WE Science Citation Index Expanded (SCI-EXPANDED)
SC Chemistry
GA Q5C2P
UT WOS:001384852100001
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PT J
AU Sun, ZY
AF Sun, Zuoyu
TI Hydrogen Energy: Development Prospects, Current Obstacles and Policy
   Suggestions under China's "Dual Carbon" Goals
SO CHINESE JOURNAL OF URBAN AND ENVIRONMENTAL STUDIES
LA English
DT Article
DE Hydrogen energy; energy transformation; net zero emissions
AB Hydrogen energy has an advantage over conventional fossil energy because of its clean and low-carbon features, while its stability gives it an advantage over renewable energy sources such as hydropower, photovoltaic (PV) power, and wind power. Using hydrogen as a fuel can achieve zero carbon emissions or even net zero emissions at the end of energy conversion. Moreover, with hydrogen as the carrier, an energy system of multi-energy complementarity will be established by coupling multiple energy systems such as power grids, gas grids and heat networks, which can realize the comprehensive utilization of renewable energy sources in an efficient, stable, and flexible manner. Based on the "dual carbon" goals, this paper targets sectors with high carbon emissions represented by electric power, steel and transportation, analyzes the feasible path of using hydrogen energy to promote deep carbon reduction, and points out the obstacles faced by hydrogen energy development in various sectors. On account of the current development and expected prospects, this paper proposes that the current focus of hydrogen energy industry is to coordinate the development of industrial sectors and regions, build a pattern that can facilitate the industry's systematic and concerted development, address key technical challenges (such as green hydrogen production or hydrogen storage and transportation via pipeline), improve industrial standards, and promote the industry's development in a balanced, coordinated and orderly way.
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PU WORLD SCIENTIFIC PUBL CO PTE LTD
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J9 CHIN J URBAN ENV STU
JI Chin. J. Urban Env. Stud.
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WC Urban Studies
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SC Urban Studies
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AF Cholewa, T.
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Salem, O.
TI Reaction kinetics for ammonia synthesis using ruthenium and iron based catalysts under low temperature and pressure conditions
SO SUSTAINABLE ENERGY & FUELS
LA English
DT Article
AB Ammonia (NH3) production using green hydrogen and its emerging application as carbon-free energy carrier or fuel is predicted to play an important role for the global energy transition. Yet, the inherently fluctuating production of hydrogen from renewable energy and the corresponding new boundary conditions for NH3 synthesis require efficient and intensified processes. A key strategy for the intensification of the NH3 synthesis is the shift of the synthesis conditions to lower temperature and pressure compared to the conventional Haber-Bosch process. In this work, the reaction kinetics of ruthenium- and iron-based catalysts are determined experimentally at pressures between 10 to 80 bar and at temperatures from 350 to 450 degrees C. Using axially resolved temperature and concentration measurement, detailed experimental data were obtained in the kinetic regime and utilized to develop kinetic models for both catalysts. Therefore, an ideal plug-flow model for a fixed bed reactor, considering the axial temperature profile, is used to estimate the kinetic parameters. The developed kinetic models are based on the extension

of the Temkin equation, which is adapted for both catalysts. Remaining deviation between simulated and experimental data is reduced to a root-mean-square error for the molar fraction of NH3 of below 0.6%. The proposed extension of the Temkin equation allowed the reduction of this deviation by 20-30% compared to the conventional Temkin expression, which underlines the relevance of the novel kinetic expressions. Based on the validated kinetic models, concepts for process intensification and modularization of the NH3 synthesis can be developed towards industrial realization.
Reaction kinetics for the synthesis of NH3 from renewable H2 under mild reaction conditions.
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FU Bundesministerium fr Bildung und Forschung [03SF0634A]; German Federal Ministry of Education and Research [FKZ 20020/671]; Deutsche Bundesstiftung Umwelt (DBU)
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NR 41
TC 2
Z9 2
U1 10
U2 19
PU ROYAL SOC CHEMISTRY
PI CAMBRIDGE
PA THOMAS GRAHAM HOUSE, SCIENCE PARK, MILTON RD, CAMBRIDGE CB4 0WF, CAMBS,
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SN 2398-4902
J9 SUSTAIN ENERG FUELS
JI Sustain. Energ. Fuels
PD MAY 14
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VL 8
IS 10
BP 2245
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DI 10.1039/d4se00254g
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WC Chemistry, Physical; Energy & Fuels; Materials Science,
   Multidisciplinary
WE Science Citation Index Expanded (SCI-EXPANDED)
SC Chemistry; Energy & Fuels; Materials Science
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PT J
AU Kapelari, S
   Gamaletsos, PN
   Pilla, G
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AF Kapelari, Stergi
   Gamaletsos, Platon N.
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TI Developing a Low-Temperature, Carbon-Lean Hybrid Valorisation Process
   for Bauxite Residue (Red Mud) Towards Metallic Fe and Al Recovery
SO JOURNAL OF SUSTAINABLE METALLURGY
LA English
DT Article
DE Bauxite residue; Red mud valorization; H-2 gas; Fe reduction; Al
   recovery
ID IRON RECOVERY; RARE-EARTHS; REDUCTION; ALUMINUM
AB The present study deals with the recovery of metallic Fe and an Al-ion-rich liquid from bauxite residue (BR), with an Naion-rich liquid phase that could potentially be recycled or recovered as NaOH. First, BR was mixed with sodium hydroxide in mass ratios of 80/20 and 74/26, respectively. Then, each mixture was roasted under pure -H2 for 2 h at 500 degrees C, 550 degrees C and 600 degrees C. The thermal products were analyzed by

powder X-ray diffraction, which revealed the formation of metallic iron, sodium aluminum silicon oxide and perovskite, among other phases, along with an amorphous phase. Subsequent water leaching of the milled products resulted in an Al- and Na-ion-rich liquid and a metal-containing Fe-rich insoluble product. Chemical analysis of the liquid phase of the sample with the mass ratio of 74/26 after roasting at 600 degrees C showed that Al recovery was as high as 77%, while the average Fe content of the solid fraction reached approximately 38.5 wt%. A similar Fe content was also observed at lower temperatures, but the Al recovery was lower. The composition of the remaining solid phase consisted mainly of Ca, Si, Ti and some undissolved Na and Al, which accounted for less than 6 wt%. The findings of this study suggest that hydrogen reduction of BR is not only as efficient as carbothermic reduction, perhaps even more so, but also that it has the added advantage of producing significantly less -CO2 emissions, especially when green hydrogen is used in the process.
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FU European Community's Horizon 2020 Programme (H2020/2014-2019) (MSCA-ETN REDMUD) [636876]; Vlaio TOGETHER project
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NR 38
TC 11
Z9 11
U1 5
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PU SPRINGER
PI NEW YORK
PA ONE NEW YORK PLAZA, SUITE 4600, NEW YORK, NY, UNITED STATES
SN 2199-3823
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J9 J SUSTAIN METALL
JI J. SUST. METALL.
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IS 2
BP 578
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WC Green & Sustainable Science & Technology; Metallurgy & Metallurgical
   Engineering
WE Science Citation Index Expanded (SCI-EXPANDED)
SC Science & Technology - Other Topics; Metallurgy & Metallurgical
   Engineering
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PT J
AU Dongre, S
   Zuccante, G
   Muhyuddin, M
   Vecchio, CL
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AF Dongre, Sumanth
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   Balakrishna, R. Geetha
   Santoro, Carlo
TI Innovative biochar-based electrocatalysts from chilli plants and fruits
   for sustainable oxygen reduction and hydrogen evolution reactions
SO ELECTROCHIMICA ACTA
LA English
DT Article
DE Oxygen reduction reaction; Alkaline media; Platinum group metal-free
   electrocatalysts; Hydrogen evolution reaction; Biochar electrocatalysts
ID ACTIVATED CARBON; BIOMASS; FE; TECHNOLOGIES; CATALYSTS; ALKALINE

AB The rapid population growth and the subsequent energy demands have led to a surge in fossil fuel usage, resulting in unprecedented environmental challenges due to carbon emissions. Green hydrogen seems to be a promising avenue to tackle the negative effects of fossil fuels to achieve an environment-friendly and sustainable energy source. In this study, we present the development of iron and nickel-based electrocatalysts derived from biochar obtained from chilli plants and their fruits for cathodic oxygen reduction reaction (ORR) and hydrogen evolution reaction (HER). The biochar was produced by pyrolyzing the biomass at 600 degrees C and 800 degrees C, followed by KOH activation and functionalization with iron(II) phthalocyanine for ORR and nickel nanopowder for HER. Electrochemical tests in alkaline media (0.1 M KOH for ORR and 1 M KOH for HER) demonstrated significant electrocatalytic activity. The Plant-Fe 800 electrocatalyst achieved an onset potential of 0.97 V (vs RHE) and a half-wave potential of 0.87 V (vs RHE) for ORR with minimal peroxide yield. For HER, the Chilli-Ni 800 electrocatalyst showed an overpotential of roughly 0.41 V (vs RHE). The high performance of these biochar-based electrocatalysts can be attributed to their large surface area, effective Fe-Nx active site dispersion, and the presence of nitrogen-related defects within the carbon matrix. This study highlights the potential of using sustainable, biomass-derived materials to create efficient and cost-effective electrocatalysts, paving the way for green energy.
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FU Ministry of Foreign Affairs and International Cooperation (MAECI), Italian Government; European Union Next-Generation EU [PE00000004, 1551.11-10-2022]; Italy's Recovery and Resilient Plan; EU Recovery Plan; NextGeneration EU; Cariplo Foundation Call for Circular Economy through the project Transformation of plastic waste in Electrocatalysts, Supported by exhausted gases recovery Layout (TESLA)
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NR 59
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WC Electrochemistry
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SC Electrochemistry
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ER

PT J
AU Prieto, N
   da Silva, EL
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   Cuna, A
AF Prieto, N.
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   Cuna, A.
TI Synthesis and characterization of non-noble metal cathode
   electrocatalysts for PEM water electrolysis
SO ELECTROCHIMICA ACTA
LA English
DT Article
DE Water electrolysis; Hydrogen evolution reaction; Electrochemical
   impedance spectroscopy; Faradaic efficiency; Fe2P/C electrocatalyst
ID EFFICIENT HYDROGEN; IRON PHOSPHIDE; FE2P NANOPARTICLES; EVOLUTION;
   PERFORMANCE; NANOSHEETS; GRAPHENE; CATALYST; SUPPORT; ENERGY
AB The development of new cathode materials for electrolyzers is one of the important current challenges to lower the costs of green hydrogen (H2) production. In this work, a new and easy route for Fe2P-based electrocatalysts synthesis was proposed and studied for its application in the hydrogen evolution reaction (HER). The materials were prepared from an iron salt and activated biocarbon, involving different chemical and thermal treatments. The samples were characterized by chemical, morphological, structural and textural analysis. The electrocatalytical performance of the samples was tested in acid media by linear voltammetry experiments, electrochemical impedance spectroscopy (EIS) and chronoamperometric analysis, and compared with a commercial Pt/ C electrocatalyst. The Fe(20)/CHP700 sample presented the lower Eonset (-179 mV vs. RHE), a Tafel slope of 108 mV dec � 1, a charge transfer resistance about 1.7 ohm cm2 with a good electrocatalytic stability. However, these results are worse than those presented by the commercial Pt/C. EIS results reveals that the best performance of the electrocatalysts can be related with a higher surface capacitance of the sample. H2 production evaluation in galvanostatic mode reveals a direct proportion between the FE values with the applied current density, reaching a maximum of 84 % at -344.8 mA cm-2 for our used measurement setup. In conclusion, the synthesis proposed in this article allowed to obtain promising free noble metal based electrocatalyst for HER, but its requires improvements in some of the aforementioned aspects to be used in PEM water electrolysis.
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OI Cuna Suarez, Andres/0000-0002-1343-2772; Prieto, Natalia/0009-0007-5966-7992
FU Uruguayan Basic Sciences Development Program (PEDEClBA-Qumica); CSIC-Universidad de la Republica (CSIC I + D Project); [22520220100147UD]
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NR 53
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AU Hidalgo, D
Martín-Marroquín, JM
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TI The role of magnetic nanoparticles in dark fermentation
SO BIOMASS CONVERSION AND BIOREFINERY
LA English
DT Review
DE Additives; Green hydrogen; Nanomaterials; Magnetism; Renewable gases; Trace metals
ID ENHANCED BIOHYDROGEN PRODUCTION; IRON-OXIDE NANOPARTICLES; BIO-HYDROGEN PRODUCTION; NICKEL NANOPARTICLES; ETHANOLIGENENS-HARBINENSE; HEMATITE NANOPARTICLES; ANAEROBIC-DIGESTION; ELECTRON-TRANSFER; ESCHERICHIA-COLI; MIXED CULTURE
AB Dark fermentation holds great promise as a game-changing strategy in the field of biological hydrogen generation. With its ability to utilize a diverse range of organic feedstocks as a starting material, it offers the added advantage of waste valorization. Despite this, it has long been plagued by a low yield of hydrogen production when compared to traditional thermochemical processes. Recently, researchers have explored the use of nanoparticles as a means of intensifying the fermentation process. In this paper, the latest research on the use of metallic additives in dark fermentation, with a specific focus on naturally magnetic additives such as iron, nickel, and cobalt, is critically reviewed. The influence of these additives on the hydrogen generation process and the mechanisms that make it all happen are evaluated in detail. Optimal dosages for each additive type are also explored based on previous research. Finally, insightful suggestions for future research in this field are put forth. The conclusion is drawn that metal nanoparticles with natural magnetism, such as Fe, Ni, and Co, can improve hydrogen production, process stability, system start-up, and substrate utilization in dark fermentation. However, further research is needed to address various issues, including optimal dosage, operating conditions, microbial population dynamics, use of unconventional substrates, metal toxicity, morphology of metal additives, and potential risks generated by metals that remain in the system after fermentation. The exploration of combining several additives with complementary characteristics or properties is also proposed as an interesting line of research.

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TI Sustainable Hydrogen Generation Facilitated through Ethylene Glycol
   Oxidation in Fresh/Seawater with Cobalt- and Iron-Based Fluorinated
   Nanosheets
SO ENERGY & FUELS
LA English
DT Article
ID WATER OXIDATION; METAL; OXYGEN; REDUCTION; CHEMISTRY; MECHANISM;
   CATALYST; STORAGE; ARRAY
AB Replacing the kinetically sluggish and energy-intensive oxygen evolution reaction (OER) at the anode with the oxidation of more kinetically and thermodynamically favorable small organic molecules is a promising strategy for boosting hydrogen production. This study focuses on sustainable hydrogen generation at the cathode facilitated by the ethylene glycol oxidation reaction (EGOR) at the anode, coupled with the production of value-added formate. For this, we designed and deposited cobalt- and iron-based fluorinated two-dimensional (2D)-nanosheets (2D-CoFe@OF) through a straightforward hydrothermal method onto a nickel foam substrate (NF). The resulting 2D-CoFe@OF/NF exhibits an anodic potential that is 100 mV lower in a 0.5 M EG-added 1.0 M KOH electrolyte to achieve a benchmark electrolysis current density of 10 mA cm-2, compared to a pure 1.0 M KOH electrolyte. Additionally, assembling two identical 2D-CoFe@OF/NF||2D-CoFe@OF/NF electrode-based electrolyzers resulted in a 150 mV reduction in operating cell voltage when electrolyzing at 150 mA cm-2, particularly when the OER was replaced by EGOR, thereby demonstrating a significant improvement in energy efficiency. Under this condition, the electrolyzer demonstrated a nearly 100% Faradaic current efficiency for the hydrogen evolution reaction (HER). Furthermore, the practical application of this system studied with an EG-seawater electrolyzer suggests its potential to replace freshwater with abundant seawater, thereby expanding the horizon for sustainable hydrogen generation. This study, thus, highlights the promising potential of the 2D-CoFe@OF nanosheets on EGOR in seawater, advancing green hydrogen technology toward a more sustainable future.
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AU Ahmad, W
Koley, P
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Lakshman, R
Shin, YK
van Duin, ACT
Shrotri, A
Tanksale, A
AF Ahmad, Waqar
Koley, Paramita
Dwivedi, Swarit
Lakshman, Rajan
Shin, Yun Kyung
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Shrotri, Abhijit
Tanksale, Akshat
TI Aqueous phase conversion of CO₂ into acetic acid over
thermally transformed MIL-88B catalyst
SO NATURE COMMUNICATIONS
LA English
DT Article
ID METAL-ORGANIC FRAMEWORK; CARBON-DIOXIDE HYDROGENATION; EFFICIENT
SYNTHESIS; LOW-TEMPERATURE; FORMIC-ACID; IRON; METHANATION; FE;
PURIFICATION; FORMALDEHYDE
AB Sustainable production of acetic acid is a high priority due to its high global manufacturing capacity and numerous applications. Currently, it is predominantly synthesized via carbonylation of methanol, in which both the reactants are fossil-

derived. Carbon dioxide transformation into acetic acid is highly desirable to achieve net zero carbon emissions, but significant challenges remain to achieve this efficiently. Herein, we report a heterogeneous catalyst, thermally transformed MIL-88B with Fe-0 and Fe3O4 dual active sites, for highly selective acetic acid formation via methanol hydrocarboxylation. ReaxFF molecular simulation, and X-ray characterisation results show a thermally transformed MIL-88B catalyst consisting of highly dispersed Fe-0/Fe(II)-oxide nanoparticles in a carbonaceous matrix. This efficient catalyst showed a high acetic acid yield (590.1 mmol/g(cat).L) with 81.7% selectivity at 150 degrees C in the aqueous phase using LiI as a co-catalyst. Here we present a plausible reaction pathway for acetic acid formation reaction via a formic acid intermediate. No significant difference in acetic acid yield and selectivity were noticed during the catalyst recycling study up to five cycles. This work is scalable and industrially relevant for carbon dioxide utilisation to reduce carbon emissions, especially when green methanol and green hydrogen are readily available in future.

Carbon dioxide conversion into chemicals is essential for carbon capture and utilization. Here, the authors present a novel iron-based catalyst, synthesized from the thermal treatment of a parent metal-organic framework (MIL-88B), to produce a dual-active site for carbon dioxide reduction into acetic acid.
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OI Dwivedi, Swarit/0000-0002-4639-5576; Tanksale, Akshat/0000-0002-7087-0912; Shrotri, Abhijit/0000-0001-9850-7325; KOLEY, PARAMITA/0000-0001-7422-7767
FU Faculty of Engineering, Monash University; Australian Research Council [DP170104017]; Institute for Catalysis, Hokkaido University; Cooperative Research Program of Institute for Catalysis, Hokkaido University [19A1005]

