

# 1- Evolution of water structures in metal-organic frameworks for improved atmospheric water harvesting

# By:

Hanikel, N (Hanikel, Nikita) [1], [2]; Pei, XK (Pei, Xiaokun) [1], [2]; Chheda, S (Chheda, Saumil) [3], [4] ; Lyu, H (Lyu, Hao) [1], [2]; Jeong, W (Jeong, WooSeok) [4], [5]; Sauer, J (Sauer, Joachim) [6]; Gagliardi, L (Gagliardi, Laura) [7], [8]; Yaghi, OM (Yaghi, Omar M.) [1], [2] (provided by Clarivate) Volume 374 Issue 6566 Page 454-+ DOI 10.1126/science.abj0890 Published OCT 22 2021 Indexed 2021-11-11 **Document Type** Article

# Abstract

Although the positions of water guests in porous crystals can be identified, determination of their filling sequence remains challenging. We deciphered the water-filling mechanism for the state-of-the-art water-harvesting metal-organic framework MOF-303 by performing an extensive series of single-crystal x-ray diffraction measurements and density functional theory calculations. The first water molecules strongly bind to the polar organic linkers; they are followed by additional water molecules forming isolated clusters, then chains of clusters, and finally a water network. This evolution of water structures led us to modify the pores by the multivariate approach, thereby precisely modulating the binding strength of the first water molecules and deliberately shaping the water uptake behavior. This resulted in higher water productivity, as well as tunability of regeneration temperature and enthalpy, without compromising capacity and stability.

Keywords Keywords Plus TOTAL-ENERGY CALCULATIONSADSORPTION PROPERTIESSORPTION



2- Adsorption-based atmospheric water harvesting By: Ejeian, M (Ejeian, M.) [1]; Wang, RZ (Wang, R. Z.) [1] (provided by Clarivate) Volume 5 Issue 7 Page 1678-1703 DOI 10.1016/j.joule.2021.04.005 Published JUL 21 2021 Indexed 2021-08-02 **Document Type** Review

## Abstract

Atmospheric water harvesting (AWH) is a promising solution to the world's water shortage. Meanwhile, adsorption-based atmospheric water harvesting (ABAWH) has shown a higher ability to supply water in arid areas using clean and cheap energy. Numerous modern adsorbents for this application have been introduced so far, and many prototypes have been provided. However, there is still a long way to go for widespread and practical use of this technology. Dedicated designs, operating strategies, environmental compatibility, and energy supply are issues that still need further consideration. This article has tried to summarize what has been achieved so far in ABAWH, analyze the challenges ahead, and provide solutions to continue the path.

## Keywords

Keywords Plus METAL-ORGANIC FRAMEWORKSCOMPOSITE DESICCANT MATERIALHUMID AIRDROPWISE CONDENSATIONAMBIENT HUMIDITYPOTABLE WATERMOIST AIRDESALINATIONSYSTEMENERGY



# 3- Applications of water-stable metal-organic frameworks in the removal of water pollutants: A review

## By:

<u>Zhang, S</u> (Zhang, Shu) [1]; <u>Wang, JQ</u> (Wang, Jiaqi) [1]; <u>Zhang, Y</u> (Zhang, Yue) [1]; <u>Ma, JZ</u> (Ma, Junzhou) [1]; <u>Huang, LT</u> (Huang, Lintianyang) [1]; <u>Yu, SJ</u> (Yu, Shujun) [2]; <u>Chen, L</u> (Chen, Lan) [1]; <u>Song, G</u> (Song, Gang) [3]; <u>Qiu, MQ</u> (Qiu, Muqing) [4]; <u>Wang, XX</u> (Wang, Xiangxue) [1], [5]

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# Abstract

Because the pollutants produced by human activities have destroyed the ecological balance of natural water environment, and caused severe impact on human life safety and environmental security. Hence the task of water environment restoration is imminent. Metal-organic frameworks (MOFs), structured from organic ligands and inorganic metal ions, are notable for their outstanding crystallinity, diverse structures, large surface areas, adsorption performance, and excellent component tunability. The water stability of MOFs is a key requisite for their possible actual applications in separation, catalysis, adsorption, and other water environment remediation areas because it is necessary to safeguard the integrity of the material structure during utilization. In this article, we comprehensively review state-of-the-art research progress on the promising potential of MOFs as excellent nanomaterials to remove contaminants from the water environment. Firstly, the fundamental characteristics and preparation methods of several typical water-stable MOFs include UiO, MIL, and ZIF are introduced. Then, the removal property and mechanism of heavy metal ions, radionuclide contaminants, drugs, and organic dyes by different MOFs were compared. Finally, the application prospect of MOFs in pollutant remediation prospected. In this review, the synthesis methods and application in water pollutant removal are explored, which provide ways toward the effective use of water-stable MOFs in materials design and environmental remediation.

Keywords Author Keywords



Water-stable MOFsUiOMILZIFEnvironmental remediation

**Keywords Plus** 

ZEOLITIC IMIDAZOLATE FRAMEWORK-8SOLID-PHASE EXTRACTIONPHOTOCATALYTIC CO2 REDUCTIONLIGHT-DRIVEN PHOTOCATALYSTROOM-TEMPERATURE SYNTHESISHIGHLY EFFICIENT REMOVALAQUEOUS-SOLUTIONHEAVY-METALADSORPTIVE REMOVALFACILE SYNTHESIS



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3- Design and Applications of Water-Soluble Coordination Cages
By:
Percastegui, EG (Percastegui, Edmundo G.) [1], [2], [3]; Ronson, TK (Ronson, Tanya K.) [1]; Nitschke, JR
(Nitschke, Jonathan R.) [1]
(provided by Clarivate)
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Abstract
Compartmentalization of the aqueous space within a cell is necessary for life. In similar fashion to the
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nanometer-scale compartments in living systems, synthetic water-soluble coordination cages (WSCCs) can isolate guest molecules and host chemical transformations. Such cages thus show promise in biological, medical, environmental, and industrial domains. This review highlights examples of threedimensional synthetic WSCCs, offering perspectives so as to enhance their design and applications. Strategies are presented that address key challenges for the preparation of coordination cages that are soluble and stable in water. The peculiarities of guest binding in aqueous media are examined, highlighting amplified binding in water, changing guest properties, and the recognition of specific molecular targets. The properties of WSCC hosts associated with biomedical applications, and their use as vessels to carry out chemical reactions in water, are also presented. These examples sketch a blueprint for the preparation of new metal-organic containers for use in aqueous solution, as well as guidelines for the engineering of new applications in water.

# Keywords

# **Keywords Plus**

METAL-ORGANIC CAGESH BOND ACTIVATIONPOST-ASSEMBLY MODIFICATIONHYDROPHOBIC EFFECT DRIVESAZA-COPE REARRANGEMENTHIGH-ENERGY WATERMOLECULAR RECOGNITIONSUPRAMOLECULAR HOSTGUEST EXCHANGEDIELS-ALDER



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4- Design and Applications of Water-Soluble Coordination Cages
By:
Percastegui, EG (Percastegui, Edmundo G.) [1], [2], [3]; Ronson, TK (Ronson, Tanya K.) [1]; Nitschke, JR
(Nitschke, Jonathan R.) [1]
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Abstract
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nanometer-scale compartments in living systems, synthetic water-soluble coordination cages (WSCCs) can isolate guest molecules and host chemical transformations. Such cages thus show promise in biological, medical, environmental, and industrial domains. This review highlights examples of threedimensional synthetic WSCCs, offering perspectives so as to enhance their design and applications. Strategies are presented that address key challenges for the preparation of coordination cages that are soluble and stable in water. The peculiarities of guest binding in aqueous media are examined, highlighting amplified binding in water, changing guest properties, and the recognition of specific molecular targets. The properties of WSCC hosts associated with biomedical applications, and their use as vessels to carry out chemical reactions in water, are also presented. These examples sketch a blueprint for the preparation of new metal-organic containers for use in aqueous solution, as well as guidelines for the engineering of new applications in water.

# Keywords

# **Keywords Plus**

METAL-ORGANIC CAGESH BOND ACTIVATIONPOST-ASSEMBLY MODIFICATIONHYDROPHOBIC EFFECT DRIVESAZA-COPE REARRANGEMENTHIGH-ENERGY WATERMOLECULAR RECOGNITIONSUPRAMOLECULAR HOSTGUEST EXCHANGEDIELS-ALDER



5- Current scenario and challenges in adsorption for water treatment By: Dotto, GL (Dotto, Guilherme L.) [1]; McKay, G (McKay, Gordon) [2] (provided by Clarivate) Volume 8 Issue 4 **Article Number** 103988 DOI 10.1016/j.jece.2020.10.3988 Published AUG 2020 Indexed 2020-09-08 **Document Type** Article

## Abstract

In this opinion paper, the current scenario and the main challenges in adsorption for water treatment are presented shortly. It is expected that this discussion paper will serve as a fast literature directive to support new ideas and novel investigations in the field. A general background about the topic is first presented. Subsequently, some important aspects that are well developed in literature are discussed, including adsorbent materials, adsorption operation mode, modeling, regeneration, and process operation with real samples. In the last section, it has been pointed out what should likely be the next steps required to advance in this knowledge.

## Keywords

Author Keywords adsorbent materialsadsorptionmodelingprocesseswater treatment Keywords Plus INORGANIC HYBRID SORBENTPERSONAL CARE PRODUCTSEQUILIBRIA. WRONG USEFIXED-BED ADSORPTIONLOW-COST ADSORBENTSVANT HOOF EQUATIONURBAN WASTE-WATERREACTIVE RED 141AQUEOUS-SOLUTIONACTIVATED CARBON



6- MOF based engineered materials in water remediation: Recent trends By: Rego, RM (Rego, Richelle M.) [1]; Kuriya, G (Kuriya, Gangalakshmi) [1]; Kurkuri, MD (Kurkuri, Mahaveer D.) [1]; Kigga, M (Kigga, Madhuprasad) [1] (provided by Clarivate) Volume 403 **Article Number** 123605 DOI 10.1016/j.jhazmat.2020.123605 Published FEB 5 2021 Indexed 2021-01-11 **Document Type** Review

## Abstract

The significant upsurge in the demand for freshwater has prompted various developments towards water sustainability. In this context, several materials have gained remarkable interest for the removal of emerging contaminants from various freshwater sources. Among the currently investigated materials for water treatment, metal organic frameworks (MOFs), a developing class of porous materials, have provided excellent platforms for the separation of several pollutants from water. The structural modularity and the striking chemical/physical properties of MOFs have provided more room for targetspecific environmental applications. However, MOFs limit their practical applications in water treatment due to poor processability issues of the intrinsically fragile and powdered crystalline forms. Nevertheless, growing efforts are recognized to impart macroscopic shapability to render easy handling shapes for realtime industrial applications. Furthermore, efforts have been devoted to improve the stabilities of MOFs that are subjected to fragile collapse in aqueous environments expanding their use in water treatment. Advances made in MOF based material design have headed towards the use of MOF based aerogels/hydrogels, MOF derived carbons (MDCs), hydrophobic MOFs and magnetic framework composites (MFCs) to remediate water from contaminants and for the separation of oils from water. This review is intended to highlight some of the recent trends followed in MOF based material engineering towards effective water regeneration.

## Keywords

## Author Keywords

<u>Metal organic framework (MOF)Emerging contaminantsWater</u> remediationAerogelsHydrogelsHydrophobic MOF



## **Keywords Plus**

METAL-ORGANIC-FRAMEWORKNANOPOROUS CARBON MATERIALSLAYERED DOUBLE HYDROXIDESSOLID-PHASE EXTRACTIONTARGETED DRUG-DELIVERYPERSONAL CARE PRODUCTSADSORPTIVE REMOVALPOROUS CARBONGRAPHENE OXIDEAQUEOUS-SOLUTION



## Abstract

Metallic nanostructures with low dimensionality (one-dimension and two-dimension) possess unique structural characteristics and distinctive electronic and physicochemical properties including high aspect ratio, high specific surface area, high density of surface unsaturated atoms and high electron mobility. These distinctive features have rendered them remarkable advantages over their bulk counterparts for surface-related applications, for example, electrochemical water splitting. In this review article, we highlight the recent research progress in low-dimensional metallic nanostructures for electrochemical water splitting including hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). Fundamental understanding of the electrochemistry of water splitting including HER and OER is firstly provided from the aspects of catalytic mechanisms, activity descriptors and property evaluation metrics. Generally, it is challenging to obtain low-dimensional metallic nanostructures with desirable characteristics for HER and OER. We hereby introduce several typical methods for synthesizing onedimensional and two-dimensional metallic nanostructures including organic ligand-assisted synthesis, hydrothermal/solvothermal synthesis, carbon monoxide confined growth, topotactic reduction, and templated growth. We then put emphasis on the strategies adopted for the design and fabrication of highperformance low-dimensional metallic nanostructures for electrochemical water splitting such as alloying, structure design, surface engineering, interface engineering and strain engineering. The underlying structure-property correlation for each strategy is elucidated aiming to facilitate the design of more advanced electrocatalysts for water splitting. The challenges and perspectives for the development of electrochemical water splitting and low-dimensional metallic nanostructures are also proposed.