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NR 55
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Z9 21
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AU Gao, ZX
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AF Gao, Zixiang
   Zeng, Dewang
   Wu, Shiliang
   Ren, Shaojun
   Zhou, Fu
   Gao, Ming
   Song, Feng
   Zhai, Yunfei
   Xiao, Rui
TI High-purity hydrogen production from real biomass pyrolysis vapors
   <i>via</i> a chemical looping process
SO SUSTAINABLE ENERGY & FUELS
LA English
DT Article
ID BIO-OIL; IRON-OXIDE; OXYGEN CARRIERS
AB H-2 production from renewable bio-oil is a promising way to supply green hydrogen; however, this technology suffers from the high viscosity, high corrosiveness, and complex compositions of the bio-oil. Thus, in the present study, we propose a novel method that converts real biomass pyrolysis vapors into H(2)via a chemical looping process. Fe-Al-Ni composite oxide pellets were prepared in a simple and industrial way and then used as the oxygen carrier (OC), and their redox activity and cycle stability were assessed in a fixed-bed reactor system under different conditions with pine sawdust volatiles as the fuel. The results indicated that the Fe-Al-Ni composites exhibited nearly 99% CO2 selectivity in the reduction stage and high H-2 purity (>98%) in the H-2 production stage when the redox temperature was higher than 850 degrees C. X-ray diffraction (XRD) analysis of the Fe-Al-Ni composite oxide pellets at different bed layers indicated that Fe2O3 can be reduced to FeO by sawdust pyrolysis vapors, and an inert spinel phase of Fe-Al-O was formed concurrently. Coke deposited on the OC would hinder reduction, thereby decreasing the fuel conversion and H-2 energy efficiency, but it can be improved by increasing the pyrolysis temperature. Long cycling tests showed that a relatively stable H-2 energy efficiency of 20% and a H-2 purity of 98% could be obtained in whole tests; nevertheless, the conversion of CH4 declined rapidly after 25 cycles, which could be attributed to the interior sintering, iron migration to the outer surface and garnet phase (Al3Fe5O12) formation of the OC according to the scanning electron micrograph, micro texture, and XRD analysis of the OC with different cycling tests.
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NR 37
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U1 8
U2 46
PU ROYAL SOC CHEMISTRY
PI CAMBRIDGE
PA THOMAS GRAHAM HOUSE, SCIENCE PARK, MILTON RD, CAMBRIDGE CB4 0WF, CAMBS,
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JI Sustain. Energ. Fuels
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AF Chang, Jiuli
Song, Fengfeng
Xu, Fang
Wu, Dapeng
Hou, Yan
Jiang, Kai
Guo, Yuming
Gao, Zhiyong
TI Enhanced electrocatalytic efficiencies for water electrolysis and para-nitrophenol hydrogenation by self-supported nickel cobalt phosphide-nickel iron layered double hydroxide p-n junction
SO JOURNAL OF COLLOID AND INTERFACE SCIENCE
LA English
DT Article
DE Phosphide; Layered double hydroxide; P-n junction; Hydrogen evolution reaction; Oxygen evolution reaction; Para-nitrophenol hydrogenation
ID METAL PHOSPHIDE; EVOLUTION; NANOSHEETS; REDUCTION; ALKALINE
AB Charge redistribution across heterointerfaces is an important tactic to enhance the catalytic activities and bifunctionality of hybrid catalysts, especially for green hydrogen production from water electrolysis and harmless electrocatalytic valorization of organics. Herein, a self-supported p-n junction catalytic electrode was constructed by tandem electrodeposition of nickel cobalt phosphide (NiCoP) and nickel iron layered double hydroxide (NiFe LDH) onto Ni foam (NF) substrate, denoted as NiCoP@NiFe LDH/NF, to enhance the electro catalytic capabilities for water electrolysis and hydrogenation of an organic, para-nitrophenol (4-NP). Benefitting from the charge redistribution across the p-n junction, high electrocatalytic efficiencies for oxygen evolution reaction (OER, overpotential of 388 mV at 100 mA cm-2) and hydrogen evolution reaction (HER, overpotential of 132 mV at 10 mA cm-2) could be achieved concurrently by the NiCoP@NiFe LDH/NF electrode, and both overpotentials were located within the mainstream levels in this domain. The bifunctional catalytic features enabled a full water electrolysis response of 10 mA cm-2 at 1.61 V. In addition, the p-n junction electrode- catalyzed the hydrogenation of 4-NP at a conversion of 100%, para-aminophenol (4-AP) selectivity of 90% and faradaic efficiency (FE) of 88% at-0.18 V. The current work offers a feasible strategy for fulfilling electro-chemical H2 production and hydrogenation valorization of 4-NP pollutant by constructing a self-supported p-n junction catalytic electrode.
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AU Gaikwad, A
   Maga, D
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TI Influence of RED-II Calculation Rules on the Carbon Footprint of
   Methanol E-Fuel
SO CHEMIE INGENIEUR TECHNIK
LA English
DT Article
DE Carbon capture and utilization; Hydrogen; Life cycle assessment;
   Methanol; RED-II
AB The carbon footprint of methanol from cradle-to-grave is evaluated using three process concepts to capture CO2, i.e., one using CO2 from direct air capture (DAC) and the other two utilizing CO2 from a steel mill's blast furnace gas (BFG). Hydrogen is supplied by onsite electrolysis, or from a German offshore wind park, or an Australian solar park with ammonia as hydrogen carrier. The study is of interest to life cycle assessment (LCA) practitioners, policymakers, and industries' management who are involved in regulating, planning, implementing, and operating projects which aim to produce fuels using hydrogen from electrolysis (so-called 'e-fuels'). The influence of assumptions in the RED-II delegated act regarding recycled carbon fuels and renewable liquid and gaseous fuels of

non-biological origin on the carbon footprint results is examined. The RED-II assumption regarding the credits for captured CO2 after 2041 indicate that DAC-based concepts are advantageous with respect to BFG, although the LCA results indicate the opposite. Using green hydrogen from nearby locations reduces carbon footprints more than faraway locations due to transport-related emissions.
The RED-II directive has different assumptions to calculate life cycle emissions of fuels from traditional life cycle assessment. Its influence on the carbon footprint of e-methanol is examined with the help of three concepts to produce methanol from CO2: (a) CO2 from air, CO2 from blast furnace gas with (b) carbon capture, and (c) water-gas shift pathway. image
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AU Lindquist, GA
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AF Lindquist, Grace A.
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TI Performance and Durability of Pure-Water-Fed Anion Exchange Membrane Electrolyzers Using Baseline Materials and Operation
SO ACS APPLIED MATERIALS & INTERFACES
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DT Article
DE water electrolysis; membrane electrolysis; anion exchange membrane; ionomer stability; membrane conditioning
ID LAYERS; ACTIVATION; HYDROGEN
AB Water electrolysis powered by renewable electricity produces green hydrogen and oxygen gas, which can be used for energy, fertilizer, and industrial applications and thus displace fossil fuels. Pure-water anion-exchange-membrane (AEM) electrolyzers in principle offer the advantages of commercialized proton-exchange-membrane systems (high current density, low cross over, output gas compression, etc.) while enabling the use of less-expensive steel components and nonprecious metal catalysts. AEM electrolyzer research and development, however, has been limited by the lack of broadly accessible materials that provide consistent cell performance, making it difficult to compare results across studies. Further, even when the same materials are used, different pretreatments and electrochemical analysis techniques can produce different results. Here, we report an AEM electrolyzer comprising commercially available catalysts, membrane, ionomer, and gas-diffusion layers operating near 1.9 V at 1 A cm(-2) in pure water. After the initial break in, the performance degraded by 0.67 mV h(-1) at 0.5 A cm(-2) at 55 degrees C. We detail the key preparation, assembly, and operation techniques employed and show further performance improvements using advanced materials as a proof-of-concept for future AEM-electrolyzer development. The data thus provide an easily reproducible and comparatively high-performance baseline that can be used by other laboratories to calibrate the performance of improved cell components, nonprecious metal oxygen evolution, and hydrogen evolution catalysts and learn how to mitigate degradation pathways.
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ID METAL-SURFACES; NH3 ADSORPTION; DECOMPOSITION; NITROGEN; FE(100);
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AB Being rich in hydrogen and easy to transport, ammonia is a promising hydrogen carrier. However, a microscopic characterization of the ammonia cracking reaction is still lacking, hindered by extreme operando conditions. Leveraging state-of-the-art molecular dynamics, machine learning potentials, and enhanced sampling methods, we offer an atomistic view of the adsorption, diffusion, and dehydrogenation processes of a single NHx (x = 1, 3) molecule on two representative surfaces at the operando temperature of 700 K. We elucidate the effects of the dynamics on all the steps of decomposition. On the stable (110) surface, we found that the reaction intermediate diffusions are favored over dehydrogenation, with non-negligible effects on the reactivity for one intermediate. The role is even more dramatic on the (111) surface, where the mobility of Fe surface atoms introduces unexplored adsorption sites and significantly alters the dehydrogenation barriers. In both cases, a detailed analysis of reactive events shows that there is never a single transition state, but it is always an ensemble. Notwithstanding, a unified mechanism can be identified by following the charge transfer along the different reaction pathways.
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TI In-situ grown metal-organic framework-derived carbon-coated Fe-doped
   cobalt oxide nanocomposite on fluorine-doped tin oxide glass for acidic
   oxygen evolution reaction
SO APPLIED CATALYSIS B-ENVIRONMENTAL
LA English
DT Article
DE Water electrolysis; Metal-organic framework (MOF); Noble metal-free
   catalyst; Acidic water oxidation; Free-standing
ID ELECTROCATALYSTS; CO3O4; ROBUST; FILMS; FOAM
AB Development of stable and efficient non-noble metal based electrocatalysts for oxygen evolution reaction (OER) in acidic media is of great importance for proton exchange membrane based water electrolysis, which is indispensable for green hydrogen production. Herein, iron-doped, carbon-coated Co3O4 nanocomposite derived from a cobalt metal-organic framework, is grown in-situ on fluorine-doped tin oxide (FTO) glass (Fe-Co3O4@C/FTO) as an efficient and a stable binder-free electrode for acidic OER. Fe doping enhances both catalytic efficiency and stability of carbon coated Co3O4 toward acidic OER, through inducing small primary particle sizes and suitably modulated electronic structure of Co3O4, and better catalyst/substrate adhesion. Fe-Co3O4@C/FTO exhibits impressive electrocatalytic performances in 0.5 M H2SO4, with a low overpotential of 396 mV at 10 mA cm(-2) and a small Tafel slope of 68.6 mV dec(-1) . Its electrochemical performances remain stable for over 50 h at 10 mA cm(-2), making it a promising non-noble metal based electrocatalyst for acidic OER.
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TI Decarbonizing the European energy system in the absence of Russian gas: Hydrogen uptake and carbon capture developments in the power, heat and industry sectors
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DT Article
DE Stochastic programming; Energy transition; Carbon capture and storage; Hydrogen; Energy crisis
ID OPTIMIZATION; ELECTRICITY; TRANSMISSION
AB Hydrogen and carbon capture and storage are pivotal to decarbonize the European energy system in a broad range of pathway scenarios. Yet, their timely uptake in different sectors and distribution across countries are affected by supply options of renewable and fossil energy sources. Here, we analyse the decarbonization of the European energy system towards 2060, covering the power, heat, and industry sectors, and the change in use of hydrogen and carbon capture and storage in these sectors upon Europe's decoupling from Russian gas. The results indicate that the use of gas is significantly reduced in the power sector, instead being replaced by coal with carbon capture and storage, and with a further expansion of renewable generators. Coal coupled with carbon capture and storage is also used in the steel sector as an intermediary step when Russian gas is neglected, before being fully decarbonized with hydrogen. Hydrogen production mostly relies on natural gas with carbon capture and storage until natural gas is scarce and costly at which time green hydrogen production increases sharply. The disruption of Russian gas imports has significant consequences on the decarbonization pathways for Europe, with local energy sources and carbon capture and storage becoming even more important. Given the highlighted importance of carbon capture and storage in reaching the climate targets, it is essential that policymakers ameliorate regulatory challenges related to these value chains.
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TI Metal-organic framework derived iron-nickel sulfide nanorods for oxygen
evolution reaction
SO INTERNATIONAL JOURNAL OF HYDROGEN ENERGY

LA English
DT Article
DE Metal-organic framework; Oxygen evolution reaction; Electrocatalyst;
FeNi sulfide; FeNi (oxy)hydroxides; Amorphous
ID BIFUNCTIONAL ELECTROCATALYSTS; CARBON; WATER; REDUCTION; NANOSHEETS;
NANOTUBES; OXIDATION; CATALYST; COBALT
AB Highly efficient oxygen evolution reaction (OER) on noble metal-free catalysts is a major challenge for green hydrogen production. We report herein a rational preparation strategy for MOF-derived chalcogenide electrocatalysts. The optimal sulfuration time is 12 h under the conditions of the theoretical Fe/Ni ratio of 1:1 and treatment temperature at 120 degrees C. In this case, the pyrite Fe0.75Ni0.25S2 nanorods combining with amorphous FeNiOOH formed in situ exhibit a low overpotential of 247 mV with a small Tafel slope of 47.6 mV dec(-1) at a current density of 10 mA cm(-2) in alkaline media along with high electrochemical stability for OER. The enhanced performance is derived from the synergistic effect between FeNi sulfide with favorable electrical conductivity and generated (oxy)hydroxides with high intrinsic activity. More importantly, the more active sites and appropriate mesoporous structure further facilitate electrocatalytic activity due to improved mass transfer. This facile synthesis method is a potential pathway for MOF derived highly efficient electrocatalysis for sustainable hydrogen product. (C) 2021 Hydrogen Energy Publications LLC. Published by Elsevier Ltd. All rights reserved.
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   Fabregat-Santiago, Francisco
TI Pencil graphite rods decorated with nickel and nickel-iron as low-cost
   oxygen evolution reaction electrodes
SO SUSTAINABLE ENERGY & FUELS
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DT Article
ID ELECTROCHEMICAL EVOLUTION; OXIDE CATALYSTS; IMPEDANCE; FILM;
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AB Society is demanding clean energy to substitute greatly polluting carbon-based fuels. As an alternative, the use of green hydrogen produced by electrocatalysis constitutes a nice strategy as its products and reactants are not toxic to the environment. However, the use of scarce materials and high overpotentials to accomplish the oxygen evolution reaction (OER) make electrocatalysis an uncompetitive process. To solve these challenges, a low-cost procedure for the preparation of earth-abundant Ni, Fe and NiFe decorated electrodes has been developed. For this purpose, pencil graphite rods have been selected as highly porous substrates. A reasonable performance is achieved when they are employed for the OER. Furthermore, for the first time, a detailed analysis of impedance spectroscopy allows the association of the Ni redox transitions Ni2+/Ni3+ and Ni3+/Ni4+ (including the identification of the hydrated alpha-gamma and the non-hydrated beta phases) with an electrochemical redox capacitance response. Additionally, the Ni3+/Ni4+ redox peak capacitance together with a quick decrease in the charge transfer resistance indicates the implication of Ni4+ in the OER. These results show the utility of impedance spectroscopy as a non-destructive and non-invasive technique to study these electrochemical systems in detail under operating conditions.
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TI A 3D hierarchical network derived from 2D Fe-doped NiSe nanosheets/carbon nanotubes with enhanced OER performance for overall water splitting
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DT Article
ID OXYGEN EVOLUTION REACTION; LAYERED DOUBLE HYDROXIDE; HIGHLY EFFICIENT; CARBON NANOTUBES; ONE-STEP; NICKEL FOAM; NANOPARTICLES; ELECTROCATALYSTS; SELENIDE; ELECTRODE
AB Designing an earth-abundant electrode material with high activity and durability is a major challenge for water splitting to produce clean and green hydrogen energy. In this study, we report a novel high-performance electrocatalyst derived from a unique three-dimensional hierarchical network of two-dimensional iron-doped nickel selenide nanosheets (2D Fe-doped NiSe NSs) and high-quality carbon nanotubes (CNTs) grown on a carbon paper substrate. The synergistic effects derived from Fe doping and interfering effects between 2D NSs and CNTs produce an enrichment of electroactive sites and good electrical conductivity, thereby significantly improving the electrocatalytic oxygen evolution activities. As a result, the catalyst requires an overpotential of only 282.7 mV to achieve 10 mA cm(-2) in 1.0 M KOH electrolyte. An electrolyzer of Pt/C(-)//Fe-doped NiSe NSs/CNTs(+) demonstrates a cell voltage of 1.57 V and effective durability, superior to the state-of-the-art Pt/C(-)//RuO2/C(+) system (1.66 V) as well as recently reported catalysts. The achievements indicate a prospective catalyst for enhancing the OER in overall water splitting application.
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TI Ni-Fe-Cu-layered double hydroxides as high-performance electrocatalysts
for alkaline water oxidation
SO INTERNATIONAL JOURNAL OF ENERGY RESEARCH
LA English
DT Article
DE electrocatalyst; layered double hydroxide; oxygen evolution reaction;
self‐ supported catalyst; water splitting

AB Alkaline oxygen evolution reaction (OER) electrocatalysts have been widely studied for improving the efficiency and green hydrogen production through electrochemical water splitting. Currently, iron-doped nickel-LDHs (NF-LDHs) are regarded as the benchmark electrocatalyst for alkaline OER, primarily owing to the physicochemical synergetic effects between Ni and Fe. Here, the third element addition into NF-LDHs is designed to further enhance the electrocatalytic performance through the modulation of electronic property. Cu-doped NF-LDHs (NFC-LDHs) are developed with the self-supported structure on porous supports. NFC-LDHs can be grown on carbon cloth (CC) in an intriguing 2D nanosheet structure, wherein the surface electronic configuration is suitably modulated by interactions among Ni-Fe-Cu. Importantly, activation energy for OER can be lowered by adding Cu into NF-LDHs. Thereby, the NFC-LDHs exhibited enhanced OER activity and improved stability than those of nickel-LDHs (Ni-LDHs) and NF-LDHs. For NFC-LDHs, small overpotentials of only 230 and 250 mV yield current densities of 50 and 100 mA cm(-2), respectively. In addition, excellent electrochemical stability is demonstrated during long-term OER tests without any degradation demonstrating no dissolution of active metals water electrolysis due to synergetic effects among Ni-Fe-Cu.
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TI Direct conversion of CO₂ to a jet fuel over CoFe alloy catalysts
SO INNOVATION
LA English
DT Article
DE carbon dioxide hydrogenation; C-C coupling; heterogeneous catalysis; jet fuel; CoFe alloys
ID FISCHER-TROPSCH SYNTHESIS; CARBON-DIOXIDE; LIQUID FUELS; HYDROGENATION; IRON; HYDROCARBONS; SELECTIVITY; RENAISSANCE; SUPPORT; SURFACE
AB The direct conversion of carbon dioxide (CO2) using green hydrogen is a sustainable approach to jet fuel production. However, achieving a high level of performance remains a formidable challenge due to the inertness of CO2 and its low activity for subsequent C-C bond formation. In this study, we prepared a Na-modified CoFe alloy catalyst using layered double-hydroxide precursors that directly transforms CO2 to a jet fuel composed of C-8-C-16 jet-fuel-range hydrocarbons with very high selectivity. At a temperature of 240 degrees C and pressure of 3 MPa, the catalyst achieves an unprecedentedly high C-8-C-16 selectivity of 63.5% with 10.2% CO2 conversion and a low combined selectivity of less than 22% toward undesired CO and CH4. Spectroscopic and computational studies show that the promotion of the coupling reaction between the carbon species and inhibition of the undesired CO2 methanation occur mainly due to the utilization of the CoFe alloy structure and addition of the Na promoter. This study provides a viable technique for the highly selective synthesis of eco-friendly and carbon-neutral jet fuel from CO2.
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TI Dynamic chloride ion adsorption on single iridium atom boosts seawater oxidation catalysis
SO NATURE COMMUNICATIONS
LA English
DT Article
ID OXYGEN EVOLUTION; SELECTIVITY; WATER; OPPORTUNITIES; ELECTROLYSIS; TEMPERATURE; IR
AB Seawater electrolysis offers a renewable, scalable, and economic means for green hydrogen production. However, anode corrosion by Cl- pose great challenges for its commercialization. Herein, different from conventional catalysts designed to repel Cl- adsorption, we develop an atomic Ir catalyst on cobalt iron layered double hydroxide (Ir/CoFe-LDH) to tailor Cl- adsorption and modulate the electronic structure of the Ir active center, thereby establishing a unique Ir-OH/Cl coordination for alkaline seawater electrolysis. Operando characterizations and theoretical calculations unveil the pivotal role of this coordination state to lower OER activation energy by a factor of 1.93. The Ir/CoFe-LDH exhibits a remarkable oxygen evolution reaction activity (202 mV overpotential and TOF = 7.46 O2 s-1) in 6 M NaOH+2.8 M NaCl, superior over Cl--free 6 M NaOH electrolyte (236 mV overpotential and TOF = 1.05 O2 s-1), with 100% catalytic selectivity and stability at high current densities (400-800 mA cm-2) for more than 1,000 h.
The seawater oxidation reaction faces challenges from competitive chloride oxidation reaction. Herein, the authors have utilized chlorine adsorption to modulate the single-atom Ir coordination state and promote seawater oxidation and catalyst stability.
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TI Single-Site Iridium Picolinamide Catalyst Immobilized onto Silica for
   the Hydrogenation of CO₂ and the Dehydrogenation of Formic
   Acid
SO INORGANIC CHEMISTRY
LA English
DT Article
ID ENHANCED NMR-SPECTROSCOPY; LOW-PRESSURE HYDROGENATION; METAL-ORGANIC
   FRAMEWORK; DEFINED IRON CATALYST; CARBON-DIOXIDE; REVERSIBLE
   HYDROGENATION; HETEROGENEOUS CATALYSIS; HOMOGENEOUS CATALYSTS; STORAGE
   MATERIALS; WATER OXIDATION
AB The development of an efficient heterogeneous catalyst for storing H-2 into CO(2)and
releasing it from the produced formic acid, when needed, is a crucial target for
overcoming some intrinsic criticalities of green hydrogen exploitation, such as high
flammability, low density, and handling. Herein, we report an efficient heterogeneous
catalyst for both reactions prepared by immobilizing a molecular iridium organometallic
catalyst onto a high-surface mesoporous silica, through a sol-gel methodology. The
presence of tailored single-metal catalytic sites, derived by a suitable choice of
ligands with desired steric and electronic characteristics, in combination with optimized
support features, makes the immobilized catalyst highly active. Furthermore, the
information derived from multinuclear DNP-enhanced NMR spectroscopy, elemental analysis,
and Ir L-3-edge XAS indicates the formation of cationic iridium sites. It is quite
remarkable to note that the immobilized catalyst shows essentially the same catalytic
activity as its molecular analogue in the hydrogenation of CO2. In the reverse reaction
of HCOOH dehydrogenation, it is approximately twice less active but has no induction
period.
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AB Electrochemical water splitting is regarded as an effective technology for producing green hydrogen, which is crucial for addressing energy and environmental challenges. In particular, direct seawater splitting offers significant economic and environmental advantages. However, its efficiency is hindered by the high overpotential required for the oxygen evolution reaction (OER) and the competition from chloride oxidation. This review highlights the potential of interface engineering to overcome these limitations and develop efficient OER electrocatalysts. We comprehensively explore recent advancements in interface engineering for OER in both alkaline and seawater environments. We begin by introducing the mechanisms of freshwater and seawater electrolysis, emphasizing key considerations for OER catalyst design. Subsequently, we review the recent progress made in various interface engineering strategies, analyzing their impact on OER performance in both electrolytes. Finally, we outline promising future directions for developing efficient seawater oxidation catalysts through interface engineering.
   This review unravels the recent achievements in electrocatalysts for alkaline seawater oxidation through interface engineering. We define the interface types and classify them based on the interfacial configurations. Then, we summarize the recent studies on electrocatalysts developed through interface engineering to elaborate the interfacial effects on promoting the OER processes in both alkaline electrolyte and seawater. image
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AB In order to enable an emission-free society by 2050, the distribution of green hydrogen is a key element for a successful transformation of the energy supply. This paper presents the design and manufacturing of composite pipelines made of fiber-reinforced plastic (FRP) and its potential for the transport of high-pressurized gases such as hydrogen. Furthermore, the extent to which FRP-pipelines can be a potential complement to existing steel pipelines is being discussed.
   The wet winding process is an established manufacturing process for FRP-pipes which, however, provide only a fraction of all necessary requirements. Oftentimes, a trade between the different factors cost, weight, performance and feasibility is made. By means of benchmarking the alternative manufacturing approaches such as multi- supply filament winding (MFW) and radial braiding, the potential for cost-effective high-pressure composite pipelines are investigated within this paper. For the aspired operational pressure of 350 bars, suitable lay-ups are derived and validated via simulation according to ISO 14692. As pre-impregnated fibers, so-called towpregs, enable elevated winding speeds and reduced resin content variance, the study focusses on this material. Additionally, MFW allows the processing of up to 48 towpregs simultaneously and therefore, increased productivity compared to single- filament winding. Using the generated data and based on the material combinations investigated, the productivity of the MFW process is examined. The most promising design is selected for the manufacturing of a demonstrator via MFW. Finally, recommendations for the industrial upscale of composite pipeline manufacturing are presented and the manufacturing approach via radial braiding as an alternative is discussed.
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AB Hydrogen, particularly in renewable forms like green hydrogen and biohydrogen, is critical for decarbonization and sustainable development. This review provides a comprehensive overview of the multifaceted role of hydrogen and its versatility in industrial applications, energy storage, and transportation while addressing its potential to mitigate greenhouse gas emissions. The PRISMA methodology was applied, systematically analyzing over 25,000 publications and reports from 2017 to 2024, focusing on cutting-edge production methods like electrolysis and biomass conversion. Hydrogen production processes are explored, including water electrolysis, a clean method powered by renewable energy, and biohydrogen routes utilizing biomass and organic waste through thermochemical and biological conversions. These innovations align with global decarbonization targets, reducing emissions in hard-to-abate sectors like steel and aviation. The study also highlights hydrogen's evolving global market, with investments exceeding USD 680 billion and expanding project portfolios in Europe, North America, and Asia. Green finance, via tools like green bonds and sustainability-linked loans, is identified as essential for scaling hydrogen technologies. By integrating environmental, social, and governance (ESG) principles, hydrogen projects ensure socio-economic benefits, including job creation and reduced reliance on fossil fuels. Moreover, hydrogen is projected to reduce CO2 emissions by 6.5% by 2050, making it a key element in climate strategies. In conclusion, this study offers a thorough overview of hydrogen's role in achieving net-zero emissions. Its findings highlight the important interplay between technological innovation, market dynamics, and sustainable finance, providing actionable insights to aid in policy formulation and strategic decision-making. By harnessing hydrogen's potential, society can advance the energy transition and promote a resilient, lowcarbon future.
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TI Charting the Course: Navigating Decarbonisation Pathways in Greece, Germany, The Netherlands, and Spain's Industrial Sectors
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DT Review
DE energy-intensive industries; decarbonisation technologies; sector-specific analysis; economic and regulatory frameworks
ID CEMENT; DECARBONIZATION; OPTIONS; TECHNOLOGIES; STRATEGIES; CAPTURE
AB In the quest for a sustainable future, energy-intensive industries (EIIs) stand at the forefront of Europe's decarbonisation mission. Despite their significant emissions footprint, the path to comprehensive decarbonisation remains elusive at EU and national levels. This study scrutinises key sectors such as non-ferrous metals, steel, cement, lime, chemicals, fertilisers, ceramics, and glass. It maps out their current environmental impact and potential for mitigation through innovative strategies. The analysis spans across Spain, Greece, Germany, and the Netherlands, highlighting sector-specific ecosystems and the technological breakthroughs shaping them. It addresses the urgency for the industry-wide adoption of electrification, the utilisation of green hydrogen, biomass, bio-based or synthetic fuels, and the deployment of carbon capture utilisation and storage to ensure a smooth transition. Investment decisions in EIIs will depend on predictable economic and regulatory landscapes. This analysis discusses the risks associated with continued investment in high-emission technologies, which may lead to premature decommissioning and significant economic repercussions. It presents a dichotomy: invest in climate-neutral technologies now or face the closure and offshoring of operations later, with consequences for employment. This open discussion concludes that while the technology for near-complete climate neutrality in EIIs exists and is rapidly advancing, the higher costs compared to conventional methods pose a significant barrier. Without the ability to pass these costs to consumers, the adoption of such technologies is stifled. Therefore, it calls for decisive political commitment to support the industry's transition, ensuring a greener, more resilient future for Europe's industrial backbone.
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TI BLENDING HYDROGEN WITH NATURAL GAS/BIOMETHANE AND TRANSPORTATION IN
   EXISTING GAS NETWORKS
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LA English
DT Article
DE hydrogen; natural gas; biomethane; gas infrastructure; gas blends
ID RESISTANCE
AB The existing European Union (EU) natural gas network provides large capacity to integrate renewable (RGs) and low-carbon gases. Today, hydrogen contributes only a few percent to Europe's energy consumption and is almost exclusively produced from fossil fuels and used in the industry. Nevertheless, hydrogen has a significant role to play in emission reduction in hard-to-decarbonize sectors, in particular, as a fuel in transport applications and as a fuel or feedstock in certain industrial processes (steel, refining or chemical industries, the production of "green fertilizers"). Carbon dioxide (CO2) in reaction with hydrogen can also be further processed into synthetic fuels, such as synthetic kerosene in aviation. In addition, hydrogen brings other environmental co-benefits when used as fuel, such as the lack of air pollutant emissions.However, in transitional phase from fossil to RG, namely, renewable or green hydrogen, natural gas/biomethane and hydrogen blends, are needed to gradually replace natural in existing gas transmission and distribution networks. The gas networks are believed to be able to use natural gas/biomethane and hydrogen blends with 5-20 % of hydrogen by volume. Most systems and applications are able to handle it without a need for major infrastructure upgrades or end-use appliance retrofits or replacements. The promotion of hydrogen network such as European Hydrogen backbone (EHB) is gaining momentum in Europe. To decarbonize the natural gas grids, the threshold of hydrogen in the existing grid systems must be increased, which can be done by means of wider natural gas/biomethane and hydrogen blending and simultaneous transportation in currently operational gas networks.
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NR 37
TC 6
Z9 6
U1 2
U2 6
PU SCIENDO
PI WARSAW
PA BOGUMILA ZUGA 32A, WARSAW, MAZOVIA, POLAND
SN 0868-8257
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J9 LATV J PHYS TECH SCI
JI Latv. J. Phys. Tech. Sci.
PD OCT 1
PY 2023
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IS 5
BP 43
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DI 10.2478/lpts-2023-0030
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WC Physics, Applied
WE Emerging Sources Citation Index (ESCI)
SC Physics
GA T5YQ6
UT WOS:001078747300004
OA gold
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ER

PT J
AU Luzzo, I
Cirilli, F
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Gambato, A
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AF Luzzo, Irene
   Cirilli, Filippo
   Jochler, Guido
   Gambato, Alessio
   Longhi, Jacopo
   Rampinini, Gabriele
TI Feasibility study for the utilization of natural gas and hydrogen blends
   on industrial furnaces
SO MATERIAUX & TECHNIQUES
LA English
DT Article
DE hydrogen; oxidability; descaling susceptibility; decarbonisation; CO2
AB In the deep steel industry decarbonization, green hydrogen plays a pivotal role as alternative energy to replace natural gas and carbon bearing materials. In this frame, technical aspects and in general criticalities relevant to the use of mixtures of hydrogen and natural gas in industrial processes were investigated: in particular its effect was analyzed on employ of existing industrial burners for treatment furnace and on oxidability and descaling susceptibility of forged material as Grade F22V and Inconel(R) 625. The experimental campaign on burner using blends with 30% and 50%vol. of hydrogen in natural gas highlighted that it is possible to ignite the burner for both mixtures, but that the burner is more stable with the 30%vol. of hydrogen in natural gas. The detected emissions of nitrogen oxides compared to the natural gas increase up to 15%. The results indicated that selected high speed burner should be used in industrial plant with a 30% of hydrogen in volume with no need of hardware modifications. The oxidation investigation on atmospheres deriving from the combustion of 100% of hydrogen, at 1230 degrees C, showed a moderate scale increase up to 14% for F22V grade and 8% for Inconel(R) 625. This increase of scale growth has not detrimental effect on the scale removability. For the selected reference industrial scenario, the burner was positively tested in industrial furnace with a 30% of hydrogen in volume with no need of hardware modifications. Moderate scale growth was observed, but with no detrimental effect on the scale removability. Moreover, the H-2 addition allows to get CO2 reductions, without any noticeable drawback on other process parameters or product quality for this industrial scenario.
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CR Birks N., 1983, INTRO HIGH TEMPERATU
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U1 1
U2 11
PU EDP SCIENCES S A
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PA 17, AVE DU HOGGAR, PA COURTABOEUF, BP 112, F-91944 LES ULIS CEDEX A,
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WC Materials Science, Multidisciplinary
WE Emerging Sources Citation Index (ESCI)
SC Materials Science
GA ZC5AI
UT WOS:000757532500002
OA hybrid
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ER

PT J
AU Nguyen, TX
Ting, NH
Ting, JM
AF Nguyen, Thi Xuyen
Ting, Nai-Hsin
Ting, Jyh-Ming
TI Multi-metal phosphide as bi-functional electrocatalyst for enhanced water splitting performance
SO JOURNAL OF POWER SOURCES
LA English
DT Article
DE Multi-metal phosphides; Bi-functional electrocatalyst; Overall water splitting
ID NICKEL; COBALT; EFFICIENT; IRON; NANOBOXES; OXIDATION; PROGRESS; STATE; CO2P; XPS
AB Developing cost effective and highly efficient electrocatalyst for water splitting is vital for green hydrogen production. Transition metal phosphides have attracted significant attentions for electrochemical water splitting owing to their desired conductivity, catalytic activity, and stability. Meanwhile, multi-metal compound provides unique tailorable properties as result of its nearly unlimited compositional space. In this study, we have therefore investigated the effect of incorporating a sixth metal of Ti, V, and Zn into a quinary-metal phosphide containing Cr, Mn, Fe, Ni, and Co. We show that the resulting senary-metal phosphides exhibit better oxygen evolution reaction (OER) performances than the quinary-metal phosphide and baseline samples of binary FeCo phosphide and commercial IrO2. We further demonstrate that the addition of Ti into the quinary-metal phosphide (5MT-P) shows the best performance by giving outstanding bi-functional catalytic activity and durability in alkaline media. The 5MT-P catalyst yields a current density of 50 mA cm(-2) at overpotentials of 226 and 220 mV for OER and hydrogen evolution reaction (HER), respectively. For overall water splitting, a 5MT-P parallel to 5MT-P electrolyzer requires a low cell voltage of 1.69 V to achieve a current density of 100 mA cm(-2) and exhibits excellent 100-h durability.
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FU National Science and Tech- nology Council in Taiwan; [MOST 111-2224-E-006-005]
FX This work has been supported by the National Science and Tech- nology Council in Taiwan under Grant No. MOST 111-2224-E-006-005.
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NR 73
TC 28
Z9 29
U1 11
U2 95
PU ELSEVIER
PI AMSTERDAM
PA RADARWEG 29, 1043 NX AMSTERDAM, NETHERLANDS
SN 0378-7753
EI 1873-2755
J9 J POWER SOURCES
JI J. Power Sources
PD DEC 30
PY 2022
VL 552
AR 232249
DI 10.1016/j.jpowsour.2022.232249
EA OCT 2022
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WC Chemistry, Physical; Electrochemistry; Energy & Fuels; Materials
   Science, Multidisciplinary
WE Science Citation Index Expanded (SCI-EXPANDED)
SC Chemistry; Electrochemistry; Energy & Fuels; Materials Science
GA 5Z8QP
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ER

PT J
AU Salehabadi, A
   Zanganeh, J
   Moghtaderi, B
AF Salehabadi, Ali
   Zanganeh, Jafar
   Moghtaderi, Behdad
TI Mixed metal oxides in catalytic ammonia cracking process for green
   hydrogen production: A review
SO INTERNATIONAL JOURNAL OF HYDROGEN ENERGY
LA English
DT Review
DE Ammonia; Hydrogen storage; Hydrogen production; Catalyst; Mixed metal
   oxide
ID COX-FREE HYDROGEN; DECOMPOSITION KINETICS; NH3 DECOMPOSITION; LANTHANUM
   OXIDES; H-2 PRODUCTION; NI; IRON; RU; GENERATION; NANOSTRUCTURES
AB Hydrogen, a versatile energy carrier, is a promising alternative to replace the environmentally harmful and unsustainable use of fossil fuels. This much-touted fuel of the future may however have pitfalls, such as issues associated with hydrogen production, storage, and distribution. Hydrogen storage and distribution are concerned with various technical, environmental and safety issues. Indirect hydrogen storage methods such as - in solidstate materials, ammonia, and methanol/ethanol - are recently being considered by academic and industry parties. Ammonia (NH3) can be a promising carbon-free carrier with a high energy density, established transportation network, high hydrogen contents and high flexibility. Hydrogen production from NH3 decomposition requires catalyst/support such as metal oxides. In binary metal oxides like perovskites and spinels, their unique morphologies and structural flexibility enable to apply defined control over the reaction profile through detailed engineering material design. The focus of this study is to conduct a comprehensive review on the existing and emerging mixed metal oxides catalysts used in the NH3 decomposition process in hydrogen production. The activity of various mixed metal oxide catalysts is critically assessed, and their resulting performances are

discussed in detail. Furthermore, this study covers challenges associated with hydrogen production through the catalytic NH3 cracking process.
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TI Techno-economic assessment of gasoline production from Fe-assisted lignocellulosic biomass hydrothermal liquefaction process with minimized waste stream
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DE Red mud; Pinewood; Aspen plus; Techno-economic analysis; Life cycle assessment
ID ENVIRONMENTAL-IMPACT ASSESSMENT; HYDROGEN-PRODUCTION; BIO-OIL; AQUEOUS-PHASE; FUELS; FEASIBILITY; TEMPERATURE; MICROALGAE; HTL
AB Techno-economic analyses were conducted on an iron-assisted hydrothermal liquefaction (HTL) process for converting lignocellulosic biomass into gasoline, comparing two approaches for minimizing by-product streams. The primary difference between the two approaches lies in their hydrogen (H2) source for upgrading bio-crude to bio-gasoline. Scheme 1 utilizes residual water-soluble and gaseous compounds from the process to generate the H2 needed for upgrading. Scheme 2, on the other hand, converts these waste streams into heat to supply part of the required energy, while external H2 from steam methane reforming (with or without CO2 capture) or water electrolysis (green hydrogen) is used for upgrading. Both schemes use pinewood and red mud as feedstocks. Red mud, after the reduction of Fe2O3 3 to metallic iron, is employed in the HTL reactor as a hydrogen producer, enhancing both the yield and quality of the bio-crude while minimizing the H2 2 consumption in the upgrading unit. The HTL reactor was modeled based on optimal operating conditions experimentally determined while sensitivity analyses were performed on the other scheme's units to determine their optimal conditions. A Life Cycle Assessment (LCA) was also conducted to measure the environmental impact of the two scenarios. Both schemes produce 459 tonnes of gasoline equivalent per day, consuming 33 tonnes of H2. 2 . Scheme 2 achieves a minimum fuel selling price (MFSP) of $0.94 per liter of gasoline equivalent (LGE), with methane reforming and CO2 capture providing the lowest emissions (1.13 kg CO2-Eq per kg of LGE). Scheme 1 has a slightly higher MFSP of $0.96 per LGE but is more environmentally sustainable, with a LCA showing 1.11 kg CO2Eq per kg of LGE.
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TI Directed Surface Reconstruction of Fe Modified
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SO ADVANCED MATERIALS
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DE cation leaching; CV activation; oxygen evolution reaction; surface
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AB Affordable highly efficient catalysts for electrochemical oxygen evolution reaction
(OER) play pivotal roles in green hydrogen production via water electrolysis. Regarding
the non-noble metal-based electrocatalysts, considerable efforts are made to decipher the

cation leaching and surface reconstruction; yet, little attention is focused on correlating them with catalytical activity and stability. Herein, in situ reconstruction of Fe-modified Co2VO4 precursor catalyst to form a highly active (Fe,V)-doped CoOOH phase for OER is reported, during which partial leaching of V accelerates the surface reconstruction and the V reserved in the reconstructed CoOOH layer in the form of alkali-resistant V2O3 serves for dynamic charge compensation and prevention of excessive loss of lattice oxygen and Co dissolution. Fe substitution facilitates Co pre-oxidation and endows the catalysts with structural flexibility by elevating O 2p band level; hence, encouraging participation of lattice oxygen in OER. The optimized Co2Fe0.25V0.75O4 electrode can afford current densities of 10 and 500 mA cm(-2) at low overpotentials of 205 and 320 mV, respectively, with satisfactory stability over 600 h. By coupling with Pt/C cathode, the assembled alkaline electrolyzer can deliver 500 mA cm(-2) at a low cell voltage of 1.798 V, better than that of commercial RuO2 (+) || Pt/C (-).
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FU National Natural Science Foundation of China; National Science and Technology Major Project [2021YFB4000300]; [22072009]
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NR 62
TC 17
Z9 17
U1 62
U2 124
PU WILEY-V C H VERLAG GMBH
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PA POSTFACH 101161, 69451 WEINHEIM, GERMANY
SN 0935-9648
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J9 ADV MATER
JI Adv. Mater.
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WC Chemistry, Multidisciplinary; Chemistry, Physical; Nanoscience & Nanotechnology; Materials Science, Multidisciplinary; Physics, Applied; Physics, Condensed Matter
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SC Chemistry; Science & Technology - Other Topics; Materials Science; Physics
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PT J
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TI Graphene Materials from Coke-like Wastes as Proactive Support of
   Nickel-Iron Electro-Catalysts for Water Splitting
SO MOLECULES
LA English
DT Article
DE waste; graphene; 3D electrode; electrocatalysis; NiFe; water splitting;
   OER
ID OXYGEN EVOLUTION REACTION; ENERGY-CONVERSION; GRAPHITE;
   ELECTROCATALYSTS; CHEMISTRY; DESIGN
AB Graphene materials, used as electrocatalyst support in green hydrogen production, contribute to increasing the efficiency and robustness of various systems. However, the preparation of a hybrid catalyst containing graphene materials from industrial wastes is still a challenge due to the heterogeneity of the waste. We report the synthesis of 3D electrodes using graphene oxides (GOs) from industrial waste (IW) prepared by immersion onto Toray carbon paper as a 3D support onto GO suspensions and electrodepositing NiFe layered double hydroxides (LDHs). Standard graphite was also used as the reference. The morphology of the two hybrid electrodes was determined by SEM, HRTEM, XPS. Although very similar in both, the sample containing graphene from IW (higher Csp3 hybridization in the graphene layer) has a NiFe phase with less crystallinity and larger presence of Fe2+ ions. These electrodes exhibited similar activity and stability as electrocatalysts of the oxygen evolution reaction (OER), demonstrating the proactive effect of the graphene into the 3D electrode even when this is prepared from heterogeneous industrial waste. Moreover, the defective graphenic structure of the waste GO enhances the reaction kinetics and improves the electron transfer rate, possibly due to the small differences in the electrodeposited NiFe LDH structure.
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FX No Statement Available
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U1 5
U2 14
PU MDPI
PI BASEL
PA ST ALBAN-ANLAGE 66, CH-4052 BASEL, SWITZERLAND
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J9 MOLECULES
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TI A simple postsynthetic in-situ cation exchange strategy to construct
   Fe-doped Ni₃Se₄ nanoarray for enhanced oxygen
   evolution reaction
SO COLLOIDS AND SURFACES A-PHYSICOCHEMICAL AND ENGINEERING ASPECTS
LA English
DT Article
DE Electrocatalysis; Metal -organic frameworks; Iron modulation; Oxygen
   evolution reaction; Ni3Se4
ID NICKEL SELENIDE; ELECTROCATALYSTS; EFFICIENT; PERFORMANCE; HYDROGEN;
   ENERGY; CARBON
AB For industrial high-purity green hydrogen production, it is necessary to develop efficient, economical and stable non-precious metal-based alkaline media oxygen evolution reaction (OER) electrocatalysts. In this study, a simple stepwise synthesis strategy was proposed to construct a hierarchical MOF-based Prussian blue analogue by Ni-BPDC and derived from it to grow Fe-doped Ni3Se4 in situ on nickel foam (Fe-Ni3Se4/NF) as an efficient and stable alkaline OER electrocatalyst. Fe doping enables better modulation of the electronic structure of Ni(3)Se(4)and increases the number of active sites and electrochemical surface area to improve the OER activity. Fe- Ni3Se4/ NF exhibits remarkable electrocatalytic performance in 1 M KOH with low overpotential (211 mV at 10 mA cm(-2)) and small Tafel slope (34.44 mV dec(- 1)), which is superior to that of commercial RuO2 catalysts. Its electrochemical characteristics are stable at 10 mA cm-2 for more than 24 h, making it a viable non-precious metal-based electrocatalyst for alkaline OER. This synthetic approach could open up new possibilities for the fabrication of MOF-based hierarchical Prussian blue analogs as well as derivatives to be oriented for applications in various fields.
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OI Yang, Yaoxia/0000-0002-4891-6910; Wang, Qingtao/0000-0003-3525-3422
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   Scientific Research Ability Promotion Program of Young Teachers of
   Northwest Normal University (NWNU-LKQN-18-18) .
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NR 71
TC 3
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U1 9
U2 46
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PA RADARWEG 29, 1043 NX AMSTERDAM, NETHERLANDS
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PT J
AU Nassereddine, Y
   Ousaleh, HA
   Baba, YF
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AF Nassereddine, Yassine
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TI Synthesis, Experimental, and Theoretical Study of Co3-XNiXO4 Mixed
   Oxides: Potential Candidates for Hydrogen Production via Solar Redox
   Cycles
SO ACS OMEGA
LA English
DT Article
ID THERMOCHEMICAL CYCLES; IRON-OXIDE; WATER; ENERGY; STEP
AB Recently, green hydrogen production via solar thermochemical water splitting (STWS) as a clean and sustainable method is becoming a subject of interest to many researchers. Great efforts are being made to develop materials for STWS with suitable operating conditions, low cost, and good cycling stability. In this context, the study of mixed cobalt and nickel oxides with the general formula Co3-xNixO4 (0 < x < 1) was carried out, where four mixed metal oxides Co2.75Ni0.25O4, Co2.5Ni0.5O4, Co2.25Ni0.75O4, and Co2NiO4 have been successfully synthesized through the sol-gel method modified Pechini route. The structural investigation demonstrated that pure spinel structures were obtained for 0 < x < 0.75. A deep study was carried out with the main goal of finding the best phase that provides low redox temperature. Interesting reduction temperatures for all the compositions have been found, and the lowest values of 675 and 710 degrees C have been reported for Co2.25Ni0.75O4 and Co2.5Ni0.5O4, respectively. The thermal cycling results of this latest material using TGA measurement have proven attractive cycling stability of which the complete reoxidation of the samples was achieved. In addition, thermodynamic