# Keywords

**Keywords Plus** 

HYDROGEN-EVOLUTION REACTIONDENSITY-FUNCTIONAL THEORYENHANCED ELECTROCATALYTIC PERFORMANCEULTRATHIN NICKEL NANOSHEETSOXYGEN EVOLUTIONTRANSITION-METALHIGHLY EFFICIENTSURFACE INTERROGATIONELECTRONIC-STRUCTURECATALYTIC-ACTIVITY



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8- Global terrestrial water storage and drought severity under climate change
By:
Pokhrel, Y (Pokhrel, Yadu) [1]; Felfelani, F (Felfelani, Farshid) [1]; Satoh, Y (Satoh, Yusuke) [2], [3]
; Boulange, J (Boulange, Julien) [2]; Burek, P (Burek, Peter) [3]; Gadeke, A (Gaedeke, Anne) [4]; Gerten,
D (Gerten, Dieter) [4], [5]; Gosling, SN (Gosling, Simon N.) [6]; Grillakis, M (Grillakis, Manolis) [7]
; <u>Gudmundsson, L</u> (Gudmundsson, Lukas) [8];
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Abstract
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Terrestrial water storage (TWS) modulates the hydrological cycle and is a key determinant of water availability and an indicator of drought. While historical TWS variations have been increasingly studied, future changes in TWS and the linkages to droughts remain unexamined. Here, using ensemble hydrological simulations, we show that climate change could reduce TWS in many regions, especially those in the Southern Hemisphere. Strong inter-ensemble agreement indicates high confidence in the projected changes that are driven primarily by climate forcing rather than land and water management activities. Declines in TWS translate to increases in future droughts. By the late twenty-first century, the global land area and population in extreme-to-exceptional TWS drought could more than double, each increasing from 3% during 1976-2005 to 7% and 8%, respectively. Our findings highlight the importance of climate change mitigation to avoid adverse TWS impacts and increased droughts, and the need for improved water resource management and adaptation.

## Keywords

Keywords Plus <u>GROUNDWATER DEPLETIONINTEGRATED MODELBIAS</u> <u>CORRECTIONGRACEMULTIMODELCMIP5LANDTRENDSSTATESWELL</u>



9- MXenes as emerging nanomaterials in water purification and environmental remediation By: Yu, SJ (Yu, Shujun) [1], [2]; Tang, H (Tang, Hao) [2]; Zhang, D (Zhang, Di) [2]; Wang, SQ (Wang, Shuqin) [1]; <u>Qiu, MQ</u> (Qiu, Muqing) [1]; <u>Song, G</u> (Song, Gang) [4]; <u>Fu, D</u> (Fu, Dong) [3]; <u>Hu, BW</u> (Hu, Baowei) [1] ; Wang, XK (Wang, Xiangke) [1], [2] Volume 811 **Article Number** 152280 DOI 10.1016/j.scitotenv.2021.152280 Published MAR 10 2022 Indexed 2022-03-04 **Document Type** Review

## Abstract

Environmental pollution has accelerated and intensified because of the acceleration of industrialization, therefore fabricating excellent materials to remove hazardous pollutants has become inevitable. MXenes as emerging transition metal nitrides, carbides or carbonitrides with high conductivity, hydrophilicity, excellent structural stability, and versatile surface chemistry, become ideal candidates for water purification and environmental remediation. Particularly, MXenes reveal excellent sorption capability and efficient reduction performance for various contaminants of wastewater. In this regard, a comprehensive understanding of the removal behaviors of MXene-based nanomaterials is necessary to explain how they remove various pollutants in water. The eliminate process of MXene-based nanomaterials is collectively influenced by the physicochemical properties of the materials themselves and the chemical properties of different contaminants. Therefore, in this review paper, the synthesis strategies and properties of MXenebased nano materials are briefly introduced. Then, the chemical properties, removal behaviors and interaction mechanisms of heavy metal ions, radionuclides, and organic pollutants by MXene-based nanomaterials are highlighted. The overview also emphasizes associated toxicity, secondary contamination, the challenges, and prospects of the MXene-based nano materials in the applications of water treatment. This review can supply valuable ideas for fabricating versatile MXene nanomaterials in eliminating water pollution.

## Keywords

Author Keywords <u>MXeneHeavy metal ionRadionuclidesOrganic pollutantsEnvironmental remediation</u> Keywords Plus



2-DIMENSIONAL TITANIUM CARBIDETI3C2TX MXENEPHOTOCATALYTIC DEGRADATIONHIGHLY EFFICIENTTETRACYCLINE DEGRADATIONHEXAVALENT CHROMIUMACTIVATED CARBONSREMOVALADSORPTIONCOMPOSITES



# 10- Photocatalytic water splitting with a quantum efficiency of almost unity By: Takata, T (Takata, Tsuyoshi) [1]; Jiang, JZ (Jiang, Junzhe) [2]; Sakata, Y (Sakata, Yoshihisa) [2] ; Nakabayashi, M (Nakabayashi, Mamiko) [3]; Shibata, N (Shibata, Naoya) [3]; Nandal, V (Nandal, Vikas) [4]; Seki, K (Seki, Kazuhiko) [4]; Hisatomi, T (Hisatomi, Takashi) [1]; Domen, K (Domen, Kazunari) [1], [5] (provided by Clarivate) Volume 581 Issue 7809 Page 411-+ DOI 10.1038/s41586-020-2278-9 Published MAY 28 2020 Indexed 2020-10-16 **Document Type** Article

## Abstract

Overall water splitting, evolving hydrogen and oxygen in a 2:1 stoichiometric ratio, using particulate photocatalysts is a potential means of achieving scalable and economically viable solar hydrogen production. To obtain high solar energy conversion efficiency, the quantum efficiency of the photocatalytic reaction must be increased over a wide range of wavelengths and semiconductors with narrow bandgaps need to be designed. However, the quantum efficiency associated with overall water splitting using existing photocatalysts is typically lower than ten per cent(1,2). Thus, whether a particulate photocatalyst can enable a quantum efficiency of 100 per cent for the greatly endergonic water-splitting reaction remains an open question. Here we demonstrate overall water splitting at an external quantum efficiency of up to 96 per cent at wavelengths between 350 and 360 nanometres, which is equivalent to an internal quantum efficiency of almost unity, using a modified aluminium-doped strontium titanate (SrTiO3:Al) photocatalyst(3,4). By selectively photodepositing the cocatalysts Rh/Cr2O3 (ref.(5)) and CoOOH (refs.(3,6)) for the hydrogen and oxygen evolution reactions, respectively, on different crystal facets of the semiconductor particles using anisotropic charge transport, the hydrogen and oxygen evolution reactions could be promoted separately. This enabled multiple consecutive forward charge transfers without backward charge transfer, reaching the upper limit of quantum efficiency for overall water splitting. Our work demonstrates the feasibility of overall water splitting free from charge recombination losses and introduces an ideal cocatalyst/photocatalyst structure for efficient water splitting.



Keywords Keywords Plus DOPED SRTIO3OPTICAL-PROPERTIESSINGLE-CRYSTALSION



11- Hydrogels and Hydrogel-Derived Materials for Energy and Water Sustainability By: Guo, YH (Guo, Youhong) [1]; Bae, J (Bae, Jiwoong) [1]; Fang, ZW (Fang, Zhiwei) [1]; Li, PP (Li, Panpan) [1] ; <u>Zhao, F</u> (Zhao, Fei) [1]; <u>Yu, GH</u> (Yu, Guihua) [1] (provided by Clarivate) Volume 120 Issue 15 Page 7642-7707 DOI 10.1021/acs.chemrev.0c00345 Published AUG 12 2020 Indexed 2020-09-07 **Document Type** Review

## Abstract

Energy and water are of fundamental importance for our modern society, and advanced technologies on sustainable energy storage and conversion as well as water resource management are in the focus of intensive research worldwide. Beyond their traditional biological applications, hydrogels are emerging as an appealing materials platform for energy- and water-related applications owing to their attractive and tailorable physiochemical properties. In this review, we highlight the highly tunable synthesis of various hydrogels, involving key synthetic elements such as monomer/polymer building blocks, cross-linkers, and functional additives, and discuss how hydrogels can be employed as precursors and templates for architecting three-dimensional frameworks of electrochemically active materials. We then present an indepth discussion of the structure-property relationships of hydrogel materials based on fundamental gelation chemistry, ultimately targeting properties such as enhanced ionic/electronic conductivities, mechanical strength, flexibility, stimuli-responsiveness, and desirable swelling behavior. The unique interconnected porous structures of hydrogels enable fast charge/mass transport while offering large surface areas, and the polymer-water interactions can be regulated to achieve desirable water retention, absorption, and evaporation within hydrogels. Such structure- derived properties are also intimately coordinated to realize multifunctionality and stability for different target devices. The plethora of stimulating examples is expounded with a focus on batteries, supercapacitors, electrocatalysts, solar water purification, and atmospheric water harvesting, which showcase the unprecedented technological potential enabled by hydrogels and hydrogel-derived materials. Finally, we study the challenges and



potential ways of tackling them to reveal the underlying mechanisms and transform the current development of hydrogel materials into sustainable energy and water technologies.

# Keywords

**Keywords Plus** 

OXYGEN-REDUCTION REACTIONCONDUCTIVE POLYMER GELSEQUILIBRIUM SWELLING PROPERTIESDOUBLE-NETWORK HYDROGELSCROSS-LINKED HYDROGELSLITHIUM-ION BATTERYHIGH-PERFORMANCEMECHANICAL-PROPERTIESCONTROLLED-RELEASEDRUG-DELIVERY



# **12-** Amorphous type FeOOH modified defective BiVO4 photoanodes for photoelectrochemical water oxidation

## By:

Lu, XY (Lu, Xinyu) [1]; Ye, KH (Ye, Kai-hang) [2], [3]; Zhang, SQ (Zhang, Siqi) [1]; Zhang, JN (Zhang, Jingnan) [2]; Yang, JD (Yang, Jindong) [2]; Huang, YC (Huang, Yongchao) [1]; Ji, HB (Ji, Hongbing) [2] Volume

428 Article Number 131027 DOI 10.1016/j.cej.2021.131027 Published JAN 15 2022 Early Access JUL 2021 Indexed 2021-11-14 Document Type Article

# Abstract

Herein, a new approach of inducing oxygen vacancy in BiVO4/FeOOH nanostructures is designed, where metal trichalcogenide is introduced. The strategy involves integration of Bi2S3 quantum dots (QDs) in BiVO4/FeOOH to construct defect-rich BiVO4/FeOOH (denoted Vo-BiVO4/FeOOH) as high-performance photoanode for photoelectrochemical water oxidation. Both experimental and theoretical analysis confirm that the excellent PEC performance is due to the introduction of oxygen vacancies and FeOOH cocatalyst, which significantly improves the charge separation. As a result, the obtained Vo-BiVO4/FeOOH photoanode not only demonstrates an optimized Photoelectrochemical (PEC) performance for water oxidation, with photocurrent density of 4.71 mA cm(-2) at 1.23 V versus RHE under AM 1.5 G illumination but the interaction of BiVO4 with FeOOH cocatlayst also significantly enhance the stability for Vo-BiVO4/FeOOH without any decrease after 11 h. The oxygen vacancy and FeOOH can effectively enhance the light conversion efficiency, charge transfer efficiencies and charge separation efficiency. This work highlights an effective strategy towards achieving efficient and stable BiVO4 photoanode for sustainable solar energy conversion.

Keywords Author Keywords BiVO4Water oxidationOxygen vacancyPhotoanode Keywords Plus



OXYGEN VACANCIESZ-SCHEMEHYDROGENFILMSPERFORMANCEFABRICATIONEFFICIENCYNANOSHEETSSELENIDECARRIERS



# 13- Plasma-activated water: generation, origin of reactive species and biological applications By:

<u>Zhou, RW</u> (Zhou, Renwu) [1], [2], [3]; <u>Zhou, RS</u> (Zhou, Rusen) [1], [2]; <u>Wang, PY</u> (Wang, Peiyu) [1], [2]; <u>Xian, YB</u> (Xian, Yubin) [4]; <u>Mai-Prochnow, A</u> (Mai-Prochnow, Anne) [3]; <u>Lu, XP</u> (Lu, Xinpei) [4]; <u>Cullen, PJ</u> (Cullen, P. J.) [3]; <u>Ostrikov, K</u> ((Ken) Ostrikov, Kostya) [1], [2]; <u>Bazaka, K</u> (Bazaka, Kateryna) [1], [2], [5] (provided by Clarivate) **Volume** 

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## Abstract

Novel plasma-based technologies that offer maximum efficiency at minimal environmental costs are expected to further promote the sustainable societal and economic development. Unique transfer of chemical reactivity and energy from gaseous plasmas to water takes place in the absence of any other chemicals, but results in a product with a notable transient broad-spectrum biological activity, referred to as plasma-activated water (PAW). These features make PAW a green prospective solution for a wide range of biotechnology applications, from water purification to biomedicine. Here, we present a succinct review of how novel, efficient methods based on non-equilibrium reactive plasma chemistries can be applied to low-cost natural water sources to produce a prospective product with a wide range of applications while at the same time minimising the process steps and dramatically reducing the use of expensive and/or hazardous reagents. Despite the recent exciting developments in this field, there presently is no topical review which specifically focuses on the underlying physics and chemistry related to plasma-activated water. We focus specifically on the PAW generation, origin of reactive species present in PAW, its related analytical chemistry and potentially different mechanisms that regulate the bio-activities of PAW in different biotech-applications and their roles in determining PAW efficacy and selectivity. We then review recent advances in our understanding of plasma-water interactions, briefly outlining current and proposed applications of PAW in agriculture, food and biomedicine. Finally, we outline future research directions and challenges that may hinder translation of these technologies into real-life applications. Overall, this review will provide much needed insights into the fundamental aspects of PAW chemistry



required for optimization of the biochemical activity of PAW and translation of this environment- and human-health-friendly, and energy-efficient strategy into real life applications.