analysis of a reduction step was performed and good agreement of the theoretical reduction temperature of Co2.25Ni0.75O4 with the experimental one has been found.
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PT J
AU Upadhyay, P
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TI Physical insight into the enhanced urea electrooxidation using Ni and
   Fe-based LDH, LDO, and hydroxides under different dissolved gas
   saturation conditions in electrolyte
SO INTERNATIONAL JOURNAL OF HYDROGEN ENERGY
LA English
DT Article
DE Nickel-iron; Layered double hydroxide; Electrooxidation; Urea;
   Electrocatalytic
ID LAYERED DOUBLE HYDROXIDE; ELECTROCHEMICAL IMPEDANCE; METHANOL
   ELECTROOXIDATION; POSITIVE ELECTRODE; OXIDATION; NANOPARTICLES;
   NANOSHEETS; NI(OH)(2); MECHANISM; CATALYST
AB The production of green hydrogen is one of the most demanding and challenging for modern technology. A promising and an effective approach is electrocatalytic anodic urea oxidation reaction to generate hydrogen at cathode under alkaline electrolysis condition. However, it remains crucial for the development of active and stable electrocatalysts for efficient urea oxidation. In this study, we employed the hydrothermal synthesis route for NiFe LDH, NiFe LDO, and Ni(OH)(2). The superior performance of NiFe LDH compared to other catalysts is observed due to easy charge transfer facilitated by Fe ions. Moreover, Fe incorporation prevents surface poisoning of the electrocatalyst, resulting in increased activity and stability for electrocatalytic urea oxidation reaction. The influence of different electrolyte environments on the performance of urea-based electrolyzers for sustainable hydrogen production and management of urea-rich wastewater has been measured for the first time by varying oxygen saturation and nitrogen purging conditions. In cyclic voltammetry studies, O-2-saturated and purging conditions outperformed N-2 gas saturation or purging. The findings of this study provide valuable insight into the design of practical and environmentally friendly urea electrooxidation systems.
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AU Lee, WS
   Maeda, H
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TI Spontaneous-Spin-Polarized 2D π-d Conjugated Frameworks Towards Enhanced
   Oxygen Evolution Kinetics
SO SMALL
LA English
DT Article; Early Access
DE bimetallic p-d conjugation; coordination frameworks; electrocatalysts;
   oxygen evolution reaction; spin-polarization
ID WATER OXIDATION; MAGNETIC-FIELD; METAL; ELECTROCATALYSIS; CONDUCTIVITY;
   DISCOVERY; CATALYST; HYDROGEN; DESIGN

AB Alternative strategies to design sustainable-element-based electrocatalysts enhancing oxygen evolution reaction (OER) kinetics are demanded to develop affordable yet high-performance water-electrolyzers for green hydrogen production. Here, it is demonstrated that the spontaneous-spin-polarized 2D pi-d conjugated framework comprising abundant elements of nickel and iron with a ratio of Ni:Fe = 1:4 with benzenehexathiol linker (BHT) can improve OER kinetics by its unique electronic property. Among the bimetallic NiFex:y-BHTs with various ratios with Ni:Fe = x:y, the NiFe1:4-BHT exhibits the highest OER activity. The NiFe1:4-BHT shows a specific current density of 140 A g-1 at the overpotential of 350 mV. This performance is one of the best activities among state-of-the-art non-precious OER electrocatalysts and even comparable to that of the platinum-group-metals of RuO2 and IrO2. The density functional theory calculations uncover that introducing Ni into the homometallic Fe-BHT (e.g., Ni:Fe = 0:1) can emerge a spontaneous-spin-polarized state. Thus, this material can achieve improved OER kinetics with spin-polarization which previously required external magnetic fields. This work shows that a rational design of 2D pi-d conjugated frameworks can be a powerful strategy to synthesize promising electrocatalysts with abundant elements for a wide spectrum of next-generation energy devices.

The spontaneous-spin-polarized 2D pi-d conjugated framework that contains nickel and iron with a Ni:Fe ratio of 1:4 and is synthesized by a benzenehexathiol linker (BHT), exhibits enhanced oxygen evolution reaction (OER) kinetics without additional magnetic fields due to its distinctive electronic characteristic. This study provides a rational strategy to realize competent and affordable electrocatalysts with abundant elements. image
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TI Interstitial Manganese-Tuned Nickel-Iron Diselenide Anode for Efficient and Durable Anion Exchange Membrane Water Electrolysis
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DE anion exchange membrane water electrolysis; heteroatom doping; hydrogen production; oxygen evolution reaction; transition metal selenides
ID HYDROGEN; REACTIVITY
AB Anion exchange membrane water electrolysis (AEMWE) employing Ir/Ru-free anodes emerges as a bright prospect for green hydrogen society. Here, a Ni0.8Fe0.2Mn0.1Se2 nanosheet electrocatalyst is reported, in situ grown on stainless-steel paper, as an efficient and durable self-supporting AEMWE anode for oxygen evolution reaction (OER). The interstitial [MnSe4] tetrahedra elevate the Fermi level and narrows the band gap of the electrocatalyst, thereby expediting electrode reaction kinetics and increasing the electrical conductivity. In addition, the interstitial Mn atoms attenuate the electron density of Ni and Fe and motivate phase transition to actual active (Mn, Fe)-doped gamma-NiOOH species. The downward d-band center of Ni active center facilitates the rate-limiting *OOH desorption step, refreshing the active center, and reducing the free energy barriers for OER. Accordingly, the Ni0.8Fe0.2Mn0.1Se2 electrode achieves OER overpotentials of 149 and 232 mV at 10 and 100 mA cm-2 in 1 m KOH. The AEMWE cell incorporating Ni0.8Fe0.2Mn0.1Se2 anode demonstrates high performance (1.0 A cm-2 at 1.68 Vcell) and durability (at 1 A cm-2 for 300 h), surpassing most AEMWE cells that use NiFe-based anodes. This work highlights the potential of noble-metal-free anodes for efficient and durable AEMWE.
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AF Liang, Shiheng
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TI CDs "inserted" abundant FeB-based electrode <i>via</i> "local photothermal effect" strategy toward efficient overall seawater splitting
SO INORGANIC CHEMISTRY FRONTIERS
LA English
DT Article
ID BIFUNCTIONAL ELECTROCATALYSTS; BORIDE; CATALYSTS; HYDROGEN; HOST; COB
AB The construction of high-efficiency long-stable catalytic electrodes for hydrogen by seawater splitting is a huge challenge in the field of green hydrogen generation. Herein, a matrix-type titanium dioxide nanorod (Ti/TiO2) is constructed on the titanium plate (Ti) by one-step oxidative etching, and a two-dimensional self-supporting electrode with good stability and "local photothermal effect" strategy is constructed as a self-supporting electrode by carbon quantum dots (CDs) "inserted" self-growing iron boron (CDs-FeBx@TiO2). Based on the microstructure regulated by CDs, the in situ growth of FeB with high conductivity and high authenticity activity, the effective separation of electron-hole pairs in the TiO2 structure is promoted, and efficient photothermal seawater electrolysis is realized. The performance of hydrogen/oxygen evolution reaction (HER/OER) and overall seawater splitting of the highly active CDs-FeBx@TiO2 electrode increased by 14.7%, 16.2% and 4.4% at 10 mA cm(-2) in alkaline simulated seawater. The CDs-FeBx@TiO2 electrode remains durable for 70 days at 100 mA cm(-2) and even at industrial current density, and the catalytic activity remained at 93.5%. This work provides a simple way for the preparation of catalytic electrodes with high activity and excellent stability and provides theoretical support for the practical application of high purity hydrogen from seawater.
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AU Yaseen, W
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Chen, M
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AF Yaseen, Waleed
Nie, Qixuan
Ji, Mengyi
Yusuf, Bashir Adegbemiga
Meng, Suci
Xie, Jimin
Xie, Meng
Chen, Min
Xu, Yuanguo
TI Electrodeposited Nitrate-Intercalated NiFeCe-Based (Oxy)hydroxide Heterostructure as a Competent Electrocatalyst for Overall Water Splitting
SO INORGANIC CHEMISTRY
LA English
DT Article
ID EVOLUTION; FOAM
AB Electrochemical water splitting is a promising method for the generation of "green hydrogen", a renewable and sustainable energy source. However, the complex, multistep synthesis processes, often involving hazardous or expensive chemicals, limit its broader adoption. Herein, a nitrate (NO3 -) anion-intercalated nickel-iron-cerium mixed-metal (oxy)hydroxide heterostructure electrocatalyst is fabricated on nickel foam (NiFeCeO x H y @NF) via a simple electrodeposition method followed by cyclic voltammetry activation to enhance its surface properties. The NiFeCeO x H y @NF electrocatalyst exhibited a low overpotential of 72 and 186 mV at 10 mA cm-2 for the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER), respectively, in 1.0 M KOH. In a two-electrode system, the NiFeCeO x H y @NF obtained a low voltage of 1.47 V at 10 mA cm-2 in 1.0 M KOH with robust stability. Results revealed that the notable activity of the NiFeCeO x H y @NF catalyst is primarily due to (i) hierarchical nanosheet morphology, which provides a large surface area and abundant active sites; (ii) NO3 - anion intercalation enhances electrode stability and eliminates the need for binders while simultaneously promoting a strong catalyst-substrate adhesion, resulting in decreased electrode resistance and accelerated reaction kinetics; and (iii) the unique superhydrophilic surface properties facilitate electrolyte penetration through capillary action and minimize gas bubble formation by reducing interfacial tension.
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NR 71
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PA 1155 16TH ST, NW, WASHINGTON, DC 20036 USA
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TI Multifunctional iron-cobalt heterostructure (FeCoHS) electrocatalysts: accelerating sustainable hydrogen generation through efficient water electrolysis and urea oxidation
SO NANOSCALE
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ID EVOLUTION REACTION; HIGHLY EFFICIENT; NANOSTRUCTURES; NANOSPHERES; CONVERSION
AB The urgent need to address escalating environmental pollution and energy management challenges has underscored the importance of developing efficient, cost-effective, and multifunctional electrocatalysts. To address these issues, we developed an eco-friendly, cost-effective, and multifunctional electrocatalyst via a solvothermal synthesis approach. Due to the merits of the ideal synthesis procedure, the FeCoHS@NF electrocatalyst exhibited multifunctional activities, like OER, HER, OWS, UOR, OUS, and overall alkaline seawater splitting, with required potentials of 1.48, 0.130, 1.59, 1.23, 1.40, and 1.54 V @ 10 mA cm-2, respectively. Moreover, electrolysers required only 1.40 V at 10 mA cm-2 for energy-saving urea-assisted hydrogen production, which was 190 mV lower than that of the alkaline water electrolyser. The alkaline sewage and seawater

purification setup combined with the FeCoHS@NF electrolyzer led to a novel approach of producing pure green hydrogen and water. The ultrastability of the FeCoHS@NF electrocatalyst for industrial applications was confirmed using chronopotentiometry at 10 and 100 mA cm-2 over 110 h for OER, HER, UOR, and overall water splitting. The production of hydrogen using the FeCoHS@NF electrocatalyst in alkaline sewage water and seawater offers multiple benefits, including generation of renewable hydrogen energy, purification of wastewater, reduction of environmental pollutants, and low cost and low electricity consumption of the electrolyser system.
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NR 61
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PA THOMAS GRAHAM HOUSE, SCIENCE PARK, MILTON RD, CAMBRIDGE CB4 0WF, CAMBS,
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WC Chemistry, Multidisciplinary; Nanoscience & Nanotechnology; Materials
   Science, Multidisciplinary; Physics, Applied
WE Science Citation Index Expanded (SCI-EXPANDED)
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AU Kment, S
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TI Single Atom Catalysts Based on Earth-Abundant Metals for Energy-Related Applications
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DT Review
ID EFFICIENT OXYGEN REDUCTION; ELECTROCATALYTIC CO2 REDUCTION; COVALENT ORGANIC FRAMEWORKS; ATOMICALLY DISPERSED IRON; DOPED POROUS CARBON; LONG CYCLE LIFE; HYDROGEN EVOLUTION; RECENT PROGRESS; AIR BATTERIES; ELECTRODE MATERIALS
AB Anthropogenic activities related to population growth, economic development, technological advances, and changes in lifestyle and climate patterns result in a continuous increase in energy consumption. At the same time, the rare metal elements frequently deployed as catalysts in energy related processes are not only costly in view of their low natural abundance, but their availability is often further limited due to geopolitical reasons. Thus, electrochemical energy storage and conversion with earth-abundant metals, mainly in the form of single-atom catalysts (SACs), are highly relevant and timely technologies. In this review the application of earth-abundant SACs in electrochemical energy storage and electrocatalytic conversion of chemicals to fuels or products with high energy content is discussed. The oxygen reduction reaction is also appraised, which is primarily harnessed in fuel cell technologies and metal-air batteries. The coordination, active sites, and mechanistic aspects of transition metal SACs are analyzed for two-electron and four-electron reaction pathways. Further, the electrochemical water splitting with SACs toward green hydrogen fuel is discussed in terms of not only hydrogen evolution reaction but also oxygen evolution reaction. Similarly, the production of ammonia as a clean fuel via electrocatalytic nitrogen reduction reaction is portrayed, highlighting the potential of earth-abundant single metal species.
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ID HIGH-TEMPERATURE ELECTROLYSIS; HELIOSTAT FIELD; ENERGY STORAGE; IRON-OXIDE; FUEL-CELLS; COLLECTOR; DESIGN; CYCLES; OPTIMIZATION; PERFORMANCE
AB The techno-economic analysis of hydrogen (H2) production using concentrating solar thermal (CST) technologies is performed in this study. Two distinct hydrogen production methods, namely: a) thermochemical water splitting [model 1] and b) solid oxide electrolysers [model 2], are modeled by considering the total heat requirement and supplied from a central tower system located in Jaisalmer, India. The hourly simulated thermal energy obtained from the 10 MWth central tower system is fed as an input to both these hydrogen production systems for estimating the hourly hydrogen production rate. The results revealed that these models yield hydrogen at a rate of 31.46 kg/h and 25.2 kg/h respectively for model 1 and model 2. Further, the Levelized cost of hydrogen (LCoH) for model 1 and model 2 is estimated as ranging from $ 8.23 and $ 14.25/kg of H2 and $ 9.04 and $ 19.24/kg, respectively, for different scenarios. Overall, the present work displays a different outlook on real-time hydrogen production possibilities and necessary inclusions to be followed for future hydrogen plants in India. The details of the improvisation and possibilities to improve the LCoH are also discussed in this study. (C) 2022 Hydrogen Energy Publications LLC. Published by Elsevier Ltd. All rights reserved.
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ID TRANSITION-METAL PHOSPHIDES; HYDROGEN EVOLUTION REACTION;
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AB The electrocatalytic production of "green hydrogen", such as through the electrolysis of water or urea has been vigorously advocated to alleviate the energy crisis. However, their electrode reactions including oxygen evolution reaction (OER), urea oxidation reaction (UOR), and hydrogen evolution reaction (HER) all suffer from sluggish kinetics, which urgently need catalysts to accelerate the processes. Herein, we design and prepare an OER/UOR/HER trifunctional catalyst by transforming the homemade CoO nanorod into a two-dimensional (2D) ultrathin heterojunction nickel-iron-cobalt hybrid phosphides nanosheet (NiFeP/CoP) via a hydrothermalphosphorization method. Consequently, a strong electronic interaction was found among the Ni2P/FeP4/CoP heterogeneous interfaces, which regulates the electronic structure. Besides the high mass transfer property of 2D nanosheet, Ni2P/FeP4/CoP displays improved OER/UOR/HER performance. At 10 mA cm-2, the OER overpotential reaches 274 mV in 1.0 M KOH, and the potential of UOR is only 1.389 V in 1.0 M KOH and 0.33 M urea. More strikingly, the two-electrode systems for electrolysis water and urea-assisted electrolysis water assembled by NiFeP/CoP could maintain long-term stability for 35 h and 12 h, respectively. This work may help to pave the way for upcoming research horizons of multifunctional electrocatalysts.

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AB The development of electrocatalysts with low cost, high efficiency, and long-term durability is crucial for advancing green hydrogen production. Transition metal phosphides (TMPs) have been proved to be efficient electrocatalyst, while the improvement in the performance and durability of the TMPs remains a big challenge. Employing atmospheric pressure chemical vapor deposition (APCVD) and phosphorization, FeP/Ti electrodes are fabricated featuring controllable oxygen ingredients (O-FeP/Ti). This manipulation of oxygen content fine-tunes the electronic structure of the catalyst, resulting in improved surface reaction kinetics and catalytic activity. The optimized O-FeP-400/Ti exhibits outstanding HER activity with overpotentials of 142 and 159 mV at -10 mA cm-2 in 0.5 M H2SO4 and 1 M KOH, respectively. Notably, the obtained O-FeP/Ti cathode also displays remarkable durability of up to 200 h in acidic electrolyte with surface topography remaining intact. For the first time, the low-valence titanium oxide (Ti3O) interlayer is identified in the composite electrode and ascribed for the superior connection between Ti substrate and the surface O-FeP catalyst, as supported by experimental results and density functional theory (DFT) analysis. This work has expanded the potential applications of transition metal phosphides (TMPs) as a cost-effective, highly efficient and durable catalyst for water splitting.

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TI Breaking the inactivity of MXenes to drive Ampere-level selective oxygen evolution reaction in seawater
SO MATERIALS SCIENCE & ENGINEERING R-REPORTS
LA English
DT Review
DE MXene; Metal-organic framework; 2D heterostructures; Oxygen evolution reaction; chlorine evolution; reaction; direct seawater splitting
ID EFFICIENT; CATALYST; ELECTROCATALYSTS; TI3C2TX; ANATASE; ZIF-67
AB The limited activity and stability of conventional anodes in seawater have posed a significant obstacle to sustainable green hydrogen production directly from seawater via electrolysis. To address these challenges, we engineered Ti(3)C(2)Tx-MXene by incorporating iron and boron into its matrix (tagged FBT) for selective oxygen evolution reaction (OER). Positioning B underneath the top layer induces charge disparity on the Fe-sites, which influences the subsequent growth of the ZIF-67 metal-organic framework (MOF) on the MXene surface through Fe-O-Co ionic bonds. DFT calculations reveal a favorable binding energy of -2.30 eV at the heterointerface for ZIF-67 adsorption to the surface of FBT via O-Co bond, a shortened bond length of 1.94 & Aring;, confirming the formation of ionic bonds. These ionic bonds tune the active sites for an enhanced and selective OER over chlorine evolution reaction (CER), preventing active Fe species' leaching and ensuring stability at >1.56 A cm(-2) in 6 M alkaline seawater over 370 hours. Further, FBT and ZIF-67/FBT require low overpotentials of 521.2 and 508 mV, respectively, to deliver 1 A cm(-2) in 6 M alkaline seawater. Our findings demonstrate a robust strategy to significantly expand the potential of MXenes from simple conductive substrates to efficient OER catalysts for seawater splitting and beyond.
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FU RMIT University; Australian Synchrotron; National Computational Infrastructure (NCI)
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AU Park, KR
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AF Park, Kyoung Ryeol
   Tran, Duy Thanh
   Nguyen, Thanh Tuan
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TI Copper-Incorporated heterostructures of amorphous
   NiSe_x/Crystalline NiSe₂ as an efficient
   electrocatalyst for overall water splitting
SO CHEMICAL ENGINEERING JOURNAL
LA English
DT Article
DE Amorphous-crystalline heterostructures; Copper-nickel selenides;
   Core@shell nanostructures; Water splitting
ID HYDROGEN EVOLUTION REACTION; ENHANCED CATALYTIC-ACTIVITY; BIFUNCTIONAL
   ELECTROCATALYST; MOS2 NANOSHEETS; DOPED CARBON; NICKEL FOAM;
   METAL-OXIDE; FILMS; ARRAY; IRON
AB In this research, we designed a novel heterostructure of porous amorphous-crystalline nickel selenide incorporated with copper (Cu-(a-NiSex/c-NiSe2)) and shelled over one-dimensional TiO2 nanorods (NRs) to simultaneously accelerate both the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) kinetics in alkaline environment. The Cu-(a-NiSex/c-NiSe2)/TiO2 NRs supported by carbon cloth displayed as an effective bifunctional catalyst, which required low overpotentials of 156.9 mV for HER and 339 mV for OER to achieve a current response of 10 mA cm-2 in 1.0 M KOH medium. An electrolyzer derived from the Cu-(a-NiSex/c-NiSe2)/ TiO2 NRs material allowed an operation voltage of 1.62 V at 10 mA cm-2 along with good long-term stability after 21.5 h operation towards water splitting in alkaline medium. This achievement was resulted from the finetuned 3D porous architecture of the amorphous NiSex-crystalline NiSe2 heterostructures doped by copper, which led to significant modulation of electronic properties as well as large surface of exposed electroactive site/types, thereby effectively promoting the catalytic performance. This study suggested a rational approach of structure and shape engineering to design a potential catalyst for producing green hydrogen via water spitting.
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FU Program for Fostering Next-Generation Researchers in Engineering [2017H1D8A2030449]; Regional Leading Research Center Program through the National Research Foundation - Ministry of Science and ICT of the Republic of Korea [2019R1A5A8080326]
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TI Intermolecular Metallic Single-Site Complexes Dispersed on
Mo₂TiC₂T<i>_x</i>/MoS₂
Heterostructure Induce Boosted Solar-Driven Water Splitting
SO ADVANCED ENERGY MATERIALS
LA English
DT Article
DE heterostructures; intermolecular complexes; MoS2; MXene; solar-driven
water splitting
ID PHTHALOCYANINE; EFFICIENT; SPECTROSCOPY; NANOSHEETS