# Keywords Author Keywords

plasma-activated waterreactive oxygen and nitrogen speciesbiological applications **Keywords Plus** <u>ELECTROLYZED WATERNONTHERMAL PLASMANITRIC-OXIDEHYDROGEN-PEROXIDEESCHERICHIA-</u> <u>COLIMICROBIAL INACTIVATIONNITRATE TRANSPORTSEED-GERMINATIONDISCHARGE PLASMAWASTE-</u> <u>WATER</u>



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14- Crystallization of CsPbBr3 single crystals in water for X-ray detection
By:
Peng, JL (Peng, Jiali) [1]; Xia, CQ (Xia, Chelsea Q.) [2]; Xu, YL (Xu, Yalun) [1]; Li, RM (Li, Ruiming) [1]; Cui,
LH (Cui, Lihao) [1]; Clegg, JK (Clegg, Jack K.) [3]; Herz, LM (Herz, Laura M.) [2]; Johnston, MB (Johnston,
Michael B.) [2]; Lin, QQ (Lin, Qiangian) [1]
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## Abstract

Metal halide perovskites have fascinated the research community over the past decade, and demonstrated unprecedented success in optoelectronics. In particular, perovskite single crystals have emerged as promising candidates for ionization radiation detection, due to the excellent opto-electronic properties. However, most of the reported crystals are grown in organic solvents and require high temperature. In this work, we develop a low-temperature crystallization strategy to grow CsPbBr3 perovskite single crystals in water. Then, we carefully investigate the structure and optoelectronic properties of the crystals obtained, and compare them with CsPbBr3 crystals grown in dimethyl sulfoxide. Interestingly, the water grown crystals exhibit a distinct crystal habit, superior charge transport properties and better stability in air. We also fabricate X-ray detectors based on the CsPbBr3 crystals, and systematically characterize their device performance. The crystals grown in water demonstrate great potential for X-ray imaging with enhanced performance metrics. Perovskite single crystals are commonly grown in organic solvents, which require relatively high temperature condition. Here, the authors develop a low-temperature crystallisation strategy to grow CsPbBr3 single crystals in water with improved charge transport properties and stability.



15- Current status, research trends, and challenges in water electrolysis science and technology By: Grigoriev, SA (Grigoriev, S. A.) [1]; Fateev, VN (Fateev, V. N.) [1]; Bessarabov, DG (Bessarabov, D. G.) [2] ; <u>Millet, P</u> (Millet, P.) [3] (provided by Clarivate) Volume 45 Issue 49 Page 26036-26058 **Special Issue** SI DOI 10.1016/j.ijhydene.2020.03.109 Published OCT 2 2020 Indexed 2020-10-12 **Document Type** Article; Proceedings Paper Conference Meeting 10th International Conference on Hydrogen Production (ICH2P) / 38th Modern Science and Energy Conference (SME) Location Cluj Napoca, ROMANIA Date MAY 15-17, 2019 Abstract

Water electrolysis has various industrial applications. Over the past years, interest in water electrolysis technologies has increased largely due to the renaissance of the nuclear-hydrogen energy concept and also the prospect of the large-scale implementation of power plants based on renewable energy sources. The purpose of this paper is to present a brief review of the state-of the-art in the field of water electrolysis science and technology, including a description of the various water electrolysis technologies, and a discussion of the associated challenges and opportunities. The three main types of water electrolyzers - alkaline, proton exchange membrane, and solid oxide - are considered and described. Their electrochemical performances and limitations are presented and analyzed. Some cost elements are also reported. Research trends in the field are discussed. Possible solutions for performance improvements



are offered. The paper concludes with a discussion of several perspectives in terms of future applications. (C) 2020 Hydrogen Energy Publications LLC. Published by Elsevier Ltd. All rights reserved.

# Keywords Author Keywords

Water electrolysisHydrogen productionNuclear-hydrogen energyRenewablesEnergy storagePower-to-X Keywords Plus HIGH-TEMPERATURE ELECTROLYSISSOLID POLYMER ELECTROLYTEGAS-EVOLVING ELECTRODESTHIN-FILM ELECTROLYTEHYDROGEN-PRODUCTIONOXYGEN EVOLUTIONCURRENT-DENSITYMASS-TRANSFERFUEL-CELLARTIFICIAL-INTELLIGENCE



16- Metal-Organic Frameworks for the Removal of Emerging Organic Contaminants in Water By: Rojas, S (Rojas, Sara) [1]; Horcajada, P (Horcajada, Patricia) [1] (provided by Clarivate) Volume 120 Issue 16 Page 8378-8415 DOI 10.1021/acs.chemrev.9b00797 Published AUG 26 2020 Indexed 2020-09-21 **Document Type** Review Abstract Water is essential in all aspects of life, being the defining characteristic of our planet and even our body. Regrettably, water pollution is increasingly becoming a challenge due to novel anthropogenic pollutants. Of particular concern are emerging organic contaminants (EOCs), the term used not only to cover newly

Of particular concern are emerging organic contaminants (EOCs), the term used not only to cover newly developed compounds but also compounds newly discovered as contaminants in the environment. Aside from anthropogenic contamination, higher temperature and more extreme and less predictable weather conditions are projected to affect water availability and distribution. Therefore, wastewater treatment has to become a valuable water resource and its reuse is an important issue that must be carried out efficiently. Among the novel technologies considered in water remediation processes, metal-organic frameworks (MOFs) are regarded as promising materials for the elimination of EOCs since they present many properties that commend them in water treatment: large surface area, easy functionalizable cavities, some are stable in water, and synthesized at large scale, etc. This review highlights the advances in the use of MOFs in the elimination (adsorption and/or degradation) of EOCs from water, classifying them by the nature of the contaminant.

#### Keywords

Keywords Plus DISINFECTION BY-PRODUCTSPERSONAL CARE PRODUCTSENHANCED ADSORPTIVE REMOVALP-ARSANILIC ACIDEFFICIENT PHOTOCATALYTIC DEGRADATIONZEOLITIC IMIDAZOLATE FRAMEWORK-



Water
<u>8GRAPHENE OXIDE NANOCOMPOSITESULTRASOUND-ASSISTED SYNTHESISFENTON-LIKE</u>
<u>DEGRADATIONCONGO RED-DYE</u>



# 17- Photocatalytic solar hydrogen production from water on a 100-m(2) scale By: Nishiyama, H (Nishiyama, Hiroshi) [1]; Yamada, T (Yamada, Taro) [1]; Nakabayashi, M (Nakabayashi, Mamiko) [2]; Maehara, Y (Maehara, Yoshiki) [3], [4]; Yamaguchi, M (Yamaguchi, Masaharu) [1] ; Kuromiya, Y (Kuromiya, Yasuko) [1]; Nagatsuma, Y (Nagatsuma, Yoshie) [1]; Tokudome, H (Tokudome, Hiromasa) [3], [5]; Akiyama, S (Akiyama, Seiji) [3], [6]; Watanabe, T (Watanabe, Tomoaki) [7]; (provided by Clarivate) Volume 598 Issue 7880 Page 304-+ DOI 10.1038/s41586-021-03907-3 Published OCT 14 2021 Early Access AUG 2021 Indexed 2021-10-14 **Document Type** Article Abstract

The unprecedented impact of human activity on Earth's climate and the ongoing increase in global energy demand have made the development of carbon-neutral energy sources ever more important. Hydrogen is an attractive and versatile energy carrier (and important and widely used chemical) obtainable from water through photocatalysis using sunlight, and through electrolysis driven by solar or wind energy(1,2). The most efficient solar hydrogen production schemes, which couple solar cells to electrolysis systems, reach solar-to-hydrogen (STH) energy conversion efficiencies of 30% at a laboratory scale(3). Photocatalytic water splitting reaches notably lower conversion efficiencies of only around 1%, but the system design is much simpler and cheaper and more amenable to scale-up(1,2)-provided the moist, stoichiometric hydrogen and oxygen product mixture can be handled safely in a field environment and the hydrogen recovered. Extending our earlier demonstration of a 1-m(2) panel reactor system based on a modified, aluminium-doped strontium titanate particulate photocatalyst(4), we here report safe operation of a 100-m(2) array of panel reactors over several months with autonomous recovery of hydrogen from the moist gas product mixture using a commercial polyimide membrane(5). The system, optimized for safety and durability, and remaining undamaged on intentional ignition of recovered hydrogen, reaches a maximum STH of 0.76%. While the hydrogen production is inefficient and energy



negative overall, our findings demonstrate that safe, large-scale photocatalytic water splitting, and gas collection and separation are possible. To make the technology economically viable and practically useful, essential next steps are reactor and process optimization to substantially reduce costs and improve STH efficiency, photocatalyst stability and gas separation efficiency.

Keywords Keywords Plus EFFICIENCYDRIVENSHEETSGAS



18- Recent advances in metal-organic framework membranes for water treatment: A review By: Yu, SJ (Yu, Shujun) [1], [2]; Pang, HW (Pang, Hongwei) [2]; Huang, SY (Huang, Shuyi) [2]; Tang, H (Tang, Hao) [2]; Wang, SQ (Wang, Shuqin) [1]; Qiu, MQ (Qiu, Muqing) [1]; Chen, ZS (Chen, Zhongshan) [2]; Yang, H (Yang, Hui) [2]; Song, G (Song, Gang) [4]; Fu, D (Fu, Dong) [3]; Volume 800 **Article Number** 149662 DOI 10.1016/j.scitotenv.2021.149662 Published DEC 15 2021 **Early Access** AUG 2021 Indexed 2021-10-06 **Document Type** Review Abstract Among many separation membranes reported to date, the favorable polymer affinity and unique physiochemical performances of metal-organic frameworks (MOFs) including ultra-high surface area, regular and highly controlled porosity have drawn widespread attention in industrial and academic communities. In this comprehensive review, the developmental timeline of MOF containing membranes for water treatment were clarified. The removal efficiencies, elimination mechanisms, as well as possible influencing factors of various MOF containing membranes that applied to water treatment were systematically summarized. The excellent removal performances of MOF containing membranes for various pollutants

were determined by the size-exclusion, pi-pi stacking interaction, electrostatic interaction, hydrogen bonding and so on. Since the progress of engineered MOF containing membranes for practical wastewater treatment applications lags, we further ana-lyzed the potential environmental application of MOF containing membranes from four aspects (stability of MOFs, antifouling performance of membranes, compatibility between MOF fillers and polymer matrix, dispersity of MOF nanoparticles in matrix), hoping to provide some meaningful insights. (c) 2021 Elsevier B.V. All rights reserved.

Keywords

Author Keywords

MOFsMembranesWater treatmentStabilityAntifoulingCompatibility Keywords Plus



MIXED MATRIX MEMBRANESCO2 SEPARATION PERFORMANCEMOF-AT-GONANOCOMPOSITE MEMBRANEANTIFOULING PROPERTIESCOMPOSITE MEMBRANESTHIN-FILMSUNDERWATER SUPEROLEOPHOBICITYULTRAFILTRATION MEMBRANESEFFICIENT REMOVAL



19- Adsorption of emerging contaminants from water and wastewater by modified biochar: A review By: <u>Cheng, N</u> (Cheng, Ning) [1]; <u>Wang, B</u> (Wang, Bing) [1], [2], [3]; <u>Wu, P</u> (Wu, Pan) [1], [2], [3]; <u>Lee, XQ</u> (Lee, Xinqing) [4]; Xing, Y (Xing, Ying) [5]; Chen, M (Chen, Miao) [1], [2], [3]; Gao, B (Gao, Bin) [6] (provided by Clarivate) Volume 273 **Article Number** 116448 DOI 10.1016/j.envpol.2021.116448 Published MAR 15 2021 **Early Access** JAN 2021 Indexed 2021-04-27 **Document Type** Review

# Abstract

Emerging contaminants (ECs), a group of relatively low-concentration but high-toxicity pollutants in the environment, have attracted widespread attention in recent years. These trace pollutants can be enriched in organisms and finally transferred to human bodies, posing a potential hazard to public health. Biochar, a low-cost and high-efficiency adsorbent, has been used to treat ECs in water. However, due to certain limitations of pristine biochar, such as poor adsorption capacity, narrow adsorption range, and other shortcomings, it is necessary to modify biochar to improve its applications in water treatment for ECs. Currently, there are a lot of reports on the removal of ECs from water by modified biochar. These studies explored different modification methods to functionalize biochar with various physicochemical properties, which resulted in distinct adsorption effects, behaviors and mechanisms of modified biochar on different ECs. There is a need to systematically review and digest the knowledge on the adsorption of ECs on modified biochar. In this review, recent biochar modification methods used in ECs removal are firstly summarized, and the adsorption performance and mechanisms of modified biochar on typical ECs are then systematically reviewed. Finally, the main research directions and trends, as well as recommendations and suggestions for future development are pointed out. (C) 2021 Elsevier Ltd. All rights reserved.

# Keywords Author Keywords Modified biocharEmerging contaminantsAdsorption mechanismsModification



20- Exclusive Strain Effect Boosts Overall Water Splitting in PdCu/Ir Core/Shell Nanocrystals By: Li, MG (Li, Menggang) [1], [2]; Zhao, ZL (Zhao, Zhonglong) [3]; Xia, ZH (Xia, Zhonghong) [1]; Luo, MC (Luo, Mingchuan) [1]; Zhang, QH (Zhang, Qinghua) [5]; Qin, YN (Qin, Yingnan) [1]; Tao, L (Tao, Lu) [1]; Yin, K (Yin, Kun) [1]; <u>Chao, YG</u> (Chao, Yuguang) [1]; <u>Gu, L</u> (Gu, Lin) [5]; (provided by Clarivate) Volume 60 Issue 15 Page 8243-8250 DOI 10.1002/anie.202016199 Published APR 6 2021 Early Access MAR 2021 Indexed 2021-03-14 **Document Type** Article Abstract

Core/shell nanocatalysts are a class of promising materials, which achieve the enhanced catalytic activities through the synergy between ligand effect and strain effect. However, it has been challenging to disentangle the contributions from the two effects, which hinders the rational design of superior core/shell nanocatalysts. Herein, we report precise synthesis of PdCu/Ir core/shell nanocrystals, which can significantly boost oxygen evolution reaction (OER) via the exclusive strain effect. The heteroepitaxial coating of four Ir atomic layers onto PdCu nanoparticle gives a relatively thick Ir shell eliminating the ligand effect, but creates a compressive strain of ca. 3.60%. The strained PdCu/Ir catalysts can deliver a low OER overpotential and a high mass activity. Density functional theory (DFT) calculations reveal that the compressive strain in Ir shell downshifts the d-band center and weakens the binding of the intermediates, causing the enhanced OER activity. The compressive strain also boosts hydrogen evolution reaction (HER) activity and the strained nanocrystals can be served as excellent catalysts for both anode and cathode in overall water-splitting electrocatalysis.

Keywords Author Keywords



Water <u>coreshell structureoverall water splittingoxygen evolution reaction (OER)nanocrystalsstrain effect</u>



21- Significance of root hairs for plant performance under contrasting field conditions and water deficit By: Marin, M (Marin, M.) [1], [2]; Feeney, DS (Feeney, D. S.) [2], [3]; Brown, LK (Brown, L. K.) [2]; Naveed, M (Naveed, M.) [1] , [4] ; Ruiz, S (Ruiz, S.) [5] ; Koebernick, N (Koebernick, N.) [5] , [6] ; Bengough, AG (Bengough, A. G.) [2], [3]; Hallett, PD (Hallett, P. D.) [1]; Roose, T (Roose, T.) [5]; Puertolas, J (Puertolas, J.) [7]; (provided by Clarivate) Volume 128 Issue 1 Page 1-16 DOI 10.1093/aob/mcaa181 Published JUN 30 2021 Indexed 2022-01-01 **Document Type** Article

# Abstract

Background and Aims: Previous laboratory studies have suggested selection for root hair traits in future crop breeding to improve resource use efficiency and stress tolerance. However, data on the interplay between root hairs and open-field systems, under contrasting soils and climate conditions, are limited. As such, this study aims to experimentally elucidate some of the impacts that root hairs have on plant performance on a field scale.

Methods: A field experiment was set up in Scotland for two consecutive years, under contrasting climate conditions and different soil textures (i.e. clay loam vs. sandy loam). Five barley (Hordeum vulgare) genotypes exhibiting variation in root hair length and density were used in the study. Root hair length, density and rhizosheath weight were measured at several growth stages, as well as shoot biomass, plant water status, shoot phosphorus (P) accumulation and grain yield.

Key Results: Measurements of root hair density, length and its correlation with rhizosheath weight highlighted trait robustness in the field under variable environmental conditions, although significant variations were found between soil textures as the growing season progressed. Root hairs did not confer a notable advantage to barley under optimal conditions, but under soil water deficit root hairs enhanced plant water status and stress tolerance resulting in a less negative leaf water potential and lower leaf abscisic acid concentration, while promoting shoot P accumulation. Furthermore, the presence of root



hairs did not decrease yield under optimal conditions, while root hairs enhanced yield stability under drought.

Conclusions: Selecting for beneficial root hair traits can enhance yield stability without diminishing yield potential, overcoming the breeder's dilemma of trying to simultaneously enhance both productivity and resilience. Therefore, the maintenance or enhancement of root hairs can represent a key trait for breeding the next generation of crops for improved drought tolerance in relation to climate change.

# Keywords

# Author Keywords

Agricultural sustainabilitybarleydrought tolerancegrain yieldHordeum vulgareplant water statusphosphorusrhizosheathroot hairssoil texture

**Keywords Plus** 

PHOSPHORUS ACQUISITIONARABIDOPSIS-THALIANARHIZOSHEATH SIZEBARLEY MUTANTGROWTHPENETRATIONEFFICIENCYTOLERANCESEEDLINGSEXTRACTS


## 22- Heterogeneous Bimetallic Phosphide Ni2P-Fe2P as an Efficient Bifunctional Catalyst for Water/Seawater Splitting By: Wu, LB (Wu, Libo) [1], [2], [3]; Yu, L (Yu, Luo) [1], [2]; Zhang, FH (Zhang, Fanghao) [1], [2]; McElhenny, B (McElhenny, Brian) [1], [2]; Luo, D (Luo, Dan) [1], [2]; Karim, A (Karim, Alamgir) [3], [4]; Chen, S (Chen, Shuo) [1], [2]; <u>Ren, ZF</u> (Ren, Zhifeng) [1], [2] (provided by Clarivate) Volume 31 Issue 1 Article Number 2006484 DOI 10.1002/adfm.202006484 Published JAN 2021 Early Access SEP 2020 Indexed 2020-10-08 **Document Type** Article

## Abstract

Developing high-performance and cost-effective bifunctional electrocatalysts for large-scale water electrolysis is desirable but remains a significant challenge. Most existing nano- and micro-structured electrocatalysts require complex synthetic procedures, making scale-up highly challenging. Here, a heterogeneous Ni2P-Fe2P microsheet is synthesized by directly soaking Ni foam in hydrochloric acid and an iron nitrate solution, followed by phosphidation. Benefiting from high intrinsic activity, abundant active sites, and a superior transfer coefficient, this self-supported Ni2P-Fe2P electrocatalyst shows superb catalytic activity toward overall water splitting, requiring low voltages of 1.682 and 1.865 V to attain current densities of 100 and 500 mA cm(-2)in 1mKOH, respectively. Such catalytic performance is superior to the benchmark IrO2 || Pt/C pair and also places this electrocatalyst among the best bifunctional catalysts reported thus far. Furthermore, its enhanced corrosion resistance and hydrophilic surface make it suitable for seawater splitting. It is able to achieve current densities of 100 and 500 mA cm(-2)in 1mKOH seawater at voltages of 1.811 and 2.004 V, respectively, which, together with its robust durability, demonstrates its great potential for realistic seawater electrolysis. This work presents a general and economic approach toward the fabrication of heterogeneous metallic phosphide catalysts for water/seawater electrocatalysis.



## Keywords

Author Keywords

heterogeneous bifunctional electrocatalysthydrophilicseawater splittingtransition-metal phosphidewater splitting

## **Keywords Plus**

DOUBLE HYDROXIDE NANOSHEETSHYDROGEN EVOLUTIONOXYGEN EVOLUTIONHIGH-PERFORMANCEFACILE SYNTHESISNANOWIRE ARRAYSWATERELECTROCATALYSTSCATHODEDESIGN



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23- Land use and climate change impacts on global soil erosion by water (2015-2070)
By:
Borrelli, P (Borrelli, Pasquale) [1], [2]; Robinson, DA (Robinson, David A.) [3]; Panagos, P (Panagos, Panos)
[4] ; Lugato, E (Lugato, Emanuele) [4] ; Yang, JE (Yang, Jae E.) [2] ; Alewell, C (Alewell, Christine) [1]
; Wuepper, D (Wuepper, David) [5]; Montanarella, L (Montanarella, Luca) [4]; Ballabio, C (Ballabio,
Cristiano) [4]
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10.1073/pnas.2001403117
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SEP 8 2020
Indexed
2020-10-08
Document Type
Article
Abstract
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Soil erosion is a major global soil degradation threat to land, freshwater, and oceans. Wind and water are the major drivers, with water erosion over land being the focus of this work; excluding gullying and river bank erosion. Improving knowledge of the probable future rates of soil erosion, accelerated by human activity, is important both for policy makers engaged in land use decision-making and for earth-system modelers seeking to reduce uncertainty on global predictions. Here we predict future rates of erosion by modeling change in potential global soil erosion by water using three alternative (2.6, 4.5, and 8.5) Shared Socioeconomic Pathway and Representative Concentration Pathway (SSP-RCP) scenarios. Global predictions rely on a high spatial resolution Revised Universal Soil Loss Equation (RUSLE)-based semiempirical modeling approach (GloSEM). The baseline model (2015) predicts global potential soil erosion rates of 43(-7)(+9.2) Pg yr(-1), with current conservation agriculture (CA) practices estimated to reduce this by similar to 5%. Our future scenarios suggest that socioeconomic developments impacting land use will either decrease (SSP1-RCP2.6-10%) or increase (SSP2-RCP4.5 +2%, SSPS-RCP8.5 +10%) water erosion by 2070. Climate projections, for all global dynamics scenarios, indicate a trend, moving toward a more vigorous hydrological cycle, which could increase global water erosion (+30 to +66%). Accepting some degrees of uncertainty, our findings provide insights into how possible future socioeconomic development will affect soil erosion by water using a globally consistent approach. This preliminary



evidence seeks to inform efforts such as those of the United Nations to assess global soil erosion and inform decision makers developing national strategies for soil conservation.

Keywords Author Keywords land degradationagricultural sustainabilitypolicy scenarios Keywords Plus RAINFALL EROSIVITYAPPLICABILITYEUROPERATES



24- Protocols for synthesis of nanomaterials, polymers, and green materials as adsorbents for water treatment technologies By: Saleh, TA (Saleh, Tawfik A.) [1] Volume 24 Article Number 101821 DOI 10.1016/j.eti.2021.101821 Published NOV 2021 Early Access AUG 2021

Indexed 2021-10-10 Document Type Article

## Abstract

Water pollution caused by numerous pollutants has become one of the critical problems globally. Different technologies and materials are used for the treatment of wastewater. There is a need for protocols and procedures that act as guidelines for researchers to develop and evaluate new adsorbent materials for wastewater treatment. This review takes a step toward developing organized protocols and procedures for the synthesis of nanomaterials, polymers, and green materials as adsorbents used for water purification. In the present review, protocols, and procedures for the synthesis of adsorbents, such as nanomaterials, waste-derived materials, and polymers are proposed Furthermore, protocols for evaluating these materials for water treatment are provided. The reported protocols and procedures will provide guidelines for researchers and industrial workers to develop and evaluate new materials for water treatment. (C) 2021 Elsevier B.V. All rights reserved.

## Keywords

Author Keywords Advanced materialsNanotechnologyRemovalAdsorptionWater purificationChemical treatment technologiesValue-added product Keywords Plus LOW-COST ADSORBENTSACTIVATED CARBONDYE REMOVALNANOPARTICLESPHOSPHORUSADSORPTIONCONVERSIONTIRESIONS



25- Exact solitary wave solution for fractal shallow water wave model by He's variational method By: Wang, KL (Wang, Kang-Le) [1] Volume 36 Issue 07 **Article Number** 2150602 DOI 10.1142/S0217984921506028 Published MAR 10 2022 Indexed 2022-03-31 **Document Type** Article

## Abstract

In this paper, the shallow water wave with unsmooth boundaries is depicted by fractal calculus, and its exact fractal solitary wave solution is successfully found by He's variational method. The numerical examples demonstrate that the method is simple, efficient and convenient. Finally, we elaborate the physical properties of the fractal solitary solution by some graphs. The novel scheme clears up the road to the exact fractal soliton, and it sheds a new light on the fractal soliton theory.

Keywords Author Keywords Fractal calculusvariational principlesemi-inverse methodvariational transform method Keywords Plus PARAMETER



26- Rh-engineered ultrathin NiFe-LDH nanosheets enable highly-efficient overall water splitting and urea electrolysis

#### By:

Sun, HCA (Sun, Huachuan) [1]; Zhang, W (Zhang, Wei) [2]; Li, JG (Li, Jian-Gang) [1]; Li, ZS (Li, Zhishan) [1] ; Ao, X (Ao, Xiang) [1]; Xue, KH (Xue, Kan-Hao) [1]; Ostrikov, KK (Ostrikov, Kostya Ken) [3], [4]; Tang, J (Tang, Jiang) [1]; <u>Wang, CD</u> (Wang, Chundong) [1], [5] (provided by Clarivate) Volume 284 Article Number 119740 DOI 10.1016/j.apcatb.2020.119740 Published MAY 5 2021 Indexed 2021-07-03 **Document Type** Article

## Abstract

Water splitting is a green strategy for hydrogen generation but greatly hindered by the sluggish anodic oxygen evolution reaction (OER). Herein, ultrathin rhodium-doped nickel iron layered double hydroxide nanosheets are successfully synthesized, which exhibit outstanding hydrogen evolution reaction (HER) and OER performance, and advanced overall water splitting. More impressively, the remarkable mass activity of 960 mA mg(-1) at 1.55 V (1.7 times larger than NiFe-LDH) for urea electro-oxidation reaction (UOR) shows the great potential to surmount the sluggish OER for overall water splitting. A urine-mediated electrolysis cell is subsequently configured, delivering a current density of 10 mA cm(-2) with a potential of 1.35 V, which is 105 mV lower than that of ureafree counterpart. The enhanced catalytic activity and cell performance are attributed to the introduction of Rh into NiFe-LDH matrix by changing the electronic structure, allowing optimization of the adsorbed species, as confirmed by experimental measurements and computational analyses.

#### Keywords

## Author Keywords

<u>Electronic modulationTransition metal hydroxidesHydrogen evolutionUrea electro-oxidation</u> <u>reactionWater splitting</u>

#### **Keywords Plus**

TOTAL-ENERGY CALCULATIONSLAYERED-DOUBLE-HYDROXIDEOXYGEN EVOLUTIONBIFUNCTIONAL ELECTROCATALYSTIRONNANOARRAYSCONVERSIONCATALYSTDESIGN



## 27- Can Social Norms Promote Recycled Water Use on Campus? The Evidence From Event-Related Potentials

## By:

Liu, XI (Liu, Xiaojun) [1], [2]; Chen, SQ (Chen, Shiqi) [1], [2], [3]; Guo, XT (Guo, Xiaotong) [1], [2], [3] ; Fu, HL (Fu, Hanliang) [1], [2], [3] (provided by Clarivate) Volume 13 Article Number 818292 DOI 10.3389/fpsyg.2022.818292 Published FEB 4 2022 Indexed 2022-03-05 Document Type Article

## Abstract

The unwillingness of college students to use recycled water has become a key barrier to sewage recycling on campus, and it is critical to strengthen their inclination to do so. This paper used college students in Xi'an as a case study and adopted event-related potential technology to explore the effect of social norms on the willingness to use recycled water and the neural mechanism of cognitive processing. The results suggested the following: (1) The existence of social norms might influence college students' willingness to use recycled water. (2) When individuals' willingness to use recycled water is lower than the social norm, there is a bigger feedback-related negative amplitude. (3) College students pay more attention to social norms in groups with closer social distance. These findings can be used to provide a scientific basis for persuading the public to use recycled water from the perspective of the social norm to drive public acceptability.