AB Successful development of an electrocatalyst capable to promote the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER) elements of water electrolysis is desirable for green hydrogen gas production. Herein, this work designs intermolecular metallic single-site complexes of iron phthalocyanine (Fe-Pc) and vanadium oxide phthalocyanine (VOPc) dually immobilized on 3D hierarchical MoS2-coated MXene Mo2TiC2Tx (MX/MoS2) heterostructures as a high-performance bifunctional electrocatalyst. The well-organized structure with an unusual coordination environment and electronic localization impressively enhances water adsorption and activation to remarkably accelerate HER and OER kinetics. Therefore, the hybrid material requires overpotentials as small as 17.4 and 300 mV to drive 10 mA cm(-2) for the HER and 50 mA cm(-2) for the OER in 1.0 m KOH media, respectively. The electrolyzer of MX/MoS2-FePcVOPc(+,-) exhibits low cell voltage of only 1.45 V to reach a current response of 10 mA cm(-2) in 7.0 m KOH at 75 degrees C along with excellent current retention stability of 99%/94% after long-term operations of 30 h at 10/50 mA cm(-2). Moreover, a solar-to-hydrogen conversion efficacy of 19.96% is achieved in a solar energy-powered water electrolysis system, highlighting the great potential of the developed MX/MoS2-FePcVOPc electrocatalyst toward water electrolysis.
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ID TOTAL-ENERGY CALCULATIONS; EVOLUTION; EFFICIENCY
AB The dissolution of active atoms under operating potential will lead to a decline in their oxygen evolution reaction (OER) performance, thus preventing the current highly active catalysts from being practically applicable in industrial water electrolysis. Here, we propose a sequential leaching strategy to utilize the dynamic restructuring and enhance the chemical bond strength for highly active and stable OER. Modeling on nickel-iron sulfides (NiFe-S), we introduced and utilized foreign Mo dopant preleaching as the sacrificial agent to alleviate the oxidation corrosion of partial M-S bonds. Operando spectroscopic reveal that foreign Mo dopant leach from the matrix and then adsorb on the surface of NiFe O(S)OH as molybdate at lower OER potential. The crystal occupation hamiltonian population analysis uncovers that the charge transfer from molybdate into NiFe O(S)OH will enhance bond energy of M-S, thus preventing further S and Fe/Ni leaching. By manipulating ion leaching, the resulting active phase achieves an ultralow overpotential of 250 mV at 400 mA cm-2 and high stability of more than 3,700 h at 100 mA cm-2. An industrial water electrolysis equipment using our catalysts delivered ultralow energy consumption of 4.30 kWh m -3H2 and record stability over 250 h (2,300 h lifetime by epitaxial method with 10% attenuation) under a high working current of 8,000 mA. The hydrogen production cost of US$2.46/kgH2 aligns with the green hydrogen cost target set by the European Commission for the coming decade.
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TI Syngas to FCC-like gasoline range hydrocarbons with upgraded light
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ID FISCHER-TROPSCH SYNTHESIS; PARTICLE-SIZE; PORE-SIZE; IRON; PERFORMANCE;
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AB The global trend toward sustainability is due to the growing demand for synthetic chemicals and fuels relying on fossil crude oil with the associated concerns of climate change. The Fischer-Tropsch synthesis (FTS) process is a key sustainable pathway for supplying light olefins, gasoline, and other petrochemicals using green hydrogen and energy. Here we report a simple, green, cost-effective synthesis strategy to prepare an iron-based metal-organic framework (Fe-BTC MOF) at room temperature with a remarkable porous structure analogous to the commercially available Basolite F300. The catalyst shows a 97% syngas conversion to gasoline-range hydrocarbons (C-5-C-12) at high

temperatures, with a selectivity of 48.3%, yield of 28%, low methane selectivity (15.5%) and low C13+ selectivity (1%). In addition, the catalyst is 29% selective to light olefin (C-2-C-4(=)), yielding 17%, besides an olefin/paraffin ratio (O/P) of 4.3 with 81% olefin selectivity of the C-2-C-4 fraction. The resulting gasoline is equivalent to gasoline produced by Fluid Catalytic Cracking (FCC) of crude oil. The highest C-5-C-12 selectivity reached 63.6%, yielding 12% at 29% CO conversion. The Fe-BTC/C catalyst showed excellent stability for time on stream >100 h and a high gas hourly space velocity (GHSV) value of 20000 mL g(cat)(-1) h(-1) with an Fe-time yield of 165 mu mol(CO) g(Fe)(-1) s(-1). The prepared Fe-BTC catalyst, with a 2-fold larger pore volume than the previously prepared Fe-MIL-88B catalyst, has a higher olefin production capability by 2-fold, 7-fold higher O/P for the light fraction and 2.3-fold higher C5+ selectivity. The sustainable synthesis of catalysts with improved porous structure may significantly foster FTS technology for being economically practical to be scaled up and commercialized for national fuel and olefin production projects.
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AU Abedi, M
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AF Abedi, Mohsen
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TI Designing core-shell heterostructure arrays based on snowflake
   NiCoFe-LTH shelled over W 2 N-WC nanowires as an advanced bi-functional
   electrocatalyst for boosting alkaline water/seawater electrolysis
SO JOURNAL OF COLLOID AND INTERFACE SCIENCE
LA English
DT Article
DE LTH nanosheet; Core-shell nanostructure; Tungsten carbide; Tungsten
   nitride; Heterostructure; Bi-functional electrocatalyst; Water splitting
ID HIGH-PERFORMANCE; EFFICIENT ELECTROCATALYSTS; OXIDE NANOCRYSTALS; IRON;
   HYDROXIDE; CONSTRUCTION; MODULATION; NANOSHEETS; CATALYSTS
AB The pursuit of efficient and sustainable hydrogen production through water splitting has led to intensive research in the field of electrocatalysis. However, the impediment posed by sluggish reaction kinetics has served as a significant barrier. This challenge has inspired the development of electrocatalysts characterized by high activity, abundance in earth ' s resources, and long-term stability. In addressing this obstacle, it is imperative to meticulously fine-tune the structure, morphology, and electronic state of electrocatalysts. By systematically manipulating these key parameters, the full potential of electrocatalysts can unleash, enhancing their catalytic activity and overall performance. Hence in this study, a novel heterostructure is designed, showcasing core - shell architectures achieved by covering W 2 N-WC nanowire arrays with tri-metallic Nickel -Cobalt -Iron layered triple hydroxide nanosheets on carbon felt support (NiCoFe-LTH/W 2 N-WC/CF). By integrating the different virtue such as binder free electrode design, synergistic effect between different components, core - shell structural advantages, high exposed active sites, high electrical conductivity and heterostructure design, NiCoFe-LTH/W 2 N-WC/ CF demonstrates striking catalytic performances under alkaline conditions. The substantiation of all the mentioned advantages has been validated through electrochemical data in this study. According to these results NiCoFe-LTH/W 2 N-WC/CF achieves a current density of 10 mA cm -2 needs overpotential values of 101 mV for HER and 206 mV for OER, respectively. Moreover, as a bi-functional electrocatalyst for overall water splitting, a two -electrode device needs a voltage of 1.543 V and 1.569 V to reach a current density of 10 mA cm -2 for alkaline water and alkaline seawater electrolysis, respectively. Briefly, this research with attempting to combination of different factors try to present a promising stride towards advancing bi-functional catalytic activity with tailored architectures for practical green hydrogen production via electrochemical water splitting process.
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AU Ezhov, R
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AF Ezhov, Roman
   Bury, Gabriel
   Maximova, Olga
   Grant, Elliot Daniel
   Kondo, Mio
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TI Pentanuclear iron complex for water oxidation: Spectroscopic analysis of
   reactive intermediates in solution and catalyst immobilization into the
   MOF-based photoanode
SO JOURNAL OF CATALYSIS
LA English
DT Article
DE Water oxidation; Electro catalysis; X-ray absorption spectroscopy; X-ray
   emission spectroscopy; EPR; Reaction mechanisms
ID OXYGEN-EVOLVING COMPLEX; O BOND FORMATION; ELECTRONIC-STRUCTURE;
   PHOTOSYSTEM-II; MOLECULAR CATALYSTS; MANGANESE COMPLEX; EXCHANGE-ENERGY;
   RU-V=O; C-H; METAL
AB Photoelectrochemical water splitting can produce green hydrogen for industrial use and CO2-neutral transportation, ensuring the transition from fossil fuels to green, renewable energy sources. The iron-based electrocatalyst [FeII4FeIII(mu-3-O)(mu-L)6]3+ (LH = 3,5-bis(2-pyridyl)pyrazole) (1), discovered in 2016, is one of the fastest molecular water oxidation catalysts (WOC) based on earth-abundant elements. However, its water oxidation reaction (WOR) mechanism has not been yet fully elucidated. Here, we present in situ X-ray spectroscopy and electron paramagnetic resonance (EPR) analysis of electrochemical WOR promoted by (1) in water-acetonitrile solution. We observed transient reactive intermediates during the in situ electrochemical WOR, consistent with a coordination sphere expansion prior to the onset of catalytic current. At a pre-catalytic (-+1.1 V vs. Ag/AgCl) potential, the distinct g - 2.0 EPR signal assigned to FeIII/FeIV interaction was observed. Prolonged bulk electrolysis at catalytic (-+1.6 V vs. Ag/AgCl) potential leads to the further oxidation of Fe centers in (1). At the steady state achieved with such electrolysis, the formation of hypervalent FeV--O and FeIV--O catalytic intermediates was inferred with XANES and EXAFS fitting, detecting a short Fe--O bond at

- 1.6 angstrom. (1) was embedded into MIL-126 MOF with the formation of a (1)-MIL-126 composite. The latter was tested in photoelectrochemical WOR and demonstrated an increase in electrocatalytic current upon visible light irradiation in acidic (pH = 2) water solution. The presented spectroscopic analysis gives further insight into the catalytic pathways of multinuclear systems and should help the subsequent development of more energy- and costeffective water-splitting catalysts based on earth-abundant metals. Photoelectrocatalytic activity of (1)-MIL126 confirms the possibility of creating an assembly of (1) inside a solid support and harnessing solar irradiation towards industrial applications of the catalyst.
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TI Assessment of a multistep revamping methodology for cleaner steel production
SO JOURNAL OF CLEANER PRODUCTION
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DT Article
DE CO2 emissions; Decarbonization; Direct reduction-electric arc furnace; Green steel; Green hydrogen; Revamping methodology
ID CO2 EMISSION REDUCTION; BLAST-FURNACE; HYDROGEN; IRON; TECHNOLOGIES; SIMULATION; ENERGY; INJECTION; DESIGN
AB A novel revamping methodology is proposed to achieve the decarbonization of currently operating integrated steel mills (step 0) without reducing steel production levels. Such a method encompasses four successive steps involving cleaner and more energy efficient technological pathways for steel production.The decarbonization strategy is reported: step 1, partial replacement of coke with recycled plastic in a con-ventional Blast Furnace - Basic Oxygen Furnace (BF-BOF) plant; step 2, implementation of a Direct Reduction -Electric Arc Furnace (DR-EAF) line combined with the BF-BOF plant; step 3, complete shut-down of the BF-BOF line and full operation of two DR-EAF lines fed by CH4; step 4, installation of an alkaline electrolyzer and use of 100% green H2 as a reducing agent in the DR plants.The gradual replacement of the integrated steel mill with DR-EAF lines causes a progressive drop in CO2 emissions, ranging from 8.5 Mt/y at step 0 to a minimum of 0.68 Mt/y at step 4 (92% decrease).Coke replacement with recycled plastic in the blast furnace in step 1 leads to a slight decrease in CO2 emissions without altering

the structural layout of the plant. In step 2, the combined operation of BF-BOF and DR-EAF lines determines a 39% decrease in CO2 emission compared to the initial configuration, while keeping total steel production constant. Step 3 involves two DR-EAF lines fed by CH4 and reduces the CO2 emissions by 75% compared to the initial configuration. The operation of two DR-EAF lines increases the electricity consumption, especially when 100% green H2 is involved as a reducing agent in step 4. By increasing the scrap mass fraction in the EAFs of step 4, both electricity and H2 demands of the DR plant are expected to decrease, while the CO2 emission levels remain almost unchanged, leading to about 92% total CO2 emissions reduction compared to the initial configuration (provided that green electricity is used). By assuming an initial 10% scrap mass fraction at the EAFs inlet of step 4, the demand of green hydrogen is significant, thus requiring the installation of a 1.42 GW electrolyzer. The capital expenditure (CAPEX) estimated upon completion of the revamping methodology amounts to approximately 2.97 B euro . The transition towards a full decarbonization of steel production technologies is demonstrated to be technically feasible, though strictly dependent upon the large availability of low emissions electric power and scrap material.
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TI Vertically Oriented FeNiO Nanosheet Array for Urea and Water
   Electrolysis at Industrial-Scale Current Density
SO ACS SUSTAINABLE CHEMISTRY & ENGINEERING
LA English
DT Article
DE Self-supported catalysts; FeNiO nanosheets; Water electrolysis; Urea
   electrolysis; Industrial-scalehydrogen production; Hydrothermal
   synthesis
ID OXYGEN EVOLUTION REACTION; IN-SITU FORMATION; HYDROGEN-PRODUCTION;
   ELECTROCATALYSTS; OXIDE; OXIDATION; ENERGY; EFFICIENT; IRON; CATALYSTS
AB In addressing the challenging quest for an efficient electrocatalyst in electrochemical water splitting, we demonstrate an Fe-doped NiO nanosheet array anchored on nickel foam synthesized via a two-step process. Demonstrating exceptional performance in an alkaline electrolyte, FeNiO catalysts exhibit the oxygen evolution reaction with a low potential of 1.52 V vs RHE and the urea oxidation reaction of 1.32 V vs RHE @ 10 mA/cm(2). The bifunctional electrolyzer generates 10 mA/cm(2) current at 1.95 V for water and 1.59 V for urea electrolysis at ambient temperature. Promisingly, the FeNiO catalyst based electrolyzer generates hydrogen at an industrial-scale current density of 400 mA/cm(2) at a cell voltage of just 1.91 V in concentrated alkaline electrolyte and elevated temperature (80 degrees C) due to the dimensionally stable and robust behavior of the self-supported catalyst. The activation energy for alkaline water electrolysis is found to be 52 kJ/mol. The present catalysts also demonstrate stable performance at 300 mA/cm(2) in 4 M KOH electrolyte at 50 degrees C for more than 20 h. The synergy induced by Fe doping into NiO activates catalytic sites, expediting charge transfer and reaction kinetics. The present research report highlights the potential of catalysts as a practical and cost-effective approach for green hydrogen production via water splitting.
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AU Marimuthu, S
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TI Tailoring the Heterointerfaces of Earth-Abundant Transition-Metal
   Nanoclusters on Nickel Oxide Nanosheets for Enhanced Overall Water
   Splitting through Electronic Structure Optimization
SO LANGMUIR
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DT Article
ID OXYGEN-EVOLUTION ELECTROCATALYSTS; HYDROGEN EVOLUTION; EFFICIENT;
   NANOPARTICLES; CATALYST; ARRAYS
AB Evolving highly competent and economical electrocatalysts for alkaline water electrolysis is crucial in renewable hydrogen energy technologies. The slow hydrogen evolution reaction (HER)/oxygen evolution reaction (OER) kinetics under alkaline electrolytes, still, has troubled developments in high-performance green hydrogen production systems. Herein, we demonstrate the tailoring of the interface of earth-abundant transition-metal nanoclusters (MNCs), including iron (Fe), cobalt (Co), nickel (Ni), and copper (Cu) nanoclusters on nickel oxide nanosheets (M NCs|NiO NS) through metal-support interaction for enriched overall water splitting under an alkaline electrolyte. The strong metal-metal oxide interaction allows alteration of the binding capabilities of hydrogen ions (*H) and hydroxyl ions (*OH) on Ni electrodes. Specifically, the robust interaction between Fe and NiO reveals optimized binding of H* and OH* energies, facilitating the water-splitting reaction under an alkaline electrolyte. In addition, the improved HER/OER catalytic activity is attained with the Fe NCs|NiO NS with small overpotentials of similar to 62.0 and similar to 380.0 mV for the HER and OER, respectively, a high mass activity of similar to 90.0 A g(-1), a turnover frequency of similar to 5.94 s(-1), and long-lasting stability via offering abundant electrochemical active sites, three-dimensional (3D) morphologies, and high dispersion of nanoclusters that provide effective charge and mass transport processes. This study provides a promising strategy for the effective design of efficient bifunctional electrocatalysts based on earth-abundant materials for alkaline water electrolyzers.
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Turek, Thomas
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TI Benchmarking performance: A round-robin testing for liquid alkaline electrolysis
SO INTERNATIONAL JOURNAL OF HYDROGEN ENERGY
LA English
DT Article
DE Alkaline water electrolysis; Test protocol; Benchmarking; Round robin; Reproducibility; AFC TCP task 30
ID GREEN HYDROGEN; OXYGEN EVOLUTION; ELECTRODES
AB Liquid alkaline water electrolysis has gained considerable interest in recent years due to its promising role in an energy sector based on renewable energy sources. Its main advantage is the low investment cost of industrial alkaline water electrolyzers compared to other electrolysis technologies. A challenge remains in developing costefficient materials, stable in corrosive electrolytes, and offering competitive cell performance. Although there are many publications in liquid alkaline electrolysis, there is insufficient standardization of experimental conditions and procedures, reference materials, and hardware. As a result, comparability and reproducibility suffer, significantly slowing down research progress. This manuscript presents the initial efforts towards the development of such reference hardware and procedures within the framework of Task 30 Electrolysis in the Technology Collaboration Programme on Advanced Fuel Cells (AFC TCP) of the International Energy Agency (IEA). For this purpose, a homogenized setup including the electrolysis cell, functional materials, experimental conditions, and a test protocol was developed. The protocol and hardware were tested simultaneously at eleven different institutions in Europe and North America. To evaluate the success of this approach, polarization and run-in data were collected and analyzed for comparison, and performance differences were calculated. Significant disparities between the laboratories were observed and some key influence factors were identified: iron content in the electrolyte resulted to be a main source of deviation between experiments, along with temperature control and the conditioning of the cells. The results suggest that additional attention to detailed experimental conditions should be paid to obtain meaningful performance data in future research.
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TI Ti₃C₂T_{<i>x</i>} MXene coupled
   Co(OH)₂: a stable electrocatalyst for the hydrogen evolution
   reaction in alkaline media
SO RSC SUSTAINABILITY
LA English
DT Article
ID EFFICIENT; NANOPARTICLES; NANOSHEETS; COMPOSITE; IRON
AB Green hydrogen (H-2) production via water electrolysis is a promising technique. Within this domain, two dimensional (2D) materials are gaining more attention throughout the world particularly in energy conversion/storage devices due to their unique features. Herein, this study focuses on the development of sustainable, durable, and economical electrocatalysts based on titanium carbide (Ti3C2Tx) MXene and cobalt hydroxide (Co(OH)(2)) as a composite. Ti3C2Tx has been doped into Co(OH)(2) (CT nanostructure) with varying concentrations by the aqueous chemical growth method. The as-prepared electrocatalysts (CT-15 and CT-30) have been investigated through different physicochemical characterization studies including X-ray diffraction (XRD), scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FTIR), and electrochemical analysis in order to access their morphology, crystalline phase homogeneity, surface functionalization, and electrochemical behaviour for the HER. It is observed that the as-prepared material (CT-30) exhibits superior hydrogen evolution reaction (HER) activity in 1.0 M potassium hydroxide (KOH). The optimised electrocatalyst CT-30 demonstrates an overpotential of 380 mV at a current density of 10 mA cm(-2) with a 99 mV dec(-1) Tafel slope value, showing fast reaction kinetics. Moreover, it offers a low charge transfer resistance (Rct) accompanied by good stability, high electrochemical active surface area (ECSA), and durability for 30 h, as evident for efficient HER activity. This novel electrocatalyst can contribute to the replacement of noble metal-based electrocatalysts for practical usage in energy conversion/storage systems.
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TI In Situ Modulation of NiFeOOH Coordination Environment for Enhanced Electrocatalytic-Conversion of Glucose and Energy-Efficient Hydrogen Production
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DE doping; electrocatalytic-conversion of glucose; electrochemical activation; electrolyzer; hydrogen evolution reaction; NiFeOOH
ID ELECTROOXIDATION; OXYGEN; FORMATE; MOLYBDENUM; CATALYSTS; BIOMASS; PROTON
AB Glucose electrocatalytic-conversion reaction (GCR) is a promising anode reaction to replace the slow oxygen evolution reaction (OER), thus promoting the development of hydrogen production by electrochemical water splitting. Herein, NiFe-based metal-organic framework (MOF) is used as a precursor to prepare W-doped nickel-iron phosphide (W-NiFeP) nanosheet arrays by ion exchange and phosphorylation, which exhibit a high electrocatalytic activity toward the hydrogen evolution reaction (HER), featuring an overpotential of only -179 mV to achieve the current density of 100 mA cm-2 in alkaline media. Notably, electrochemical activation of W-NiFeP facilitates the in situ formation of phosphate groups producing W,P-NiFeOOH, which, in conjunction with the W co-doped amorphous layers, leads to a high electrocatalytic performance toward GCR, due to enhanced proton transfer and adsorption of reaction intermediates, as confirmed in experimental and theoretical studies. Thus, the two-electrode electrolyzer of the W-NiFeP/NF||W,P-NiFeOOH/NF for HER||GCR needs only a low cell voltage of 1.56 V to deliver 100 mA cm-2 at a remarkable hydrogen production efficiency of 1.86 mmol h-1, with a high glucose conversion (98.0%) and formic acid yields (85.2%). Results from this work highlight the significance of the development of effective electrocatalysts for biomass electrocatalytic-conversion in the construction of high-efficiency electrolyzers for green hydrogen production.
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NR 64
TC 0
Z9 0
U1 34
U2 34
PU WILEY
PI HOBOKEN
PA 111 RIVER ST, HOBOKEN 07030-5774, NJ USA
EI 2198-3844
J9 ADV SCI
JI Adv. Sci.
PD FEB
PY 2025
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DI 10.1002/advs.202412872
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WC Chemistry, Multidisciplinary; Nanoscience & Nanotechnology; Materials
Science, Multidisciplinary
WE Science Citation Index Expanded (SCI-EXPANDED)
SC Chemistry; Science & Technology - Other Topics; Materials Science
GA U8A5I
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OA gold
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PT J
AU Hu, B
Xu, LF
Li, Y
Sun, F
Wang, ZZ
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AF Hu, Bo
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Kong, Wenwen
Shen, Boxiong
Wang, Xin
Yang, Jiancheng
TI Biochar and Fe2+mediation in hydrogen production by water electrolysis:
Effects of physicochemical properties of biochars
SO ENERGY
LA English
DT Article
DE Water electrolysis; Hydrogen production; Biomass; Iron ions mediator
ID ACTIVATED COKE; CARBON; COAL; RAMAN; CONVERSION; EVOLUTION; BIOMASS
AB Electrolysis of water to produce hydrogen can consume excessive renewable power and generate high-value hydrogen. Biochar-assisted water electrolysis for producing pure and green hydrogen, substituting the oxygen evolution reaction at the anode with biochar oxidation reaction (BOR), could significantly reduce the starting potential and increase