## Keywords

Author Keywords

social normsrecycled waterpublic willingnessfeedback-related negativitysocial distance Keywords Plus OUTCOME EVALUATIONCONFLICTDISTANCESUPPORT



## 28- Redirecting dynamic surface restructuring of a layered transition metal oxide catalyst for superior water oxidation

## By:

<u>Wang, J</u> (Wang, Jian) [1]; <u>Kim, SJ</u> (Kim, Se-Jun) [2]; <u>Liu, JP</u> (Liu, Jiapeng) [3]; <u>Gao, Y</u> (Gao, Yang) [4]; <u>Choi,</u> <u>S</u> (Choi, Subin) [1]; <u>Han, J</u> (Han, Jeongwoo) [1]; <u>Shin, H</u> (Shin, Hyeyoung) [5]; <u>Jo, S</u> (Jo, Sugeun) [1]; <u>Kim,</u> J (Kim, Juwon) [1]; <u>Ciucci, F</u> (Ciucci, Francesco) [3], [6]; (provided by Clarivate)

Volume 4 Issue 3 Page 212-222 DOI 10.1038/s41929-021-00578-1 Published MAR 2021 Early Access MAR 2021 Indexed 2021-03-21 **Document Type** Article

## Abstract

Rationally manipulating the in situ formed catalytically active surface of catalysts remains a tremendous challenge for a highly efficient water electrolysis. Here we present a cationic redox-tuning method to modulate in situ catalyst leaching and to redirect the dynamic surface restructuring of layered LiCoO2xClx (x= 0, 0.1 or 0.2), for the electrochemical oxygen evolution reaction (OER). Chlorine doping lowered the potential to trigger in situ cobalt oxidation and lithium leaching, which induced the surface of LiCoO1.8Cl0.2 to transform into a self-terminated amorphous (oxy)hydroxide phase during the OER. In contrast, Cl-free LiCoO2 required higher electrochemical potentials to initiate the in situ surface reconstruction to spinel-type Li1 +/- xCo2O4 and longer cycles to stabilize it. Surface-restructured LiCoO1.8Cl0.2 outperformed many state-of-the-art OER catalysts and demonstrated remarkable stability. This work makes a stride in modulating surface restructuring and in designing superior OER electrocatalysts via manipulating the in situ catalyst leaching.



## 29- Clean and Affordable Hydrogen Fuel from Alkaline Water Splitting: Past, Recent Progress, and Future Prospects

#### By:

Yu, ZY (Yu, Zi-You) [1]; Duan, Y (Duan, Yu) [1]; Feng, XY (Feng, Xing-Yu) [1]; Yu, XX (Yu, Xingxing) [1]; Gao, MR (Gao, Min-Rui) [1]; Yu, SH (Yu, Shu-Hong) [1] (provided by Clarivate) Volume 33 Issue 31 **Article Number** 2007100 DOI 10.1002/adma.202007100 Published AUG 2021 **Early Access** JUN 2021 Indexed 2021-06-16 **Document Type** Review

## Abstract

Hydrogen economy has emerged as a very promising alternative to the current hydrocarbon economy, which involves the process of harvesting renewable energy to split water into hydrogen and oxygen and then further utilization of clean hydrogen fuel. The production of hydrogen by water electrolysis is an essential prerequisite of the hydrogen economy with zero carbon emission. Among various water electrolysis technologies, alkaline water splitting has been commercialized for more than 100 years, representing the most mature and economic technology. Here, the historic development of water electrolysis is overviewed, and several critical electrochemical parameters are discussed. After that, advanced nonprecious metal electrocatalysts that emerged recently for negotiating the alkaline oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) are discussed, including transition metal alloys, chalcogenides, phosphides, and carbides for the HER. In this section, particular attention is paid to the catalyst synthesis, activity and stability challenges, performance improvement, and industry-relevant developments. Some recent works about scaled-up catalyst synthesis, novel electrode designs, and alkaline seawater electrolysis are also spotlighted. Finally, an outlook on future challenges and opportunities for alkaline water splitting is offered, and potential future directions are speculated.



Keywords Author Keywords alkaline water splittinghydrogen energyhydrogen evolutionoxygen evolution Keywords Plus EFFICIENT OXYGEN-EVOLUTIONLAYERED DOUBLE-HYDROXIDETRANSITION-METAL (OXY)HYDROXIDESPOLYMER ELECTROLYTE WATERPOROUS NANOWIRE ARRAYSACTIVE EDGE SITESHIGHLY-EFFICIENTMOLYBDENUM-CARBIDEBIFUNCTIONAL ELECTROCATALYSTDOPED CARBON



# 30- Climate change will affect global water availability through compounding changes in seasonal precipitation and evaporation

By: Konapala, G (Konapala, Goutam) [1], [2], [3]; Mishra, AK (Mishra, Ashok K.) [1]; Wada, Y (Wada, Yoshihide) [4]; Mann, ME (Mann, Michael E.) [5] (provided by Clarivate) Volume 11 Issue 1 DOI 10.1038/s41467-020-16757-w Published JUN 23 2020 Indexed 2020-07-14 **Document Type** Article

#### Abstract

Both seasonal and annual mean precipitation and evaporation influence patterns of water availability impacting society and ecosystems. Existing global climate studies rarely consider such patterns from non-parametric statistical standpoint. Here, we employ a non-parametric analysis framework to analyze seasonal hydroclimatic regimes by classifying global land regions into nine regimes using late 20th century precipitation means and seasonality. These regimes are used to assess implications for water availability due to concomitant changes in mean and seasonal precipitation and evaporation changes using CMIP5 model future climate projections. Out of 9 regimes, 4 show increased precipitation variation, while 5 show decreased evaporation variation coupled with increasing mean precipitation and evaporation. Increases in projected seasonal precipitation variation in already highly variable precipitation regimes gives rise to a pattern of "seasonally variable regimes becoming more variable". Regimes with low seasonality in precipitation, instead, experience increased wet season precipitation. Adequate water availability is key to human and ecosystem sustainability. Here, the authors show that seasonally variable regimes become more variable, and the combined influence of seasonality and magnitude of climate variables will affect future water availability.

## Keywords

 Keywords Plus

 RAINFALL

 SEASONALITYCMIP5LANDEVAPOTRANSPIRATIONCLASSIFICATIONDRYENSEMBLEEXTREMESENTROPYTRE

 NDS



31- Recent advances in metal-organic frameworks for the removal of heavy metal oxoanions from water By: Zhao, XL (Zhao, Xiaoliang) [1]; Yu, XZ (Yu, Xuezheng) [1]; Wang, XY (Wang, Xueyao) [1]; Lai, SJ (Lai, Shoujuan) [1]; Sun, YY (Sun, Yuanyuan) [1]; Yang, DJ (Yang, Dongjiang) [1], [2] Volume 407 **Article Number** 127221 DOI 10.1016/j.cej.2020.127221 Published MAR 1 2021 Indexed 2021-02-03 **Document Type** Article

#### Abstract

Due to the serious threat of heavy metal oxoanions to human health and the natural environment, their efficient removal from water contaminants has become a vital issue. Currently, adsorptive removal is one of most promising approaches to purify contaminated water. Thus, the exploration of advanced adsorption materials has attracted widespread attention. Metal-organic frameworks (MOFs) with the advantages of tunable porosity, high surface area, and abundant functional groups are superior than conventional adsorbents. Herein, this review summarizes recent progress in different MOFs as outstanding adsorbents to remove heavy metal oxoanions from water, including typical SeO32-/SeO42-, HAsO42-/H2AsO4-/H3AsO3, and CrO42-/Cr2O72-. In addition, their adsorption mechanisms are also involved, which is conducive to not only understand the adsorption process between MOFs and heavy metal oxoanion contaminants but also design new MOFs-based adsorbents with excellent performance for further research.

## Keywords

## Author Keywords

<u>Metal-organic frameworksAdsorbentsHeavy metal oxoanionsWater treatmentAdsorption mechanisms</u> **Keywords Plus** 

ZEOLITIC IMIDAZOLATE FRAMEWORK-8HIGHLY EFFICIENT REMOVALANION-EXCHANGECOORDINATION POLYMERSHEXAVALENT CHROMIUMAQUEOUS-SOLUTIONADSORPTIVE PERFORMANCESELECTIVE ADSORPTIONFUNCTIONAL-GROUPSOXYGEN VACANCIES



## 32- Boron-doped nitrogen-deficient carbon nitride-based Z-scheme heterostructures for photocatalytic overall water splitting

By:

Zhao, DM (Zhao, Daming) [1]; Wang, YQ (Wang, Yiqing) [1]; Dong, CL (Dong, Chung-Li) [2]; Huang, YC (Huang, Yu-Cheng) [2], [3]; Chen, J (Chen, Jie) [1]; Xue, F (Xue, Fei) [1]; Shen, SH (Shen, Shaohua) [1] ; Guo, LJ (Guo, Liejin) [1] (provided by Clarivate) Volume 6 Issue 4 Page 388-397 DOI 10.1038/s41560-021-00795-9 Published APR 2021 **Early Access** MAR 2021 Indexed 2021-03-25 **Document Type** Article

## Abstract

Splitting water using suspensions of particulate carbon nitride-based photocatalysts may be a cheap way to produce hydrogen, but efficiencies have remained low. Now, Shen and colleagues use doped carbon nitride-based Z-scheme heterostructures to split water with a solar-to-hydrogen efficiency of 1.1% in the presence of metal-based co-catalysts.

Photocatalytic overall water splitting can be achieved using Z-scheme systems that mimic natural photosynthesis by combining dissimilar semiconductors in series. However, coupling well-suited H-2- and O-2-evolving components remains challenging. Here, we fabricate a Z-scheme system for photocatalytic overall water splitting based on boron-doped, nitrogen-deficient carbon nitride two-dimensional (2D) nanosheets. We prepare ultrathin carbon nitride nanosheets with varying levels of boron dopants and nitrogen defects, which leads to nanosheets that can act as either H-2- or O-2-evolving photocatalysts. Using an electrostatic self-assembly strategy, the nanosheets are coupled to obtain a 2D/2D polymeric heterostructure. Owing to their ultrathin nanostructures, strong interfacial interaction and staggered band alignment, a Z-scheme route for efficient charge-carrier separation and transfer is realized. The obtained heterostructure achieves stoichiometric H-2 and O-2 evolution in the presence of Pt and Co(OH)(2) co-catalysts, and the solar-to-hydrogen efficiency reaches 1.16% under one-sun illumination.



## **33-** Erythritol-based polyester loose nanofiltration membrane with fast water transport for efficient dye/salt separation

#### By:

<u>Jin, PR</u> (Jin, Pengrui) [1]; <u>Zhu, JY</u> (Zhu, Junyong) [2]; <u>Yuan, SS</u> (Yuan, Shushan) [1]; <u>Zhang, G</u> (Zhang, Gang) [3]; <u>Volodine, A</u> (Volodine, Alexander) [4]; <u>Tian, MM</u> (Tian, Miaomiao) [1]; <u>Wang, JX</u> (Wang, Jianxiu) [1] ; <u>Luis, P</u> (Luis, Patricia) [5]; <u>Van der Bruggen, B</u> (Van der Bruggen, Bart) [1], [6] (provided by Clarivate)

Volume 406 Article Number 126796 DOI 10.1016/j.cej.2020.126796 Published FEB 15 2021 Indexed 2021-05-10 Document Type Article

#### Abstract

Loose nanofiltration membranes with a remarkable water permeability are highly promising for the fractionation of dyes and salts in the treatment of textile wastewater. In this study, a novel polyester membrane with unprecedented water permeability was developed via interfacial polymerization (IP), in which meso-erythritol (ME) was utilized as an aqueous monomer. Instead of using toxic catalysts, sodium hydroxide was incorporated to the aqueous solution to catalyze the ester reaction between hydroxyl and acyl chloride. A series of characterizations demonstrated that the formed polyester film is hydrophilic and negatively charged, with microsphere structures on the surface. Due to the low-active hydroxyl groups of the aqueous monomers, the participation of ME could yield a coherent polyester film with slightly loose structure atop the polyethersulfone (PES) membrane. The resultant membrane with high water permeability exhibited both a high rejection of dyes and a high transmission of salts. The rejection of the LNFM-2 membrane with an excellent water permeability of 53.23 LMH bar(-1) for Congo red (CR), direct red 23 (DR23), reactive blue 2 (RB2), Na2SO4, NaCl was 99.6%, 95.2%, 99.6%, 11.0%, and 5.6% respectively. Furthermore, LNFM-1 has a water permeability of up to 87.13 LMH bar(-1) while maintaining a competitive dye/salt separation performance. In addition, this type of polyester membrane has a superior antifouling performance and long-term stability during the filtration of dye/salt mixtures.

The newly developed polyester LNF membranes have great application potential in the treatment of textile wastewater. This study paves the way for applying hydroxyl monomers like polyols for constructing TFC membranes for diverse separations.



## Keywords Author Keywords Loose nanofiltrationMeso-ErythritolPolyesterInterfacial polymerizationDye/salt separation



34- In-situ reconstructed Ru atom array on alpha-MnO2 with enhanced performance for acidic water oxidation

#### By:

<u>Lin, C</u> (Lin, Chao) [1], [2]; <u>Li, JL</u> (Li, Ji-Li) [3]; <u>Li, XP</u> (Li, Xiaopeng) [1]; <u>Yang, S</u> (Yang, Shuai) [4]; <u>Luo, W</u> (Luo, Wei) [1]; <u>Zhang, YJ</u> (Zhang, Yaojia) [1]; <u>Kim, SH</u> (Kim, Sung-Hae) [2]; <u>Kim, DH</u> (Kim, Dong-Hyung) [2]; <u>Shinde, SS</u> (Shinde, Sambhaji S.) [2]; <u>Li, YF</u> (Li, Ye-Fei) [3];

(provided by Clarivate) **Volume** 4 **Issue** 12 **Page** 1012-1023 **DOI** 10.1038/s41929-021-00703-0 **Published** DEC 2021 **Indexed** 2021-12-27 **Document Type** Article

#### Abstract

The development of acid-stable oxygen evolution reaction electrocatalysts is essential for highperformance water splitting. Here, we report an electrocatalyst with Ru-atom-array patches supported on alpha-MnO2 (Ru/MnO2) for the oxygen evolution reaction following a mechanism that involves only \*O and \*OH species as intermediates. This mechanism allows direct O-O radical coupling for O-2 evolution. Ru/MnO2 shows high activity (161 mV at 10 mA cm(-2)) and outstanding stability with small degradation after 200 h operation, making it one of the best-performing acid-stable oxygen evolution reaction catalysts. Operando vibrational and mass spectroscopy measurements were performed to probe the reaction intermediates and gaseous products for validating the oxygen evolution reaction pathway. First-principles calculations confirmed the cooperative catalysis mechanism with a reduced energy barrier. Time-dependent elemental analysis demonstrated the occurrence of the in-situ dynamic cation exchange reaction during the oxygen evolution reaction, which is the key for triggering the reconstruction of Ru atoms into the ordered array with high durability.

#### Keywords

 Keywords Plus

 SURFACE WALKING METHODOXYGEN EVOLUTIONTITANIA

 ANATASEMECHANISMCATALYSTEFFICIENTNANOPARTICLESREDUCTIONELECTROCATALYSTSACTIVATION



35- Water as the reaction medium in organic chemistry: from our worst enemy to our best friend By: Cortes-Clerget, M (Cortes-Clerget, Margery) [1]; Yu, JL (Yu, Julie) [3]; Kincaid, JRA (Kincaid, Joseph R. A.) [3]; Walde, P (Walde, Peter) [2]; Gallou, F (Gallou, Fabrice) [1]; Lipshutz, BH (Lipshutz, Bruce H.) [3] (provided by Clarivate) Volume 12 Issue 12 Page 4237-4266 DOI 10.1039/d0sc06000c Published MAR 28 2021 Indexed 2021-05-06 **Document Type** Review

## Abstract

A review presenting water as the logical reaction medium for the future of organic chemistry. A discussion is offered that covers both the "on water" and "in water" phenomena, and how water is playing unique roles in each, specifically with regard to its use in organic synthesis.



36- Energetic, economic and environmental assessment of zero liquid discharge (ZLD) brackish water and seawater desalination systems

By: Panagopoulos, A (Panagopoulos, Argyris) [1] (provided by Clarivate) Volume 235 **Article Number** 113957 DOI 10.1016/j.enconman.2021.113957 Published MAY 1 2021 **Early Access** MAR 2021 Indexed 2021-04-25 **Document Type** Article

#### Abstract

The discharge of brine (saline wastewater) from brackish water and seawater desalination plants poses a major threat to the natural environment. This research study presents an energetic, economic and environmental assessment of zero liquid discharge (ZLD) desalination systems in the Eastern Mediterranean. Two scenarios are considered: (i) ZLD brackish water and (ii) ZLD seawater systems, both aimed at producing saleable freshwater and mixed solid salt. Results showed that the energy consumption in scenario 1 (9.48 kWh/m3) is 2.38 times lower than in scenario 2 (22.55 kWh/m3) due to the 7 times lower feed salinity. The differentiation in energy demands is also translated to costs since scenario 2 (US\$1.04/m3) is 1.24 times more expensive than scenario 1 (US\$0.84/m3). Both scenarios are 3.18 times cheaper than the disposal method of the evaporation pond, while they are in the same cost range as the land application and deep-well injection. Whether only freshwater is sold or both freshwater and mixed solid salt are sold, both scenarios are profitable as the profit ranges from US \$215.05/day to US\$302.55/day. Concerning CO2 emissions, scenario 1 (5.91?6.45 kg CO2/m3) has lower values than scenario 2 (14.05?15.33 kg CO2/m3) as the energy demanded in scenario 1 is significantly lower.

#### Keywords

Author Keywords Zero liquid discharge (ZLD)Seawater desalinationBrackish water desalinationBrine treatmentResource recoveryDesalination brine Keywords Plus



MEMBRANE DISTILLATIONBRINE



**37-** Molecular-level insights on the reactive facet of carbon nitride single crystals photocatalysing overall water splitting

By:

Lin, LH (Lin, Lihua) [1], [2]; Lin, ZY (Lin, Zhiyou) [1]; Zhang, J (Zhang, Jian) [1]; Cai, X (Cai, Xu) [1]; Lin, W (Lin, Wei) [1]; Yu, ZY (Yu, Zhiyang) [1]; Wang, XC (Wang, Xinchen) [1] (provided by Clarivate) Volume

3 Issue 8 Page 649-655 DOI 10.1038/s41929-020-0476-3 Published AUG 2020 Early Access JUN 2020 Indexed 2020-07-14 Document Type Article

## Abstract

Unraveling how reactive facets promote photocatalysis at the molecular level remains a grand challenge, while identification of the reactive facets can provide guidelines for designing highly efficient photocatalysts and unravelling the microscopic mechanisms behind them. Recently, a series of polytriazine imides (PTIs) was reported with highly crystalline structures; all had a relatively low photocatalytic activity for overall water splitting. Here, high-angle annular dark-field scanning transmission electron microscopy, energy dispersive spectroscopy mapping, and aberration-corrected integrated differential phase contrast imaging were used to study PTI/Li+Cl- single crystals before and after in situ photodeposition of co-catalysts, showing that the prismatic {10 (1) over bar0} planes are more photocatalytically reactive than the basal {0001} planes. Theoretical calculations confirmed that the electrons are energetically favourable to transfer toward the {10 (1) over bar0} planes. Upon this discovery, PTI/Li+Cl- crystals with different aspect ratios were prepared, and the overall water splitting performance followed a linear correlation with the relative surface areas of the {10 (1) over bar0} and {0001} planes. Our controlling of the reactive facets directly instructs the development of highly efficient polymer photocatalysts for overall water splitting.



## Keywords Keywords Plus

TOTAL-ENERGY CALCULATIONSEXPOSED 001 FACETSHYDROGEN-

PRODUCTIONEFFICIENCYSEMICONDUCTORNANOSHEETSEVOLUTIONPERFORMANCEPERCENTAGECOCAT ALYST



## **38-** Interface Engineering of Hierarchical Branched Mo-Doped Ni**3S2**/NixPy Hollow Heterostructure Nanorods for Efficient Overall Water Splitting

#### By:

Luo, X (Luo, Xu) [1], [2]; Ji, PX (Ji, Pengxia) [1]; Wang, PY (Wang, Pengyan) [1]; Cheng, RL (Cheng, Ruilin) [1]; Chen, D (Chen, Ding) [1]; Lin, C (Lin, Can) [1]; Zhang, JA (Zhang, Jianan) [3]; He, JW (He, Jianwei) [1] ; <u>Shi, ZH</u> (Shi, Zuhao) [4]; <u>Li, N</u> (Li, Neng) [4]; (provided by Clarivate) Volume 10 Issue 17 Article Number 1903891 DOI 10.1002/aenm.201903891 Published MAY 2020 Indexed 2020-05-27 **Document Type** Article

#### Abstract

Rational design and construction of bifunctional electrocatalysts with excellent activity and durability is imperative for water splitting. Herein, a novel top-down strategy to realize a hierarchical branched Modoped sulfide/phosphide heterostructure (Mo-Ni3S2/NixPy hollow nanorods), by partially phosphating Mo-Ni3S2/NF flower clusters, is proposed. Benefitting from the optimized electronic structure configuration, hierarchical branched hollow nanorod structure, and abundant heterogeneous interfaces, the as-obtained multisite Mo-Ni3S2/NixPy/NF electrode has remarkable stability and bifunctional electrocatalytic activity in the hydrogen evolution reaction (HER)/oxygen evolution reaction (OER) in 1 m KOH solutions. It possesses an extremely low overpotential of 238 mV at the current density of 50 mA cm(-2) for OER. Importantly, when assembled as anode and cathode simultaneously, it merely requires an ultralow cell voltage of 1.46 V to achieve the current density of 10 mA cm(-2), with excellent durability for over 72 h, outperforming most of the reported Ni-based bifunctional materials. Density functional theory results further confirm that the doped heterostructure can synergistically optimize Gibbs free energies of H and O-containing intermediates (OH\*, O\*, and OOH\*) during HER and OER processes, thus accelerating the catalytic kinetics of electrochemical water splitting. This work demonstrates the importance of the rational combination of metal doping and interface engineering for advanced catalytic materials.



## Keywords Author Keywords bifunctional electrocatalystshydrogen evolution reactioninterface engineeringoxygen evolution reaction Keywords Plus HIGHLY EFFICIENTBIFUNCTIONAL ELECTROCATALYSTSOXYGEN EVOLUTIONNI3S2

NANOWIRESPERFORMANCENANOSHEETSHYDROGENALKALINEARRAYSFOAMS



## **39-** Engineering single-atomic ruthenium catalytic sites on defective nickel-iron layered double hydroxide for overall water splitting

By:

Zhai, PL (Zhai, Panlong) [1]; Xia, MY (Xia, Mingyue) [2]; Wu, YZ (Wu, Yunzhen) [1]; Zhang, GH (Zhang, Guanghui) [1]; Gao, JF (Gao, Junfeng) [2]; Zhang, B (Zhang, Bo) [1]; Cao, SY (Cao, Shuyan) [1]; Zhang, YT (Zhang, Yanting) [1]; Li, ZW (Li, Zhuwei) [1]; Fan, ZZ (Fan, Zhaozhong) [1]; (provided by Clarivate) Volume 12 Issue 1 Article Number 4587 DOI 10.1038/s41467-021-24828-9 Published JUL 28 2021 Indexed 2021-08-17 **Document Type** 

## Article

## Abstract

Rational design of single atom catalyst is critical for efficient sustainable energy conversion. However, the atomic-level control of active sites is essential for electrocatalytic materials in alkaline electrolyte. Moreover, well-defined surface structures lead to in-depth understanding of catalytic mechanisms. Herein, we report a single-atomic-site ruthenium stabilized on defective nickel-iron layered double hydroxide nanosheets (Ru-1/D-NiFe LDH). Under precise regulation of local coordination environments of catalytically active sites and the existence of the defects, Ru-1/D-NiFe LDH delivers an ultralow overpotential of 18mV at 10mAcm(-2) for hydrogen evolution reaction, surpassing the commercial Pt/C catalyst. Density functional theory calculations reveal that Ru-1/D-NiFe LDH optimizes the adsorption energies of intermediates for hydrogen evolution reaction and promotes the O-O coupling at a Ru-O active site for oxygen evolution reaction. The Ru-1/D-NiFe LDH as an ideal model reveals superior water splitting performance with potential for the development of promising water-alkali electrocatalysts. Rational design of single atom catalyst is critical for efficient sustainable energy conversion. Single-atomic-site ruthenium stabilized on defective nickel-iron layered double hydroxide nanosheets achieve superior HER and OER performance in alkaline media.

Keywords Keywords Plus



Water EFFICIENT ELECTROCATALYSTOXYGEN VACANCIESEVOLUTIONNANOSHEETSGRAPHENE



40- Employing extreme value theory to establish nutrient criteria in bay waters: A case study of Xiangshan Bay

#### By:

Fang, X (Fang, Xin) [1], [2]; Wang, Q (Wang, Qi) [3]; Wang, JC (Wang, Jingchen) [1]; Xiang, YY (Xiang, Yunyun) [1]; Wu, YF (Wu, Yifan) [1]; Zhang, YF (Zhang, Yifei) [1] (provided by Clarivate) Volume 603 Part D **Article Number** 127146 DOI 10.1016/j.jhydrol.2021.127146 Published DEC 2021 **Early Access** DEC 2021 Indexed 2021-12-27 **Document Type** Article

#### Abstract

The Yangtze River estuary and its surrounding seas have had the highest degree of eutrophication in China. Xiangshan Bay, located at the southern bank of the Yangtze River, is not immune from eutrophication, leading to the water quality below the control requirements for marine functional zoning. Clarifying the nutrient criteria is essential to alleviate eutmphication in Xiangshan Bay. We used a generalized Pareto distribution-based peaks over threshold model to analyze 2006-2018 survey data. Through calculation, inorganic nitrogen and reactive phosphate criteria in Xiangshan Bay at the five percentile are 0.443 mg/L and 0.025 mg/L, respectively. Additionally, we also obtained the corresponding confidence intervals. Rationality and sensitivity analyses of the calculation results proved the methods used in this study to be rational and reliable, providing a basis for subsequent monitoring and assessment of nutrient salts in bays.