the current density during water electrolysis, combining excessive renewable electricity and biomass waste utilization. However, slow BOR limits the electrolysis. In this study, the mediator of Fe2+ and biochars with different treatments were used to enhance the BOR in electrochemical experiments. Pickling pretreatment improves the performance of pyrolysis and hydrothermal biochars in BAWE containing Fe2+ media, especially the latter, which has the highest oxidation current density of 180 mA/cm2 at an anode voltage of 1.2 V vs. MSE. The effects of different oxygen-containing functional groups on the current density are determined by comparing different biochars before and after pickling. The abundance of -OH and C--O groups favors the increase of oxidation current, while the C-O groups from anhydride and ether play a negative role. Pickling allows biochars to obtain a higher specific surface area and enrich its pores, thereby improving electrolytic performance. Further activation of KOH can increase the specific surface area and make the pore structure, especially the micropores, more abundant, which is conducive to the further increase of oxidation current. This work is expected to lead to a more efficient use of biochar in the BAWE process.
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C3 Hebei University of Technology; Thermal Power Research Institute Co Ltd; Harbin Institute of Technology
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RI Sun, Fei/M-4258-2019
OI Xu, Lianfei/0000-0001-5805-0279
FU National Natural Science Foundation of China [51906058]; Joint Funds of the National Natural Science Foundation of China [U20A20302]; Natural Science Foundation of Hebei Province [E2020202213]; Innovative group projects in Hebei Province [E2021202006]; Huaneng Group Headquarters Technology Project [HNKJ21-H32]
FX The study was supported by National Natural Science Foundation of China (51906058), Joint Funds of the National Natural Science Foundation of China (U20A20302), Natural Science Foundation of Hebei Province (E2020202213), and Innovative group projects in Hebei Province (E2021202006), Huaneng Group Headquarters Technology Project (HNKJ21-H32) .
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NR 64
TC 6
Z9 7
U1 12
U2 15
PU PERGAMON-ELSEVIER SCIENCE LTD
PI OXFORD
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J9 ENERGY
JI Energy
PD JUN 15
PY 2024
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AR 131275
DI 10.1016/j.energy.2024.131275
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WC Thermodynamics; Energy & Fuels
WE Science Citation Index Expanded (SCI-EXPANDED)
SC Thermodynamics; Energy & Fuels
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PT J
AU Wang, KT
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AF Wang, Ketao
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   Zhu, Jiawei
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   Lin, Haifeng
   Wang, Lei
TI Mn Doping and P Vacancy Induced Fast Phase Reconstruction of FeP for
   Enhanced Electrocatalytic Oxygen Evolution Reaction in Alkaline Seawater
SO SMALL
LA English
DT Article
DE fast phase reconstruction; iron phosphide; oxygen evolution reaction;
   seawater splitting
ID ENVIRONMENT
AB Due to the shortage of pure water resources, seawater electrolysis is a promising strategy to produce green hydrogen energy. To avoid chlorine oxidation reactions (ClOR) and the production of more corrosive hypochlorite, enhancing OER electrocatalyst activity is the key to solving the above problem. Considering that transition metal phosphides (TMPs) are promising OER eletrocatalysts for seawater splitting, a method to regulate the electronic structure of FeP by introducing Mn heteroatoms and phosphorus vacancy on it (Mn-FePV) is developed. As an OER electrocatalyst in seawater solution, the synthesized Mn-FePV achieves extremely low overpotentials (eta 500 = 376, eta 1000 = 395 mV). In addition, the Pt/C||Mn-FePV couple only requires the voltage of 1.81 V to drive the current density of 1000 mA cm-2 for overall seawater splitting. The density functional theory (DFT) calculation shows that Mn-FePV (0.21 e-) has more charge transfer number compared with FeP (0.17 e-). In-situ Raman analysis shows that phosphorus vacancy and Mn doping can synergistically regulate the electronic structure of FeP to induce rapid phase reconstruction, further improving the OER performance of Mn-FePV. The new phase species of FeOOH is confirmed to can enhance the adsorption kinetics of OER intermediates.
   The Mn-FePV is successfully synthesized as an efficient OER electrocatalyst. In situ Raman analysis and DFT calculation show that Mn doping and phosphorus vacancy can synergistically regulate the electronic structure of FeP to induce rapid phase reconstruction.image
C1 [Wang, Ketao; Liu, Xiaobin; Yu, Qingping; Wang, Xuanyi; Zhu, Jiawei; Li, Yanyan; Chi, Jingqi; Lin, Haifeng; Wang, Lei] Qingdao Univ Sci & Technol, Coll Chem & Mol Engn, State Key Lab Base Ecochem Engn, Int Sci & Technol Cooperat Base Ecochem Engn & Gre, Qingdao 266042, Peoples R China.
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C3 Qingdao University of Science & Technology; Qingdao University of
   Science & Technology
RP Liu, XB; Wang, L (corresponding author), Qingdao Univ Sci & Technol, Coll Chem & Mol Engn, State Key Lab Base Ecochem Engn, Int Sci & Technol Cooperat Base Ecochem Engn & Gre, Qingdao 266042, Peoples R China.; Liu, XB; Wang, L (corresponding author), Qingdao Univ Sci & Technol, Coll Environm & Safety Engn, Qingdao 266042, Peoples R China.
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RI 王, 宣艺/IAP-1418-2023; Wang, Lei/AGQ-4540-2022; Liu, Xiaobin/A-4143-2019
FU National Natural Science Foundation of China; China Postdoctoral Science

Foundation; Postdoctoral Innovation Project of Shandong Province; Postdoctoral Applied Research Project of Qingdao, Outstanding Youth Foundation of Shandong Province, China [51772162, 21971132, 52072197, 22179068]; Youth Innovation and Technology Foundation of Shandong Higher Education Institutions, China [2020M682135]; Major Scientific and Technological Innovation Project [202102039]; Major Basic Research Program of Natural Science Foundation of Shandong Province [ZR2019JQ14]; The 111 Project of China [2019KJC004]
FX Financial support from the National Natural Science Foundation of China (51772162, 21971132, 52072197, and 22179068), China Postdoctoral Science Foundation (2020M682135), Postdoctoral Innovation Project of Shandong Province (202102039), Postdoctoral Applied Research Project of Qingdao, Outstanding Youth Foundation of Shandong Province, China (ZR2019JQ14), Youth Innovation and Technology Foundation of Shandong Higher Education Institutions, China (2019KJC004), Major Scientific and Technological Innovation Project (2019JZZY020405), Major Basic Research Program of Natural Science Foundation of Shandong Province under Grant (ZR2020ZD09), the 111 Project of China (Grant No. D20017), Taishan Scholar Young Talent Program (tsqn201909114), University Youth Innovation Team of Shandong Province (202201010318), Shandong Province "Double-Hundred Talent Plan" (WST2020003), and Key Research and Development Program of Jiangsu Province (BE2021070).
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NR 45
TC 16
Z9 16
U1 43
U2 181
PU WILEY-V C H VERLAG GMBH
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EI 1613-6829
J9 SMALL
JI Small
PD MAY
PY 2024
VL 20
IS 20
DI 10.1002/smll.202308613
EA DEC 2023
PG 9
WC Chemistry, Multidisciplinary; Chemistry, Physical; Nanoscience &
Nanotechnology; Materials Science, Multidisciplinary; Physics, Applied;
Physics, Condensed Matter
WE Science Citation Index Expanded (SCI-EXPANDED)
SC Chemistry; Science & Technology - Other Topics; Materials Science;
Physics
GA RN6Y5
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AU Guo, JY
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Zhao, Jia
Zhang, Yi-Fan
Hu, Chen-Xu
Lu, Jun
Yan, Hong
TI Mechanism of Autocatalytic Reduction of CO₂ over
MgCO₃ to High Value-Added Chemicals: A DFT & AIMD Study
SO LANGMUIR
LA English
DT Article
ID MOLECULAR-DYNAMICS; ELECTRON-DENSITY; X-RAY; DECOMPOSITION; MAGNESITE;
CARBONATE; CALCITE; SYNGAS; IRON; MGO
AB Calcination of MgCO3 is an important industrial reaction, but it causes significant and unfavorable CO2 production. Calcination in a reducing green hydrogen atmosphere can substantially reduce CO2 release and produce high value-added products such as CO or hydrocarbons, but the mechanism is still unclear. Here, the in situ transformation

process of MgCO3 interacting with hydrogen and the specific formation mechanism of the high value-added products are thoroughly investigated based on reaction thermodynamic, ab initio molecular dynamics (AIMD) simulations, and density functional theory (DFT) calculations. The reaction thermodynamic parameters of MgCO3 coupled with hydrogen to produce CO or methane are calculated, revealing that increasing and decreasing the thermal reductive decomposition temperature favors the production of CO and methane, respectively. Kinetically, the energy barriers of each possible production pathway for the dominant products CO and methane are further calculated in conjunction with the AIMD simulation results of the transformation process. The results suggest that CO is produced via the MgO catalytic-carboxyl pathway (CO2*-> COOH*(trans)-> COOH*(cis)-> CO*-> CO), which is autocatalyzed by MgO derived from the thermal reductive decomposition of MgCO3. For the mechanism of methane formation, it prefers to be produced by the stepwise interaction of carbonates in the MgCO3 laminates with hydrogen adsorbed on their surfaces (direct conversion pathway: sur-O-CO -> sur-O-HCO -> sur-O-HCOH -> sur-O-HC -> sur-O-CH2 -> sur-O-CH3 -> sur-O + CH4*).
C1 [Guo, Jing-Yi; He, Shi-Qi; Jie, Yao; Song, Hui-Ting; Lu, Hao; Xu, Xin-Yu; Zhao, Jia; Zhang, Yi-Fan; Hu, Chen-Xu; Lu, Jun; Yan, Hong] Beijing Univ Chem Technol, Coll Chem, State Key Lab Chem Resource Engn, Beijing 100029, Peoples R China.
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AU Christi, DS
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AF Christi, Darren Sebastian
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TI Nanocrystalline (NixCo(1-x))3(PO4)2@FeSe2/NF as a promising OER
   electrocatalyst for alkaline water electrolysis
SO INTERNATIONAL JOURNAL OF HYDROGEN ENERGY
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DT Article
DE Alkaline Water Electrolysis; Non-PGM based Electrocatalyst; OER;
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ID OXYGEN-EVOLUTION-REACTION; COBALT; CATALYSTS; EFFICIENT; PHOSPHATE;
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AB Affordable and sustainable hydrogen production is the need of the hour owing to the mounting global pursuit for the hydrogen economy. Water splitting is the premier go -to method to produce green hydrogen at a larger scale in which the half -cell Oxygen Evolution Reaction (OER) demands a larger amount of energy expenditure due to its sluggish kinetics. Hence, designing an efficient OER electrocatalyst, especially for alkaline water electrolysis that offers alternatives to the usage of precious group metals is a pressing priority. Herein, we report a novel nanocrystalline electrocatalyst consisting of two components, namely cobalt nickel phosphate and iron diselenide synthesised via a two-step electrodeposition at room temperature. The combination of the two components on the porous nickel foam substrate exhibits an overpotential of 272 mV at 100 mA/cm2 in 1 M KOH showing a low Tafel slope of a mere 38 mV/dec with appreciable retention even after 24 h of stability test at a relatively higher current density. The surface reconstruction that occurs when FeSe2 is electrodeposited on

(Ni0.35Co0.65)3(PO4)2@NF and the synergy between the two components is the primary reason for the improved performance. Thus, this work highlights the ambient synthesis of a highly durable earth -abundant metal -based electrocatalyst which exceeds the performance of the standard Ru/C by a decent margin.
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TI New benchmark for pure nickel-based oxygen-evolution electrocatalyst:
   Tailored large NiMoO4•xH2O monocrystals for complete reconstruction
SO APPLIED CATALYSIS B-ENVIRONMENT AND ENERGY
LA English
DT Article
DE Large-sized NiMoO4 center dot xH2O monocrystals; OER precatalyst;
   Complete reconstruction; Pure Nickel-Based; AEM-WEs
ID WATER-OXIDATION; NI; FE; PRECATALYSTS
AB High-performance oxygen evolution reaction (OER) catalysts are the key to the large-scale production of green hydrogen by water electrolysis. Since there is no problem of iron leaking, the durability of pure nickel-based catalyst is more promising. However, it is challenging to achieve comparable performance with pure nickel- based materials as seen in NiFe-based catalysts. In this work, a controllable, large-sized NiMoO4 center dot xH2O mono- crystal (alpha L-NiMoO4 center dot xH2O) was synthesized by reducing the dissociation (alpha) value of the reactants and gradually releasing MoO42- by adjusting the pH of the molybdate solution to 4.5. alpha L-NiMoO4 center dot xH2O undergoes a complete reconstruction (CR) process to transform into nanocrystalline-amorphous NiOOH (NCA-NiOOH) with excellent OER performance. The NCA-NiOOH electrode requires only 185 mV and 280 mV overpotentials to achieve OER current densities of 10 mA cm- 2 and 1.0 A cm- 2 , setting a new benchmark for the OER performance of pure Nibased anodes. The NCA-NiOOH showed no signs of activity decline during bulk electrolysis at 1.0 A cm- 2 for 3000 h. Anion-exchange membrane water electrolyzers (AEM-WEs) assembled with the NCA-NiOOH showed outstanding performance (1.57 V @ 1.0 A cm- 2 at 80 degrees C) and impressive stability (230 h @ 1.0 A cm- 2 at room temperature). This work not only developed a pure nickel benchmark OER catalyst for alkaline water electrolysis but also guided the rational design and controlled growth of precatalysts for CR.
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TI CoFe-loaded P, N co-doped carbon foam derived from petroleum pitch
waste: An efficient electrocatalyst for oxygen evolution reaction
SO CATALYSIS TODAY
LA English
DT Article
DE Electrocatalysts; Oxygen evolution reaction; CoFe; Carbon foam; And P; N
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ID BIFUNCTIONAL ELECTROCATALYST; ELECTROCHEMICAL OXIDATION;
HIGH-PERFORMANCE; ELECTRODE; REDUCTION; CATALYSTS; GRAPHENE; HYDROGEN
AB Designing and developing affordable, high-performance, and stable electrocatalysts for oxygen evolution reaction (OER) is decisive for pragmatic water electrolysis to produce green hydrogen energy. In this work, we report cobalt and iron incorporated in phosphorus and nitrogen co-doped carbon foam (CF) derived from petroleum pitch as a promising electrocatalyst for alkaline OER. The P, N heteroatoms co-doped carbon foam (PN-CF) was first synthesized via thermo-chemical treatment of low-cost petroleum pitch in the presence of melamine (N source) and sodium hypophosphite (P source) precursors, followed by carbonization. Then, mono and bimetals of Co and Fe were impregnated into the as-prepared composite carbon foam (PN-CF) substrate, followed by further carbonization. Among the different catalysts, the bimetallic CoFe integrated with the PN-CF (CoFe@PN-CF) reveals an outstanding electrocatalytic activity (320 mV overpotential at j = 10 mA center dot cm(-2)), low Tafel slope (48 mV center dot dec(-1)), and excellent durability during OER measurement in 1 M KOH aqueous solution. The superb performance of the CoFe@PN-CF catalyst stems from the synergetic effect of the bimetals confined on phosphorus and nitrogen co-doped carbon foam support with high specific surface area, highly porous structure, and formation of graphitic domains, which enhances the electrical conductivity. This work sheds light on the potential for valorizing petroleum pitch and provides a facile synthesis approach to synthesizing a low-cost, high-performance, and durable electrocatalyst for alkaline OER.
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TI Determining the Production and Transport Cost for H₂ on a Global Scale
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DT Article
DE H-2 electrolysis; network; techno-economic assessment; green hydrogen; hydrogen; cost

ID LIFE-CYCLE ASSESSMENT; HYDROGEN-PRODUCTION; ELECTROLYSIS; ECONOMICS; NETWORK; AMMONIA; DESIGN; SECTOR; POWER

AB Hydrogen (H-2) produced using renewable energy could be used to reduce greenhouse gas (GHG) emissions in industrial sectors such as steel, chemicals, transportation, and energy storage. Knowing the delivered cost of renewable H-2 is essential to decision-makers looking to utilize it. The cheapest location to source it from, as well as the transport method and medium, are also crucial information. This study presents a Monte Carlo simulation to determine the delivered cost for renewable H-2 for any usage location globally, as well as the most cost-effective production location and transport route from nearly 6,000 global locations. Several industrially dense locations are selected for case studies, the primary two being Cologne, Germany and Houston, United States. The minimum delivered H-2 cost to Cologne is 9.4 euro/kg for small scale (no pipelines considered), shipped from northern Egypt as a liquid organic hydrogen carrier (LOHC), and 7.6 euro/kg piped directly as H-2 gas from southern France for large scale (pipelines considered). For small-scale H-2 in Houston, the minimum delivered cost is 8.6 euro/kg trucked as H-2 gas from the western Gulf of Mexico, and 7.6 euro/kg for large-scale demand piped as H-2 gas from southern California. The south-west United States and Mexico, northern Chile, the Middle East and north Africa, south-west Africa, and north-west Australia are identified as the regions with the lowest renewable H-2 cost potential, with production costs ranging from 6.7-7.8 euro/kg in these regions. Each is able to supply differing industrially dominant areas. Furthermore, the effect of parameters such as year of construction, electrolyser, and H-2 demand is analysed. For the case studies in Houston and Cologne, the delivered H-2 cost is expected to reduce to about 7.8 euro/kg by 2050 in Cologne (no pipelines considered, PEM electrolyser) and 6.8 euro/kg in Houston.