#### Keywords

## Author Keywords

Generalized Pareto distributionPeaks over the thresholdBay water qualityConfidence intervalSensitivity analysis Keywords Plus COASTAL EUTROPHICATIONCHINAMANAGEMENTNITROGENTAILSSEA



## 41- Per- and polyfluoroalkyl substances in water and wastewater: A critical review of their global occurrence and distribution

#### By:

Kurwadkar, S (Kurwadkar, Sudarshan) [1], [2]; Dane, J (Dane, Jason) [1]; Kanel, SR (Kanel, Sushil R.) [3], [4]; Nadagouda, MN (Nadagouda, Mallikarjuna N.) [5]; Cawdrey, RW (Cawdrey, Ryan W.) [1]; Ambade, B (Ambade, Balram) [6]; Struckhoff, GC (Struckhoff, Garrett C.) [1]; Wilkin, R (Wilkin, Richard) [2] (provided by Clarivate) Volume 809 Article Number 151003 DOI 10.1016/j.scitotenv.2021.151003 Published FEB 25 2022 Indexed 2022-02-02 **Document Type** Review

## Abstract

Per- and polyfluoroalkyl substances (PFAS) are a family of fluorinated organic compounds of anthropogenic origin. Due to their unique chemical properties, widespread production, environmental distribution, long-term persistence, bioaccumulative potential, and associated risks for human health, PFAS have been classified as persistent organic pollutants of significant concern. Scientific evidence from the last several decades suggests that their widespread occurrence in the environment correlates with adverse effects on human health and ecology. The presence of PFAS in the aquatic environment demonstrates a close link between the anthroposphere and the hydrological cycle, and concentrations of PFAS in surface and groundwater range in value along the ng L-1-mu g L-1 scale. Here, we critically reviewed the research published in the last decade on the global occurrence and distribution of PFAS in the aquatic environment. Ours is the first paper to critically evaluate the occurrence of PFAS at the continental scale and the evolving global regulatory responses to manage and mitigate the adverse human health risks posed by PFAS. The review reports that PFAS are widespread despite being phased out-they have been detected in different continents irrespective of the level of industrial development. Their occurrence far from the potential sources suggests that long-range atmospheric transport is an important pathway of PFAS distribution. Recently, several studies have investigated the health impacts of PFAS exposure-they have been detected in biota, drinking water, food, air, and human serum. In response to the emerging information about PFAS toxicity, several countries have provided administrative guidelines for PFAS in water, including Canada, the United Kingdom, Sweden, Norway, Germany, and Australia. In the US, additional regulatory measures are under consideration. Further, many PFAS have now been listed



as persistent organic pollutants. This comprehensive review provides crucial baseline information on the global occurrence, distribution, and regulatory framework of PFAS.

## Keywords

Author Keywords Perfluoroalkyl substancesPolyfluoroalkyl substancesPFASEnvironmental pollutionPFOSPFOA Keywords Plus PERFLUORINATED ALKYL SUBSTANCESPERFLUOROOCTANOIC ACID PFOAPERFLUOROALKYL SUBSTANCESDRINKING-WATERAQUATIC ENVIRONMENTSURFACE-WATERGREAT-LAKESSPATIAL-DISTRIBUTIONCARBOXYLIC-ACIDSPRODUCTION PLANT



## 42- Lightweight, Superelastic, and Hydrophobic Polyimide Nanofiber /MXene Composite Aerogel for Wearable Piezoresistive Sensor and Oil/Water Separation Applications

By:

Liu, H (Liu, Hu) [1] , [2] ; Chen, XY (Chen, Xiaoyu) [1] ; Zheng, YJ (Zheng, Yanjun) [1] ; Zhang, DB (Zhang, Dianbo) [1]; Zhao, Y (Zhao, Ye) [1]; Wang, CF (Wang, Chunfeng) [2], [3]; Pan, CF (Pan, Caofeng) [2]; Liu, CT (Liu, Chuntai) [1]; Shen, CY (Shen, Changyu) [1] (provided by Clarivate) Volume 31 Issue 13 Article Number 2008006 DOI 10.1002/adfm.202008006 Published MAR 2021 Early Access JAN 2021 Indexed 2021-01-28 **Document Type** 

Article

## Abstract

Inspired by the ultralight and structurally robust spider webs, flexible nanofibril-assembled aerogels with intriguing attributes have been designed for achieving promising performances in various applications. Here, conductive polyimide nanofiber (PINF)/MXene composite aerogel with typical "layer-strut" bracing hierarchical nanofibrous cellular structure has been developed via the freeze-drying and thermal imidization process. Benefiting from the porous architecture and robust bonding between PINF and MXene, the PINF/MXene composite aerogel exhibits an ultralow density (9.98 mg cm(-3)), intriguing temperature tolerance from -50 to 250 degrees C, superior compressibility and recoverability (up to 90% strain), and excellent fatigue resistance over 1000 cycles. The composite aerogel can be used as a piezoresistive sensor, with an outstanding sensing capacity up to 90% strain (corresponding 85.21 kPa), ultralow detection limit of 0.5% strain (corresponding 0.01 kPa), robust fatigue resistance over 1000 cycles, excellent piezoresistive stability and reproductivity in extremely harsh environments. Furthermore, the composite aerogel also exhibits superior oil/water separation properties such as high adsorption capacity (55.85 to 135.29 g g(-1)) and stable recyclability due to its hydrophobicity and robust hierarchical porous structure. It is expected that the designed PINF/MXene composite aerogel can supply



a new multifunctional platform for human bodily motion/physical signals detection and high-efficient oil/water separation.

Keywords Author Keywords aerogeloil/water separationpiezoresistive sensorpolyimide nanofiber Keywords Plus POLYURETHANE SPONGEPRESSURE SENSORCARBON NANOTUBESPERFORMANCENANOCOMPOSITESDURABILITYRUBBERFOAMS



## 43- Recent advances in the highly sensitive determination of zearalenone residues in water and environmental resources with electrochemical biosensors

By:

Sohrabi, H (Sohrabi, Hessamaddin) [2]; Majidi, MR (Majidi, Mir Reza) [2]; Arbabzadeh, O (Arbabzadeh, Omid) [3] ; Khaaki, P (Khaaki, Pegah) [4] ; Pourmohammad, S (Pourmohammad, Sajjad) [3] ; Khataee, A (Khataee, Alireza) [5], [6]; Orooji, Y (Orooji, Yasin) [1] (provided by Clarivate) Volume 204 Part В Article Number 112082 DOI 10.1016/j.envres.2021.112082 Published MAR 2022 Early Access OCT 2021 Indexed 2021-10-22 **Document Type** Article

#### Abstract

Zearalenone (ZEN), a significant class of mycotoxin which is considered as a xenoestrogen, permits, similar to natural estrogens, it's binding to the receptors of estrogen resulting in various reproductive diseases especially, hormonal misbalance. ZEN has toxic effects on human and animal health as a result of its teratogenicity, carcinogenicity, mutagenicity, nephrotoxicity, genotoxicity, and immunotoxicity. To ensure water and environmental resources safety, precise, rapid, sensitive, and reliable analytical and conventional methods can be progressed for the determination of toxins such as ZEN. Different selective nanomaterial-based compounds are used in conjunction with different analytical detection approaches to achieve this goal. The current review demonstrates the state-of-the-art advances of nanomaterial-based electrochemical sensing assays including various sensing, apta-sensing and, immunosensing studies to the highly sensitive determination of ZEN in monitoring has been performed. Then, different conventional and clinical techniques and procedures to sensitive and selective sensing techniques have been reviewed and the efficient comparison of them has been thoroughly discussed. This study has also summarized the salient features and the requirements for applying various sensing and biosensing platforms and diverse immobilization techniques in ZEN detection. Finally, we have defined the



performance of several electrochemical sensors applying diverse recognition elements couples with nanomaterials fabricated using various recognition elements coupled with nanomaterials (metal NPs, metal oxide nanoparticles (NPs), graphene, and CNT) the issues limiting development, and the forthcoming tasks in successful construction with the applied nanomaterials.

#### Keywords

#### Author Keywords

<u>MycotoxinsSensing platformsElectrochemical approachesConventional approachesContaminated food</u> <u>samples</u>

#### **Keywords Plus**

ULTRASENSITIVE DETECTIONCONTAMINANT ZEARALENONEMONOCLONAL-ANTIBODYMEDICINAL-PLANTSALPHA-ZEARALENOLFOOD SAMPLESHPLC-FLDMYCOTOXINSDEOXYNIVALENOLCEREALS



## 44- Short-Range Ordered Iridium Single Atoms Integrated into Cobalt Oxide Spinel Structure for Highly Efficient Electrocatalytic Water Oxidation

#### By:

 Shan, JQ (Shan, Jieqiong) [1], [2]; Ye, C (Ye, Chao) [1], [2]; Chen, SM (Chen, Shuangming) [3]; Sun, TL (Sun, Tulai) [4], [5]; Jiao, Y (Jiao, Yan) [1], [2]; Liu, LM (Liu, Lingmei) [6]; Zhu, CZ (Zhu, Chongzhi) [4], [5]; Song, L (Song, Li) [3]; Han, Y (Han, Yu) [6]; Jaroniec, M (Jaroniec, Mietek) [7], [8]; (provided by Clarivate)

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 10.1021/jacs.1c01525

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## Abstract

Noble metals manifest themselves with unique electronic structures and irreplaceable activity toward a wide range of catalytic applications but are unfortunately restricted by limited choice of geometric structures spanning single atoms, clusters, nanoparticles, and bulk crystals. Herein, we propose how to overcome this limitation by integrating noble metal atoms into the lattice of transition metal oxides to create a new type of hybrid structure. This study shows that iridium single atoms can be accommodated into the cationic sites of cobalt spinel oxide with short-range order and an identical spatial correlation as the host lattice. The resultant Ir0.06Co2.94O4 catalyst exhibits much higher electrocatalytic activity than the parent oxide by 2 orders of magnitude toward the challenging oxygen evolution reaction under acidic conditions. Because of the strong interaction between iridium and cobalt oxide support, the Ir0.06Co2.94O4 catalyst shows significantly improved corrosion resistance under acidic conditions and oxidative potentials. This work eliminates the "close-packing" limitation of noble metals and offers promising opportunity to create analogues with desired topologies for various catalytic applications.

Keywords Keywords Plus



Water
<u>TOTAL-ENERGY CALCULATIONSHYDROGEN EVOLUTIONOXYGEN</u>
<u>EVOLUTIONCATALYSTDESIGNCOMPLEXSURFACEMETALSGOLD</u>



45- Removal of metal ions using a new magnetic chitosan nano-bio-adsorbent; A powerful approach in water treatment

## By:

Karimi, F (Karimi, Fatemeh) [1]; Ayati, A (Ayati, Ali) [1]; Tanhaei, B (Tanhaei, Bahareh) [1]; Sanati, AL (Sanati, Afsaneh L.) [2]; Afshar, S (Afshar, Safoora) [1]; Kardan, A (Kardan, Alireza) [1]; Dabirifar, Z (Dabirifar, Zeynab) [1]; Karaman, C (Karaman, Ceren) [3] (provided by Clarivate) Volume 203 **Article Number** 111753 DOI 10.1016/j.envres.2021.111753 Published JAN 2022 Early Access AUG 2021 Indexed 2021-10-22 **Document Type** Article

## Abstract

In this study, a magnetic chitosan/Al2O3/Fe3O4 (M-Cs) nanocomposite was developed by ethylenediaminetetraacetic acid (EDTA) functionalization to enhance its adsorption behavior for the removal of Cd (II), Cu(II) and Zn(II) metal ions from aqueous solution. The results revealed that the EDTA functionalization of M-Cs increased its adsorption capacity -9.1, -5.6 and -14.3 times toward Cu, Cd and Zn ions. The maximum adsorption capacity followed the order of Cd(II) > Cu(II) > Zn(II) and the maximum adsorption efficiency was achieved at pH of 5.3 with the removal percentage of 99.98, 93.69 and 83.81 %, respectively, for the removal of Cu, Cd and Zn ions. The metal ions adsorption kinetic obeyed pseudo-second-order equation and the Langmuir isothermal was found the most fitted model for their adsorption isothermal experimental data. In addition, the thermodynamic study illustrated that the adsorption process was exothermic and spontaneous in nature.

Keywords

Author Keywords RemovalMagnetic adsorbentChitosan-base adsorbentMetal ions Keywords Plus ADSORPTIVE REMOVALAQUEOUS-SOLUTIONKINETICSNANOPARTICLESCD(II)NI(II)EDTAEQUILIBRIUMPERFORMANCEMECHANISM


# 46- Nanostructured transition metal compounds coated 3D porous core-shell carbon fiber as monolith water splitting electrocatalysts: A general strategy

By:

Yang, F (Yang, Fang) [1]; Xiong, TZ (Xiong, Tuzhi) [1]; Huang, P (Huang, Peng) [1]; Zhou, SH (Zhou, Shuhui) [1]; Tan, QR (Tan, Qirong) [1]; Yang, H (Yang, Hao) [2]; Huang, YC (Huang, Yongchao) [3]; Balogun, MS (Balogun, M. -Sadeeq (Jie Tang)) [1], [3], [4] (provided by Clarivate)

Volume 423 Article Number 130279 DOI 10.1016/j.cej.2021.130279 Published NOV 1 2021 Early Access MAY 2021 Indexed 2021-08-20 Document Type Article

## Abstract

Different transition metal compounds (TMCs) nanostructures grown on conductive substrates have been considered as promising self-supportive non-precious electrocatalysts for electrochemical water splitting, but extremely challenging to develop facile and generalized approaches for rational design and enhancing their catalytic properties. Herein, we develop a general strategy to boost the hydrogen and oxygen evolution reactions (HER and OER) performance of TMCs by designing monolith electrocatalyst architectures. The monoliths comprises of TMCs integrated on carbon fiber cloth core-shell (CFC@EC) structure. The CFC@EC allows the creation of numerous lattice distortions and strong electronic interactions between CFC@EC and metal cations of the TMCs. Such lattice distortions exposes more active sites in CFC@EC/TMCs compared to the pristine CFC coated TMCs (CFC/TMC). Cobalt phosphide (CoP) nanowires and NiFe-LDH coated on CFC@EC exhibits the optimized HER and OER activities. Overall water splitting device assembled based on the optimized HER and OER electrodes also achieve low overall potential of 1.53 V at 10 mA cm-2. More importantly, we further experimentally verify that the integration of Ni3N and Ni3S2, CoS2, NiCo-LDH, NiMn-LDH with CFC@EC also reveal similar improved performance, providing a general and valuable strategy into the design of other selfsupporting electrocatalysts for water splitting and beyond.