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TI A Review on Green Hydrogen Valorization by Heterogeneous Catalytic
Hydrogenation of Captured CO₂ into Value-Added Products
SO CATALYSTS
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DE CO2 hydrogenation; power-to-gas; power-to-liquid; green methanol;
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CATALYSTS; NATURAL-GAS PRODUCTION; IRON-BASED CATALYST
AB The catalytic hydrogenation of captured CO2 by different industrial processes allows obtaining liquid biofuels and some chemical products that not only present the interest of being obtained from a very low-cost raw material (CO2) that indeed constitutes an environmental pollution problem but also constitute an energy vector, which can facilitate the storage and transport of very diverse renewable energies. Thus, the combined use of green H-2 and captured CO2 to obtain chemical products and biofuels has become attractive for different processes such as power-to-liquids (P2L) and power-to-gas (P2G), which use any renewable power to convert carbon dioxide and water into value-added, synthetic renewable E-fuels and renewable platform molecules, also contributing in

an important way to CO2 mitigation. In this regard, there has been an extraordinary increase in the study of supported metal catalysts capable of converting CO2 into synthetic natural gas, according to the Sabatier reaction, or in dimethyl ether, as in power-to-gas processes, as well as in liquid hydrocarbons by the Fischer-Tropsch process, and especially in producing methanol by P2L processes. As a result, the current review aims to provide an overall picture of the most recent research, focusing on the last five years, when research in this field has increased dramatically.
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Liu, Gang
Zhang, Shaofei
TI Fast synthesis of low Ru doped CoO_x/CeO₂ nanosheet arrays with abundant heterointerfaces for highly efficient overall water splitting
SO INTERNATIONAL JOURNAL OF HYDROGEN ENERGY
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DE Bifunctional electrocatalysts; Low Ru doping; Heterointerface; Nanosheet arrays; Water splitting
ID BIFUNCTIONAL ELECTROCATALYSTS; COMBUSTION SYNTHESIS
AB The development of a simple and large-scale strategy for enhancing the intrinsic activity and reaction kinetics of nano-electrocatalyst for water splitting is crucial but challenging. Herein, a Ru-doped CoOx/CeO2 heterojunction catalyst with nanosheet arrays grown on an iron foam (named R-Ru@CoOx/CeO2/IF) was synthesized via fast solution combustion and low-temperature reduction processes. Low Ru doping (3.56 wt%) creates the lattice strain on the catalyst and modified the electronic structure, which is essential

for optimizing the adsorption of reaction intermediates. Furthermore, benefiting from the desired nanosheet array framework, heterojunction structure, and abundant oxygen vacancies, the self-supporting electrode possesses sufficient active sites and fast mass/charge transport kinetics for promoting hydrogen and oxygen evolution reactions (HER and OER, respectively). Consequently, the R-Ru@CoOx/CeO2/IF exhibits ultralow overpotentials of 44 and 212 mV at 10 mA cm(-2) for the HER and OER, respectively, in an alkaline solution; it also exhibits excellent stability with an overall activity superior to those of most reported oxide catalysts. Particularly, the assembled R-Ru@CoOx/CeO2/IF || R-Ru@CoOx/CeO2/IF symmetric electrolyzer only requires 1.44 and 1.61 V to reach 10 and 100 mA cm(-2), respectively, and the decline in its activity is satisfactory after 100 h of durability testing at 1000 mA cm(-2). The proposed simple and large-scale strategy has potential in the development of low noble-metal doped electrocatalysts for producing high-density and green hydrogen.
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FU National Natural Science Founda-tion of China [52375422, 52101251]; Natural Science Foundation of Hebei Province [E2023208017, E2023208010, E2024208057]; Science and Technology Plan Project of </bold></p> Shijiazhuang [241791337A, 241130547A]; Science Research Project of Hebei Education Department [BJK2023058]
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TI Prussian blue analog-derived nickel iron phosphide-reduced graphene oxide hybrid as an efficient catalyst for overall water electrolysis
SO JOURNAL OF COLLOID AND INTERFACE SCIENCE
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DT Article
DE Phosphide; Oxygen evolution reaction; Hydrogen evolution reaction; Water electrolysis; Hydrophilic; Aerophobic
ID HYDROGEN EVOLUTION; BIFUNCTIONAL ELECTROCATALYSTS; NANOSHEETS; OXIDATION; FRAMEWORK; NIFEP
AB Efficient and bifunctional nonprecious catalysts for oxygen evolution reaction (OER) and hydrogen evo-lution reaction (HER) are essential for the production of green hydrogen via water electrolysis. Transition metal (Ni, Co, Fe, etc.) phosphides are frequently documented HER catalysts, whereas their bimetallic oxi-des are efficient OER catalysts, thus enabling bifunctional catalysis for water electrolysis via proper oper-ation. Herein, phosphide-reduced graphene oxide (rGO) hybrids were prepared from graphene oxide (GO)-incorporated bimetal Prussian blue analog (PBA) precursors. The hybrids could experience partial surface oxidation to create oxide layers with OER activities, and the hybrids also possessed considerable HER properties, therefore enabling bifunctional catalytic features for water electrolysis. The typical NiFeP-rGO hybrid demonstrated an overpotential of 250 mV at 10 mA cm-2 and good durability for OER, as well as moderate HER catalytic features (overpotential of 165 mV at-10 mA cm-2 and acceptable catalytic stability). Due to the bifunctional catalytic features, the NiFeP-rGO-based symmetric water elec-trolyzer demonstrated a moderate input voltage and high faradaic efficiency (FE) for O2 and H2 produc-tion. The current work provides a feasible way to prepare OER and HER bifunctional catalysts by facile phosphorization of PBA-associated precursors and spontaneous surface oxidation. Given the oxidation/ reduction bifunctional catalytic behaviors, phosphide-rGO hybrid catalysts have great potential for wide-spread application in fields beyond water electrolysis, such as electrochemical pollution abatement, sen-sors, energy devices and organic syntheses.(c) 2023 Elsevier Inc. All rights reserved.
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TI Supply risk considerations for photoelectrochemical water splitting
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ID SOLAR HYDROGEN-PRODUCTION; CUBI2O4; CELLS; PHOTOANODES; DEPOSITION;
   LAYER
AB Hydrogen is a key enabler of a carbon neutral economy. The main production route of renewable hydrogen is via renewable wind and solar power and water splitting via electrolyzers. Photoelectrochemical water splitting is an alternative production route using incoming solar radiation to produce hydrogen and oxygen via a photoabsorber material with suitable band gaps and positions. Various absorber materials are being discussed in research and further developed at the lab scale. However, these materials need to be scalable in production, with low supply risk, because of the scale of hydrogen production needed to satisfy the global need for green hydrogen. Here, we semi-quantitatively assess the short-term and long-term supply risks due to potential supply reduction, demand increase, concentration risks, and political risks of eight chemical elements contained in nine promising absorber materials for photoelectrochemical water splitting. On an element level, supply risks are lowest for iron, copper, and tantalum in the present scenario and tin in the future scenario. The supply risks are highest for bismuth in the present scenario and future scenario. On a material level, present supply risks are lowest for hematite and highest for bismuth vanadate. Bismuth vanadate has the highest future supply risks, but tin tungsten oxide achieves the lowest supply risk score in the future scenario. The results show that some frequently discussed photoelectrochemical absorber materials have higher supply risks than typically perceived. In contrast, other materials should be more intensively studied because of their promising low long-term supply risk evaluation. Our method provides a separate assessment of present and future supply risks, which was previously unavailable for the criticality assessments.
   Absorber materials for photoelectrochemical water splitting have supply risks emerging from supply, demand, concentration, and political risks.
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AB This review systematically summarizes the source of electricity, the key choice of catalyst, and the potentiality of electrolyte for prospective hydrogen generation. Each section provides comprehensive overview, detailed comparison and obvious advantages in these system configurations. The problems of hydrogen generation from electrolytic water splitting and directions of next-generation green hydrogen in the future are discussed and outlooked.

Direct regeneration method has been widely concerned by researchers in the field of battery recycling because of its advantages of in situ regeneration, short process and less pollutant emission. In this review, we firstly analyze the primary causes for the failure of three representative battery cathodes (lithium iron phosphate, layered lithium transition metal oxide and lithium cobalt oxide), targeting at illustrating their underlying regeneration mechanism and applicability. Efficient stripping of material from the collector to obtain pure cathode material has become a first challenge in recycling, for which we report several pretreatment methods currently available for subsequent regeneration processes. We review and discuss emphatically the research progress of five direct regeneration methods, including solid-state sintering, hydrothermal, eutectic molten salt, electrochemical and chemical lithiation methods. Finally, the application of direct regeneration technology in production practice is introduced, the problems exposed at the early stage of the industrialization of direct regeneration technology are revealed, and the prospect of future large-scale commercial production is proposed. It is hoped that this review will give readers a comprehensive and basic understanding of direct regeneration methods for used lithium-ion batteries and promote the industrial application of direct regeneration technology.

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TI Hydrogen Embrittlement as a Conspicuous Material Challenge-Comprehensive
   Review and Future Directions
SO CHEMICAL REVIEWS
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DT Review
ID FATIGUE-CRACK-GROWTH; THERMAL-DESORPTION SPECTROSCOPY; HIGH-STRENGTH
   STEEL; AUSTENITIC STAINLESS-STEEL; HIGH-ENTROPY ALLOY; ENHANCED
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AB Hydrogen is considered a clean and efficient energy carrier crucial for shaping the net-zero future. Large-scale production, transportation, storage, and use of green hydrogen are expected to be undertaken in the coming decades. As the smallest element in the universe, however, hydrogen can adsorb on, diffuse into, and interact with many metallic materials, degrading their mechanical properties. This multifaceted phenomenon is generically categorized as hydrogen embrittlement (HE). HE is one of the most complex material problems that arises as an outcome of the intricate interplay across specific spatial and temporal scales between the mechanical driving force and the material resistance fingerprinted by the microstructures and subsequently weakened by the presence of hydrogen. Based on recent developments in the field as well as our collective understanding, this Review is devoted to treating HE as a whole and providing a constructive and systematic discussion on hydrogen entry, diffusion, trapping, hydrogen-microstructure interaction mechanisms, and consequences of HE in steels, nickel alloys, and aluminum alloys used for energy transport and storage. HE in emerging material systems, such as high entropy alloys and additively manufactured materials, is also discussed. Priority has been particularly given to these less understood aspects. Combining perspectives of materials chemistry, materials science, mechanics, and artificial intelligence, this Review aspires to present a comprehensive and impartial viewpoint on the existing knowledge and conclude with our forecasts of various paths forward meant to fuel the exploration of future research regarding hydrogen-induced material challenges.
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TI Stabilization of Nickel-Doped Iron-oxy-hydroxide Core in Water by Heptamolybdate Ions to Improve the Electrochemical Oxygen Evolution Reaction
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AB Heterometal-doped nickel-oxy-hydroxides or high-entropy multimetallic oxides show notable electrocatalytic activity. Herein, a readily available Anderson-type polyoxometalate (POM) anion, heptamolybdate ([Mo7O24](6-)), is taken as an inorganic ligand to stabilize the nickel(II)-doped iron-oxy-hydroxide nanocore. [Mo7O24](6-)-ligated NixFe1-xO(OH) nanomaterials with different ratios of Ni(II) and Fe(III) in the core (1-3) are prepared via a hydrothermal route. ICP-MS and the subsequent PXRD study of the materials have found out that approximately 1.5-2% nickel is incorporated into the gamma-FeO(OH) core without altering its two-dimensional-layered lattice structure. The presence of numerous POMs covalently linked on the surface of 4-5 nm highly crystalline NixFe1-xO(OH) core is proven by multiple spectroscopic and microscopic techniques. Negative zeta potential of 1-3 infers the ionic surface of the materials due to the presence of negatively charged POMs which makes them highly dispersed and stable in water. Using 1-3 as electrocatalysts, oxygen evolution reaction (OER) is studied under alkaline condition. For catalytic OER, 1-3 on the nickel foam (NF) electrode require almost 20 mV less overpotential compared to the undoped core material MoxOy@FeO(OH) and the POM-free bare FeO(OH) and NixFe1-xO(OH). The better OER activity can be correlated to better electrokinetics, realized from the Tafel slope and charge-transfer resistance (R-ct). The fabricated electrode 1@NF not only shows a long-term stability under the OER condition but also can be fabricated to a water-splitting electrolyzer using a graphite rod as the cathode to produce green hydrogen with Faradaic efficiency of ca. 72%. In this study, Anderson-type POM is used as a potential ligand to derive the quantum-dot-sized NixFe1-xO(OH) core as a reactive electrocatalyst for OER. In a broad context, this

strategy, i.e., the use of POM as a pure inorganic ligand to stabilize a reactive metal oxide nanocore, can further be adapted to design a variety of multimetallic or mixed-valence metal oxide materials.
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DT Article
DE Self-Assembled Cd (II)-3D Network; Nitroaromatic Reduction; Dye
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AB A new Cd(II) based coordination polymers {[Cd(Azopy)(H2O)(4)](NDC)}(n) (1) has been designed and synthesized by using 4,4 '-Azopyridine (Azopy), and 2, 6-Naphthalene dicarboxylic acid (NDC) as a linker at ambient condition. The bulk purity of the 1 was analysed by powder X-ray diffraction (PXRD) analysis, infrared spectroscopy and further confirmed by single crystal X-ray studies. The crystal structure of 1 revealed a polythreading feature where each 2, 6-naphthalene dicarboxylate unit are trapped between two one-dimensional (1D) chain of [Cd(Azopy)(H2O)(4)](infinity) via strong hydrogen bonding interactions. The hydrogen bonding and pi pi stacking interactions of 1 play a crucial role in the formation of the infinite 3D-layered supramolecular network. Furthermore, the reduction of nitro-aromatics to their corresponding amines was performed using green hydrogen source such as D-glucose in H2O solvent at room temperature. Additionally, the dye adsorption studies revealed that 1 can adsorb Congo Red (CR) dye in a very short span of time. The kinetic study result reveals that the adsorption of CR for 1 is fitted well (R-2 =0.996) with a pseudo-second-order kinetic model. Moreover, photoluminescence of 1 shows emission in the blue region with lambda(max) at 395 nm and 408 nm at room temperature in the solid state. 1 shows multi-facet behaviour such as facile synthesis, luminescent nature in solids-state, emerged as a heterogeneous dye-adsorbent and catalyst which makes it easy to scaled-up.
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Z9 4
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U2 9
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PI WEINHEIM
PA POSTFACH 101161, 69451 WEINHEIM, GERMANY
SN 2365-6549
J9 CHEMISTRYSELECT
JI ChemistrySelect
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BP 7162
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WC Chemistry, Multidisciplinary
WE Science Citation Index Expanded (SCI-EXPANDED)
SC Chemistry
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PT J
AU Aigul, S
   Enkhbayar, E
   Gaur, A
   Han, H
AF Aigul, Sembinova
   Enkhbayar, Enkhtuvshin
   Gaur, Ashish
   Han, HyukSu
TI Cr-doped tri-metallic nano prism catalyst for efficient alkaline and
   seawater splitting
SO JOURNAL OF CRYSTAL GROWTH
LA English
DT Article
DE Water splitting; Seawater oxidation; Electrocatalyst; Nano prism
ID ELECTROCATALYSTS; EVOLUTION; COBALT
AB Electrochemical water splitting is one of the most promising methods for sustainable production of green hydrogen. The oxygen evolution reaction (OER) is a crucial step in the process of water splitting. However, it exhibits sluggish kinetics and requires a significant overpotential for functioning at reasonable reaction rates. The efficiency of the reaction can be enhanced by reducing the overpotential, lowering the energy barrier, and using an effective electrocatalyst. Transition metal-based catalysts are well studied for this purpose. Specially, nickel-cobalt (Ni-Co) based catalysts have been regarded as the best OER electrocatalysts. Therefore, several studies have been carried out to enhance the electrocatalytic efficiency of Ni-Co catalysts. While mixing other transition metals with Ni-Co is a straightforward and reliable method to improve the OER activity of Ni-Co catalysts, there is still a need for a thorough examination of the design of Ni-Co catalysts with various additional elements. Seawater electrolysis, which utilizes abundant water resources that constitute over 97% of the world's water, is highly appealing for sustainable energy production. To achieve commercial feasibility, scientists are striving to solve challenges, such as corrosion resistance, high overpotential, and the need for efficient and durable electrocatalysts. In this study, we fabricated a transition metal-based trimetallic catalyst (CNF), consisting of cobalt (Co), nickel (Ni), and iron (Fe). Furthermore, CNF was doped with chromium (Cr-doped CNF) and tested for the OER in alkaline freshwater and alkaline seawater. Our Cr-doped trimetallic CNF catalyst demonstrates exceptional performance in both seawater and freshwater, with overpotential of 320 mV and 280 mV at 10 mA cm(-2) current density, making it a promising candidate for large-scale, sustainable hydrogen production.
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   work was also supported by the National Research Foundation of Korea
   (NRF) grant funded by the Korean government (MSIT) (2021R1A2C2091497) .
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NR 30
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Z9 0
U1 10
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PA RADARWEG 29, 1043 NX AMSTERDAM, NETHERLANDS
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EI 1873-5002
J9 J CRYST GROWTH
JI J. Cryst. Growth
PD JAN 1
PY 2025
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EA OCT 2024
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WC Crystallography; Materials Science, Multidisciplinary; Physics, Applied
WE Science Citation Index Expanded (SCI-EXPANDED)
SC Crystallography; Materials Science; Physics
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AU Li, WJ
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   Yuan, XS
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AF Li, Wanjun
Zhang, Jinwei
Yuan, Xiaoshuai
Yang, Liping
Zhu, Hanxiong
Zhang, Xiaofei
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Liu, Lu
Liu, Zhenggang
Xiao, Yu
Cai, Rui
Liu, Zhongmin
TI Perspective on the low-carbon transformation pathways of fossil energy under dual carbon goals
SO CHINESE SCIENCE BULLETIN-CHINESE
LA Chinese
DT Article
DE dual carbon goals; fossil energy; low-carbon transformation; hard-to-abate sectors; technical innovation
ID SYNGAS
AB China has the world's largest carbon dioxide emissions primarily due to its reliance of the energy and industrial systems on fossil resources, especially coal. A low-carbon pathway for fossil resources not only involves reducing CO2 emissions but also the energy security and the stability of industrial and supply chains, which is of great importance to China's high-quality development. To reduce CO2 emissions from fossil fuels, it is imperative to promote their comprehensive utilization as chemical feedstock instead of fuel with multi-energy system integration. Multi-energy system integration can break through the existing barriers in the energy sector and promote the integration of the resource advantages of various energy systems. In addition, it can reconstruct the energy and heavy industry system and realize the green and low-carbon circular development of high-carbon industries in China. By promoting the integrated development of coal chemical and petrochemical industries, the safety of the petrochemical industry could be ensured, the diversified utilization of petrochemical raw materials could be promoted, and a new framework of complementary and coordinated development between coal chemical and petroleum chemical industries could be established. Integration of chemical industry with sectors such as steel and cement can achieve deep decarbonization in hard-to-abate industrial sectors. For example, utilizing carbon monoxide from steel industry exhaust gases and coupling it with chemical industry processes can co-produce steel and chemicals with significant emission reduction potential. Additionally, innovative approaches such as methane atmosphere calcination of cement clinker can effectively address process emissions in the cement industry while directly producing synthesis gas for downstream chemical production. Power to X, which refers to a bundle of ways to convert, store, and reconvert electricity, offers a great opportunity to couple renewable energy with fossil fuels. Water could be electrolyzed to produce hydrogen using renewable electricity. Hydrogen, a clean and versatile energy carrier, can be used in the industrial process reengineering to drive low- and zero-carbon transformations through technological innovation, which is crucial for deep decarbonization of hard-to-abate sectors. For example, the coupling of green hydrogen and coal-to-olefins process can eliminate the need for water-shift reaction in traditional coal gasification processes, reducing carbon emissions from the source and significantly improving coal utilization efficiency. Moreover, the green oxygen produced in the electrolysis process can be used in the gasification process and reduce the demand for air separation, consequently lowering the usage of fossil fuel energy. CO could be produced by electrocatalytic reduction of CO2 with renewable electricity, which could then be used to synthesize fuels. In the low-carbon transition path of fossil energy, the Chinese Academy of Sciences (CAS) has proactively positioned itself in addressing key scientific issues and core technologies in the energy field.

Key breakthroughs have been made in areas such as coal-to-synthesis gas selective catalytic conversion of low-carbon olefins, new-generation methanol-to-olefins technology, coal-to-methanol-to-ethanol technology, direct synthesis of high-carbon alcohols with oil co-production from synthesis gas, new-generation synthesis gas-to-oil technology, new-generation indirect coal liquefaction to oil technology, and the technique of hydroisomerization for producing high-quality lubricating base oil from

coal-based Fischer-Tropsch synthetic wax, dimethyl carbonate synthesis from methanol with a dual-site ion liquid catalyst, and non-photogas isocyanate preparation technology. The aim is to explore a low-carbon innovation and development path for fossil energy utilization that aligns with China's national conditions.
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PI BEIJING
PA 16 DONGHUANGCHENGGEN NORTH ST, BEIJING 100717, PEOPLES R CHINA
SN 0023-074X
EI 2095-9419
J9 CHIN SCI B-CHIN
JI Chin. Sci. Bull.-Chin.
PY 2024
VL 69
IS 8
BP 990
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DI 10.1360/TB-2023-0556
PG 7
WC Multidisciplinary Sciences
WE Emerging Sources Citation Index (ESCI)
SC Science & Technology - Other Topics
GA OM4I8
UT WOS:001207673800008
OA Bronze
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AU Gaddimath, S
   Aralekallu, S
   Prabhu, CPK
   Daniel, S
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   Sannegowda, LK
AF Gaddimath, Shivalingayya
   Aralekallu, Shambhulinga
   Prabhu, C. P. Keshavanada
   Daniel, Shantharaja
   Giddaerappa
   Sannegowda, Lokesh Koodlur
TI Developments in cobalt-based soft materials as electrocatalysts for
   oxygen evolution reaction
SO INTERNATIONAL JOURNAL OF HYDROGEN ENERGY
LA English
DT Article
DE Oxygen evolution reaction; N 4-macrocycles; Electrocatalysts; Water
   electrolysis; Green hydrogen; Long-term stability
ID METAL-ORGANIC FRAMEWORK; SINGLE-ATOM CATALYSTS; WALLED CARBON NANOTUBES;
   BIFUNCTIONAL ELECTROCATALYSTS; HETEROGENEOUS CATALYSIS; REDUCTION
   REACTION; ENERGY-CONVERSION; PHTHALOCYANINE; HYDROGEN; IRON
AB The search for sustainable, clean, and highly efficient energy sources is underway at a faster phase to meet the energy needs of modern society. Among the various sustainable energy technologies, water electrolysis emerges as a promising approach to pave the way for tomorrow's green energy fulfilment. In water electrolysis, hydrogen evolves on the cathode side, and oxygen evolves on the anode side. The oxygen evolution reaction (OER) process is crucial as it is highly sluggish compared to the hydrogen evolution reaction (HER) towards efficient, clean and green energy production. The traditional benchmark catalysts such as IrO2 and RuO2 face challenges of high cost and limited abundance. Therefore, the search for efficient and cost-effective alternate electrocatalysts has been intensified. To improve the gas evolution efficiency, researchers have developed numerous advanced electrocatalysts, leading to significant progress in understanding the fundamental mechanism of the OER and essential requirements of a good electrocatalyst. This review inspects the current progress in the electrocatalysis of OER. It presents the theoretical principles and critical parameters for evaluating OER catalysts. Then, latest developments in catalyst materials for performing OER activity, including precious and non-precious materials have been discussed. Further, a thorough review of the Co-based-N4 macromolecules for OER applications has been carried out with respect to the simplicity of synthesis and ability to fine-tune their electronic properties through the substitution of axial/peripheral groups. Attention is also paid to the single atom catalyst (SAC) approach for attaining significant electrocatalytic behavior for OER. The mechanism of OER has been enumerated from the perspective of recent experimental studies. Finally, the strategies for improving the OER performance for future research are presented.
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TI Spinel-type high-entropy oxides for enhanced oxygen evolution reaction activity in anion exchange membrane water electrolyzers
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DE High-entropy oxides; Spinel structure modulation; Oxygen evolution reaction; Rotating disk electrode study; Anion exchange membrane water electrolyzers
ID JAHN-TELLER DISTORTION; OXIDATION-STATE; LATTICE OXYGEN; COBALT OXIDE; MCO2O4 M; IRON; XPS; ELECTROCATALYSTS; METAL; MN
AB Developing efficient and cost-effective approaches to synthesize platinum group metal-free (PGM-free) electrocatalysts with high performance toward the sluggish oxygen evolution reaction (OER) is crucial for commercializing anion exchange membrane water electrolyzers (AEMWEs) to produce green hydrogen. Here, we propose a facile method to produce an emergent family of catalysts for the OER at the anode of AEMWEs. Spinel-type high entropy oxides (HEOs) based on Mg, Ni, Co, Mn, and Fe were synthesized by different methods, roomtemperature or hydrothermal-assisted coprecipitation, using different coprecipitating agents (NH3 solution vs. urea) and calcination conditions. Furthermore, HEO composition was tailored by modulating the metal's stoichiometry. Rietveld refinement and high-resolution transmission electron microscopy, coupled with energydispersive X-ray spectroscopy (HRTEM-EDX), indicated that single-phase HEOs with highly crystalline nanoparticles and homogeneous distribution of the metals were obtained by coprecipitation at room temperatures using NH3, combined with the rapid quenching of the HEOs after treatment at 750 degrees C. Notably, the catalyst's performance was significantly enhanced (EJ10 = 1.62 V vs. RHE), modulating the content of Ni, Co, and Mn, promoting their surface reconstruction and activation during OER with the formation of (oxy)hydroxides. AEMWE single-cell tests were carried out by integrating the optimized HEO as an anode catalyst of a catalystcoated membrane, using the piperION (R) as a polymeric membrane and ionomer and Pt/C as a cathode catalyst. A remarkable performance was indicated with a high current density (J = 1.57 Acm-2) at 1.8 V, with a maximum value (J = 4.14 Acm-2) being reached at 2.2 V, outperforming highly active PGM-free catalysts reported in the literature.
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TI <i>Meta</i>-kinks are key to binder performance of poly(arylene piperidinium) ionomers for alkaline membrane water electrolysis using non-noble metal catalysts
SO JOURNAL OF MATERIALS CHEMISTRY A
LA English
DT Article
ID ANION-EXCHANGE-MEMBRANE; QUATERNARY AMMONIUM CATIONS; OXYGEN EVOLUTION REACTION; HYDROGEN; DEGRADATION; STABILITY; POLY(TERPHENYLENE); ELECTROCATALYSTS; POLYAROMATICS; CONDUCTIVITY
AB Anion-exchange membrane water electrolysis (AEMWE) is a key technology for the production of green hydrogen at high current densities without the necessity of noble metal catalysts. AEMWE technology does not only rely on chemically stable and highly hydroxide-conducting membranes, but also on ionomer binders, to which additional criteria apply related to swelling, mechanical properties, gas permeability and porosity to form a triple phase boundary with catalyst particles on top of an membrane electrode assembly (MEA). Here, we investigate seven poly(arylene piperidinium)s (PAPs) with different ratios of meta-/para-terphenyl building blocks as binders for non-noble NiFe-LDH catalysts. We first analyze the materials comprehensively in pristine form and subsequently as binders. With increasing content of meta-terphenyl, specific surface area, water uptake, swelling ratio and ion-conductivity increase continuously, with the latter ranging from 145 to 216 mS cm(-1) at 80(degrees)C. We elucidate binder performance from rotating disk electrode experiments of oxygen evolution reactions (OER) catalysed by nickel-iron layered double hydroxides (NiFe-LDH) under AEMWE working potentials. Here, an increasing content of meta-kinks leads to improved catalyst utilization, superior OER performance and improved electrode stability. Finally, AEMWE single cell tests show a strong improvement in current density when altering binders from exclusively para- to meta-terphenyl in the polymer backbone. Current densities as high as 1000 to 1700 mA cm(-2) at 1.8 V and 3000 mA cm(-2)at 2.0 V are measured for the binder with exclusive meta-terphenyl kinks. The results highlight the role of the binder for AEMWE performance as well as the importance of its individual optimization aside from membrane properties.
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TI Thin Nickel Coatings on Stainless Steel for Enhanced Oxygen Evolution and Reduced Iron Leaching in Alkaline Water Electrolysis
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DE alkaline water electrolysis; electrodeposition; Fe leaching; oxygen evolution reaction; stainless steel
ID ELECTRODES; NI; ELECTROCATALYSTS; CATALYST; ARRAY; MESH
AB One of the most mature technologies for green hydrogen production is alkaline water electrolysis. However, this process is kinetically limited by the sluggish oxygen evolution reaction (OER). Improving the OER kinetics requires electrocatalysts, which can offer superior catalytic activity and stability in alkaline environments. Stainless steel (SS) has been reported as a cost-effective and promising OER electrode due to its ability to form active Ni-Fe oxyhydroxides during OER. However, it is limited by a high Fe-to-Ni ratio, leading to severe Fe-leaching in alkaline environments. This affects not only the electrode activity and stability but can also be detrimental to the electrolyzer system. Therefore, we investigate the effect of different Ni-coatings on both pure Ni- and SS-supports on the OER activity, while monitoring the extent of Fe-leaching during continuous operation. We show that thin layers of Ni enable enhanced OER activities compared to thicker ones. Especially, a less than 1 mu m thick Ni layer on an SS-support shows superior OER activity and stability with respect to the bare supports. X-ray photoelectron spectroscopy reveals traces of oxidized Fe species on the catalyst surface after OER, suggesting that Fe from the SS may be incorporated into the layer during operation, forming active Ni-Fe oxyhydroxides with a very low Fe leaching rate. Utilizing inductively coupled plasma-optical emission spectroscopy, we prove that thin Ni layers on SS decrease Fe leaching whereas the Fe from the uncoated SS-support dissolves into the electrolyte during operation. Thus, OER active and stable electrodes can be obtained while maintaining a low Fe concentration in the electrolyte. This is particularly relevant for application in high-performance electrolyzer systems.
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TI Boosting the Oxygen Evolution Reaction Performance of Ni-Fe-Electrodes
   by Tailored Conditioning
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DT Article
DE Alkaline Water Electrolysis; Electrocatalyst Preparation; In-situ
   Electrode Conditioning; Electrode Activation; Online Dissolution
ID ELECTROCHEMICAL GROWTH; POLARIZATION TIME; SURFACE OXIDES; NICKEL; IRON;
   REDOX; ELECTROCATALYSTS; FILMS; BEHAVIOR; BASE
AB To meet the rising demand for green hydrogen, efficient alkaline water electrolysis demands highly active and low-cost electrocatalysts for the oxygen evolution reaction (OER). We address this issue by focusing our work on optimizing the conditioning of promising Ni-(Fe)-based electrodes to improve their electrocatalytic performances. Systematic parameter variation for cyclic voltammetry conditioning revealed that a large potential window, low scan rate, and a high number of cycles result in improved activation. If the conditioning time is fixed, a high scan rate was found beneficial. A remarkable 47 +/- 6 mV potential drop at 10 mA cm-2 was achieved for Ni70Fe30 when conditioning between -0.35-1.6 V at 100 mV s-1 for just 30 min. We could demonstrate that this activation persisted over 100 h at 100 mA cm-2, underscoring its enduring efficacy. We suggest that this activation effect results from the growth of a hydrous hydroxide layer, which is supported by energy dispersive X-ray spectroscopy and X-ray photoelectron spectroscopy. Fe incorporation or dissolution played only a minor role in the differences in electrode activation, as demonstrated by variation of the Fe content in the electrolyte. Our work stresses the importance of conditioning in enhancing OER performance and explores how to improve the catalysts ' effectiveness by tailoring oxides.
   Cost-efficient, active, and stable electrodes for the alkaline oxygen evolution reaction remain a challenge. Herein, electrochemical conditioning of Ni-Fe-based electrodes is introduced as a promising design method. Conditioning was optimized regarding scan rate, potential limits, hold times, and treatment time. After 100 h operation at 100 mA cm-2, the overpotential was 320 mV lower than that of an unconditioned electrode. image
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TI The Study of Groundwater in the Zhambyl Region, Southern Kazakhstan, to
   Improve Sustainability
SO SUSTAINABILITY
LA English
DT Article
DE groundwater; water sustainability; white hydrogen; natural hydrogen;
   Kazakhstan; Central Asia
ID NATURAL PROCESSES; URBANIZED AREA; CHEMISTRY; AQUIFERS
AB Water resources are scarce and difficult to manage in Kazakhstan, Central Asia (CA). Anthropic activities largely eliminated the Aral Sea. Afghanistan's large-scale canal construction may eliminate life in the main stream of the Amu Darya River, CA. Kazakhstan's HYRASIA ONE project, with a EUR 50 billion investment to produce green hydrogen, is targeted to withdraw water from the Caspian Sea. Kazakhstan, CA, requires sustainable programs that integrate both decision-makers' and people's behavior. For this paper, the authors investigated groundwater resources for sustainable use, including for consumption, and the potential for natural "white" hydrogen production from underground geological "factories". Kazakhstan is rich in natural resources, such as iron-rich rocks, minerals, and uranium, which are necessary for serpentinization reactions and radiolysis

decay in natural hydrogen production from underground water. Investigations of underground geological "factories" require substantial efforts in field data collection. A chemical analysis of 40 groundwater samples from the 97 wells surveyed and investigated in the T. Ryskulov, Zhambyl, Baizak and Zhualy districts of the Zhambyl region in South Kazakhstan in 2021-2022 was carried out. These samples were compared with previously collected water samples from the years 2020-2021. The compositions of groundwater samples were analyzed, revealing various concentrations of different minerals, natural geological rocks, and anthropogenic materials. South Kazakhstan is rich in natural mineral resources. As a result, mining companies extract resources in the Taraz-Zhanatas-Karatau and the Shu-Novotroitsk industrial areas. The most significant levels of minerals found in water samples were found in the territory of the Talas-Assinsky interfluve, where the main industrial mining enterprises are concentrated and the largest groundwater deposits have been explored. Groundwater compositions have direct connections to geological rocks. The geological rocks are confined to sandstones, siltstones, porphyrites, conglomerates, limestones, and metamorphic rocks. In observation wells, a number of components can be found in high concentrations (mg/L): sulfates-602.0 (MPC 500 mg/L); sodium-436.5 (MPC 200 mg/L); chlorine-465.4 (MPC 350 mg/L); lithium-0.18 (MPC 0.03 mg/L); boron-0.74 (MPC 0.5 mg/L); cadmium-0.002 (MPC 0.001 mg/L); strontium-15, 0 (MPC 7.0 mg/L); and TDS-1970 (MPC 1000). The high mineral contents in the water are natural and comprise minerals from geological sources, including iron-rich rocks, to uranium. Proper groundwater classifications for research investigations are required to separate potable groundwater resources, wells, and areas where underground geological "factories" producing natural "white" hydrogen could potentially be located. Our preliminary investigation results are presented with the aim of creating a large-scale targeted program to improve water sustainability in Kazakhstan, CA.
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NR 65
TC 4
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U1 5
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under a wide range of pressure and temperature extremes. The fundamental objective and goal of the separation membrane is to be used in membrane reactors for synchronous hydrogen production and purification. Other competing methods, such as pressure swing adsorption and cryogenic distillation, do not compare favorably to the membrane separation approach at lower operating temperatures. This is because membrane separation takes fewer resources than other competing technologies, particularly ones that have been around for a longer time. This article discusses the various membranes that can be used for substance separation, how hydrogen separation membranes can be made using a variety of technologies, the challenges that are inherent in doing so, and the prospects for the future, particularly in terms of increasing the efficiency of hydrogen separation.
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TI Gas Diffusion Layers: Experimental and Modeling Approach for Morphological and Transport Properties
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ID FUEL-CELLS; THERMAL-CONDUCTIVITY; COMPRESSION; PERFORMANCE; EVAPORATION;
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AB CONSPECTUS: Electrochemical technologies are key to decarbonizing the energy sector. Electrification of the energy sector is underway with battery technologies dominating the lightduty electric vehicles market. It is more challenging to decarbonize historically difficult to decarbonize sectors, such as heavy-duty transportation, planes, ships, and the chemical manufacturing industry (ammonia, cement, steel). Green hydrogen produced via electrolysis will be used as a fuel and a feedstock in some of these processes. At the heart of the hydrogen economy are polymer electrolyte fuel cells (PEFCs), devices that convert hydrogen into electricity. Gas diffusion layers (GDLs) have an integral role in PEFCs, as they are porous carbon layers that transport reactants and products and also remove heat and conduct electricity. To improve the PEFCs' performance and reduce degradation of materials, an understanding of coupled morphological properties and transport phenomena in the GDLs is needed. In this Account, we emphasize the integration of experimental and modeling approaches to achieve complete understanding of materials and transport properties of the GDLs. Our approach builds in complexity from simpler ex situ experiments to in situ and last to 3-D integrated modeling predictions. GDL morphology is complex, as its fabrication includes several stochastic steps (immersion of GDL in various baths to achieve the desired surface wettability) and only 3-D techniques, such as X-ray computed tomography can capture morphology correctly. Porosity, pore-size distribution, tortuosity, and formation factor are the most important morphological properties of the GDLs. For PEFC applications, water is generated in the catalyst layers and is transported through the GDLs. Therefore, GDL wettability directly impacts water permeability through the GDLs. Using in situ water injection experiments, we directly observe which pores water fill at what liquid pressure. This result provides information about the GDL's affinity to intake water. GDLs are typically of mixed wettabilities, and internal wettability until recently has been unknown. Having images of water inside the GDL enabled us to track the triple-phase boundary at the fiber- water-air interface to obtain local contact angles in the locations where water was present. The percentage of contact angles that were hydrophilic correlated well to the percentage of surface oxides on the GDL surface using X-ray photoelectron spectroscopy (XPS). We envision many other groups using the method of XPS to determine internal surface wettability of the GDLs, as it is relatively fast. Heat transport and evaporation/condensation of water in the GDL is studied using in situ X-ray CT experiments. These provide direct insight into pore-scale water transport under thermal gradients. Three-dimensional geometries of GDLs are exported for transport simulations using the lattice Boltzmann method (LBM). Similarly, we advocate for building the LBM simulations, from water injection studies first to validate the model only to operando PEFC models later. LBM coupling with a continuum model enables a computational saving, allowing us to map local temperature, reactant, and product distributions in the GDLs.

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TI Non-Noble Bifunctional Amorphous Metal Boride Electrocatalysts for
Selective Seawater Electrolysis
SO CHEMCATCHEM
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DT Article
DE Electrocatalyst; Hydrogen evolution reaction; Oxygen evolution reaction;
Seawater electrolysis; Transition metal borides
ID SINGLE-ATOM CATALYSTS; CO OXIDATION; ADSORPTION; MODEL; CUXO/CU(111);
SUPPORT; DFT; AU
AB The global scarcity of freshwater resources has recently driven the need to explore abundant seawater as an alternative feedstock for hydrogen production by water-splitting. This route comes with new challenges for the electrocatalyst, which has to withstand harsh saline water conditions with selectivity towards oxygen evolution over other competing reactions. Herein, a series of amorphous metal borides based on the iron triad metals (Co, Ni, and Fe), synthesized by a simple one-step chemical reduction method, displayed excellent bifunctional activity for overall seawater splitting. Amongst the chosen catalysts, amorphous cobalt boride (Co-B) showed the best overpotential values of 182 mV for HER and 305 mV for OER, to achieve 10 mA/cm2, in alkaline simulated seawater. This superior activity was owed to the enrichment of the metal site with excess electrons (HER) and the in-situ surface transformation (OER), as confirmed by various means. In alkaline simulated seawater, the overall cell voltage required to achieve 100 mA/cm2 was 1.85 V for the Co-B catalyst when used in a 2-electrode assembly. The Co-B catalyst showed negligible loss in activity even after 1000 cycles and 50 h potentiostatic tests, thus demonstrating its industrial viability. The selectivity of the catalyst was established with Faradaic efficiency of above 99 % for HER and 96 % for OER, with no detection of chloride products in the spent electrolyte. This study using the mono-metallic boride catalysts will turn to be a precursor to exploit other complex metal boride systems as potential candidates for seawater electrolysis for large-scale hydrogen production.

Green hydrogen production from seawater is highly feasible since approximately 96.5 % of the Earth's surface is covered by water resource. It is necessary to develop an effective electrocatalyst that can withstand the harsh seawater condition. Meanwhile, monometallic amorphous transition metal borides synthesized by one step facile chemical reduction method shows a superior activity, stability and similar to 99 % selectivity for seawater electrolysis. Amongst three TMBs, amorphous Co-B electrocatalyst exhibited an overpotential of 182 mV and 305 mV, respectively at 10 mA/cm2 for HER and OER in alkaline simulated seawater. The optimized Co-B catalyst were extensively studied in three different alkaline media where it showed negligible decrease in the activity. The overall cell voltage of the Co-B outperforms the benchmark electrocatalyst Pt/RuO2 at higher current density. Also, Co-B sustains 50 long hours stability for both HER and OER without degradation which makes them suitable for commercial applications. image
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TI Recent Advances in Self-Supported Transition-Metal-Based Electrocatalysts for Seawater Oxidation
SO ACTA PHYSICO-CHIMICA SINICA
LA English
DT Review
DE Seawater electrolysis; Self-supported nanoarray; Transition metal-based catalyst; Anti-corrosion; Oxygen evolution reaction
ID HYDROGEN EVOLUTION; NANOWIRE ARRAYS; EFFICIENT; ENERGY; OXYGEN; DESIGN; ALKALINE; ELECTROLYSIS; HYDROXIDE; IRON
AB Seawater electrolysis is a promising and sustainable technology for green hydrogen production. However, some disadvantages include sluggish kinetics, competitive chlorine evolution reaction at the anode, chloride ion corrosion, and surface poisoning, which has led to a decline in activity and durability and low oxygen evolution reaction (OER) selectivity of the anodic electrodes. Benefiting from the lower interface resistance, larger active surface, and superior stability, the self-supported nanoarrays have emerged as advanced catalysts compared to conventional powder catalysts. Self-supported catalysts have more advantages than powder catalysts, particularly in practical large-scale hydrogen production applications requiring high current density. During electrolysis, due to the influx of bubbles generated on the electrode surface, the powdered nanomaterial is peeled off easily, resulting in reduced catalytic activity and even frequent replacement of the catalyst. In contrast, self-supported nanoarray possessing strong adhesion between the active species and the substrates ensures good electronic conductivity and high mechanical stability, which is conducive to long-term use and recycling. This minireview

summarizes the recent progress of self-supported transition-metal-based catalysts for seawater oxidation, including (oxy)hydroxides, nitrides, phosphides, and chalcogenides, emphasizing the strategies in response to the corrosion and competitive reactions to ensure high activity and selectivity in OER processes. In general, constructing three-dimensional porous nanostructures with high porosity and roughness can enlarge the surface areas to expose more active sites for oxygen evolution, which is an efficient strategy for improving mass transfer and catalytic efficiency. Furthermore, the Cl- barrier layer on the surface of catalyst, particularly that with both catalytic activity and protection, can effectively inhibit the competitive oxidation and corrosion of Cl-, thereby delivering enhanced catalytic activity, selectivity, and stability of the catalysts. Moreover, developing super hydrophilic and hydrophobic surfaces is a promising strategy to increase the permeability of electrolytes and avoid the accumulation of large amounts of bubbles on the surface of the self-supported electrodes, thus promoting the effective utilization of active sites. Finally, perspectives and suggestions for future research in OER catalysts for seawater electrolysis are provided. In particular, the medium for seawater electrolysis should be transferred from simulated saline water to natural seawater. Considering the challenges faced in natural seawater splitting, in addition to designing and synthesizing self-supported catalysts with high activities, selectivity, and stability, developing simple and low-cost natural seawater pretreatment technologies to minimize corrosion and poisoning issues is also an important topic for the future development of seawater electrolysis. More importantly, a standardized, feasible evaluation system for self-supported electrocatalysts should be established. In addition, factors such as the intrinsic activity, density of accessible active sites, size, mass loading, substrate effects, and test conditions of the catalyst should be fully considered.
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