## Keywords



## Author Keywords

<u>Monolith electrocatalystCore-double-shell engineeringTransition metal compoundLattice</u> <u>distortionElectronic interaction</u>

**Keywords Plus** 

OXYGEN EVOLUTION KINETICSLAYERED DOUBLE HYDROXIDENICKEL FOAMCATALYTIC-ACTIVITYEFFICIENTARRAYSCONSTRUCTIONNANOSHEETNANOTUBESOER



## 47- Water in waste-derived oil emulsion fuel with cetane improver: Formulation, characterization and its optimization for efficient and cleaner production

#### By:

<u>Vellaiyan, S</u> (Vellaiyan, Suresh) [1]; <u>Subbiah, A</u> (Subbiah, Arunkumar) [2]; <u>Kuppusamy, S</u> (Kuppusamy, Shanmugavel) [3]; <u>Subramanian, S</u> (Subramanian, Saravanan) [4]; <u>Devarajan, Y</u> (Devarajan, Yuvarajan) [5], [6]

(provided by Clarivate) Volume 228 Article Number 107141 DOI 10.1016/j.fuproc.2021.107141 Published APR 2022 Early Access DEC 2021 Indexed 2022-02-10 Document Type Article

## Abstract

The present study aims to formulate the water emulsified waste-derived biodiesel with cetane improver and find its optimum concentration for an efficient and cleaner production from the diesel engines. A waste-derived Lemon peel oil (LPO) is emulsified in diesel fuel along with water, and 2-Ethylhexyl nitrate (EHN). Four levels of each parameter have been chosen for the fuel preparation. The experiments are performed in a naturally aspirated diesel engine at maximum brake power conditions based on the L16 orthogonal array. A grey-relational analysis is opted to optimize the performances and emissions responses, and the statistical influence of the operating parameters is estimated based on the analysis of variance. A comprehensive study has also been conducted to understand the improvement in performance and emission parameters at the optimum level. From the results, the optimum condition of LPO, water, and EHN is identified as 20%, 10%, and 2%, respectively. The water concentration in base fuel has a contribution of 65.94% on overall engine behavior, whereas the contribution of LPO and EHN is 26.72% and 7.34%, respectively. Besides, the confirmation experiment at the optimum condition shows that the signal-to-noise ratio is improved by 40.8% compared to the initial best condition.

Keywords Author Keywords



Lemon peel oilWater emulsionCetane improverMultiple response optimizationEnergy impactEnvironmental impact Keywords Plus LEMON PEEL OILCOMBUSTION CHARACTERISTICSPERFORMANCEBIODIESELEMISSIONPARAMETERSIGNITION



## 48- Low temperature extrusion promotes transglutaminase cross-linking of whey protein isolate and enhances its emulsifying properties and water holding capacity

By:

<u>Li, JP</u> (Li, Jinpeng) [1]; <u>Fu, JF</u> (Fu, Jinfeng) [1]; <u>Ma, Y</u> (Ma, Yue) [1]; <u>He, YT</u> (He, Yanting) [1]; <u>Fu, RX</u> (Fu, Runxiao) [1]; <u>Qayum, A</u> (Qayum, Abdul) [1]; <u>Jiang, ZM</u> (Jiang, Zhanmei) [1]; <u>Wang, LZ</u> (Wang, Lizhe) [2] **Volume** 

125 Article Number 107410 DOI 10.1016/j.foodhyd.2021.107410 Published APR 2022 Early Access DEC 2021 Indexed 2022-01-20 Document Type Article

## Abstract

Impact of extrusion pretreatment (50, 70, 90, 110 and 130 degrees C) on physicochemical, emulsifying properties and water holding capacity (WHC) of transglutaminase (TGase) cross-linked whey protein isolate (WPI) were investigated in this study. The results of molecular size distribution and SDS-PAGE proved that there were more macromolecular polymers formed in TGase cross-linked WPI after extrusion pretreatment (E-WPI-TGase) and the consumption of free amino groups for E-WPI-TGase was the largest at the extrusion temperature of 50 degrees C and 70 degrees C. As the extrusion temperature increased from 90 degrees C to 130 degrees C, particle size of WPI after extrusion pretreatment (E-WPI) was not changed significantly, compared with that of E-WPI-TGase were higher than those of WPI cross-linked by TGase (WPI-TGase) (p < 0.05). Significantly, the emulsifying activity, surface hydrophobicity and WHC of E-WPI-TGase, respectively. Therefore, these results indicated that low temperature (50 degrees C and 70 degrees C) extrusion pretreatment could promote the cross-linking degree of TGase-catalyzed WPI, and improve its emulsifying properties, WHC and surface hydrophobicity.

Keywords Author Keywords



Extrusion pretreatmentWhey protein isolateTransglutaminasePhysicochemical propertiesEmulsifying properties

**Keywords Plus** 

FUNCTIONAL-PROPERTIESSOY PROTEINMICROBIAL TRANSGLUTAMINASEPHYSIOCHEMICAL PROPERTIESMOLECULAR-STRUCTURESPHYSICAL-PROPERTIESFOOD PROTEINSPROTEOLYSISULTRASOUNDQUALITY



## 49- NiFe Layered-Double-Hydroxide Nanosheet Arrays on Graphite Felt: A 3D Electrocatalyst for Highly Efficient Water Oxidation in Alkaline Media

By:

Ding, P (Ding, Peng) [1], [2]; Meng, CQ (Meng, Chuqian) [1]; Liang, J (Liang, Jie) [1]; Li, TS (Li, Tingshuai) [1]; Wang, Y (Wang, Yan) [1]; Liu, Q (Liu, Qian) [3]; Luo, YL (Luo, Yonglan) [3]; Cui, GW (Cui, Guanwei) [4]; Asiri, AM (Asiri, Abdullah M.) [5], [6]; Lu, SY (Lu, Siyu) [2]; (provided by Clarivate)

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 AUG 2021

 Indexed

 2021-10-02

 Document Type

## Abstract

Article

It is of great importance to rationally design and develop earth-abundant nanocatalysts for high-efficiency water electrolysis. Herein, NiFe layered double hydroxide was in situ grown hydrothermally on a 3D graphite felt (NiFe LDH/GF) as a high-efficiency catalyst in facilitating the oxygen evolution reaction (OER). In 1.0 M KOH, NiFe LDH/GF requires a low overpotential of 214 mV to deliver a geometric current density of 50 mA cm(-2) (eta(50 mA cm-2) = 214 mV), surpassing that NiFe LDH supported on a 2D graphite paper (NiFe LDH/GF; eta(50 mA cm-2) = 301 mV). More importantly, NiFe LDH/GF shows good durability at 50 mA cm(-2) within 50 h of OER catalysis testing and delivers a faradaic efficiency of nearly 100% in the electrocatalysis of OER.

## Keywords

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Keywords Plus
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OXYGEN EVOLUTIONPERFORMANCESURFACEELECTRODENANOARRAYCATALYSTHYDROGEN



50- Ecological risk assessment of soil and water loss by thermal enhanced methane recovery: Numerical study using two-phase flow simulation By: Xue, Y (Xue, Yi) [1]; Liu, J (Liu, Jia) [1]; Liang, X (Liang, Xin) [1]; Wang, SH (Wang, Songhe) [1]; Ma, ZY (Ma, Zongyuan) [1] (provided by Clarivate) Volume 334 **Article Number** 130183 DOI 10.1016/j.jclepro.2021.130183 Published FEB 1 2022 Indexed 2022-04-19 **Document Type** Article

#### Abstract

Thermal enhanced methane recover y inevitably aggravates the soi I and water loss, causing severe harm to the sustainability of groundwater environment and the surrounding ecosystem. Therefore, quantitative analysis of the effect of thermal enhanced methane recover y on groundwater loss and ecological risk of coalbed methane development zone is necessary. In this study, a coupling model of gas drainage and groundwater loss is estab-lished. The model considers the dynamic gas diffusion of coal matrix, the twophase flow of water and gas, and the influence of temperature on such flow. Based on this model, characteristics of groundwater loss of coal seam reservoir caused by enhanced methane recover y are analyzed, and the ecological risk assessment of methane recovery zone is realized. Results indicate that during heat injection, the permeability of the coal seam increases with distance from the borehole due to the competition between two-phase flow and temperature. High tem-perature develops the permeability, gas production, and water production of the reservoir. The change rules of water and gas productions are similar with initial increases and subsequent declines. The influence of coal gas diffusion on groundwater loss has a certain time lag. In the early stage, the dynamic attenuation of gas dif f usion is not apparent. In the later stage, the supplement rate of gas from matrix to fracture decreases. The initial saturation has a significant influence on the water production rate in the early stage. A large Langmuir volume constant not only strengthens the peak value of gas drainage rate but also the gas drainage rate itsel f in the later declining period. Large scale coalbed methane development will face ecological risks such as water environment pollution, habitat destruction and soi I degradation, which is the key aspect of ecological environment man-agement and risk prevention.



Keywords Author Keywords Enhanced methane recoveryHeat injectionGroundwater lossPermeability evolutionNumerical investigation Keywords Plus: GAS



# 51- Rational design of multifunctional electrocatalyst: An approach towards efficient overall water splitting and rechargeable flexible solid-state zinc-air battery

By:

<u>Ramakrishnan, S</u> (Ramakrishnan, Shanmugam) [1]; <u>Velusamy, DB</u> (Velusamy, Dhinesh Babu) [2], [3]; <u>Sengodan, S</u> (Sengodan, Sivaprakash) [4]; <u>Nagaraju, G</u> (Nagaraju, Goli) [4]; <u>Kim, DH</u> (Kim, Do Hwan) [1], [5], [6]; <u>Kim, AR</u> (Kim, Ae Rhan) [1], [7]; <u>Yoo, DJ</u> (Yoo, Dong Jin) [1], [7]

(provided by Clarivate) Volume 300 Article Number 120752 DOI 10.1016/j.apcatb.2021.120752 Published JAN 2022 Early Access OCT 2021 Indexed 2021-10-28 Document Type Article

## Abstract

Constructing an electrocatalyst with highly durable active and cost-effective core-shell with a porous carbon nanosheet for the development of high efficiency energy conversion and storage devices. Herein, we developed core-shell nickel-iron oxide on a highly porous N-doped carbon nanosheet (CS-NFO@PNC) via a facile solvothermal calcination route. The optimized CS-NFO@PNC-700 showed remarkable electrocatalytic activity towards ORR (0.85 V vs RHE), OER r10 = 217 mV, and HER r10 = 200 mV with excellent durability towards the corresponding half-cell reactions. Further, we investigated the ORR, OER, and HER mechanistic pathways of the electrocatalyst using the density functional theory. Finally, we fabricated a rechargeable liquid electrolyte-based zinc-air battery with CS-NFO@PNC-700 as the cathode which displayed an improved power density of 130 mW cm-2 at 217 mA cm-2 with excellent durability of 180 h. The rechargeable flexible quasi-solid-state zinc-air battery with CS-NFO@PNC-700 air cathode, which exhibited excellent long term durability over 40 h at 5 mA cm-2.

Keywords

Author Keywords <u>Multifunctional electrocatalystNickel-iron oxideOverall water splittingDensity functional theory</u> Keywords Plus



OXYGEN REDUCTIONPOROUS CARBONBIFUNCTIONAL CATALYSTEVOLUTION REACTIONMOF COMPOSITEACTIVE-SITESNANOSHEETSNICKELCOBALTOXIDE



52- Bilinear auto-Backlund transformations and soliton solutions of a (3+1)-dimensional generalized nonlinear evolution equation for the shallow water waves

By: Shen, Y (Shen, Yuan) ; Tian, B (Tian, Bo) [1] Volume 122 **Article Number** 107301 DOI 10.1016/j.aml.2021.107301 Published DEC 2021 **Early Access** AUG 2021 Indexed 2021-09-17 **Document Type** Article

## Abstract

Waves are seen in the atmosphere, oceans, etc. As one of the most common natural phenomena, water waves attract the attention of researchers. For the shallow water waves, a (3+1)-dimensional generalized nonlinear evolution equation is hereby investigated via the symbolic computation. Based on the Hirota method, we present three bilinear auto-Backlund transformations, along with some soliton solutions. Our results depend on the water-wave coefficients in that equation. (C) 2021 Elsevier Ltd. All rights reserved.

#### Keywords

## **Author Keywords**

<u>Shallow water waves(3+1)-dimensional generalized nonlinear evolution equationHirota methodSymbolic</u> <u>computationBilinear auto-Backlund transformationSoliton solution</u>



## 53- Efficient Photocatalytic Overall Water Splitting Induced by the Giant Internal Electric Field of a g-C3N4/rGO/PDIP Z-Scheme Heterojunction

By:

Chen, XJ (Chen, Xianjie) [1]; Wang, J (Wang, Jun) [2]; Chai, YQ (Chai, Yongqiang) [3]; Zhang, ZJ (Zhang, Zijian) [1]; Zhu, YF (Zhu, Yongfa) [1] (provided by Clarivate) Volume 33 Issue 7 **Article Number** 2007479 DOI 10.1002/adma.202007479 Published FEB 2021 **Early Access** JAN 2021 Indexed 2021-02-08 **Document Type** Article

## Abstract

A graphitic carbon nitride/rGO/perylene diimide polymer (g-C3N4/rGO/PDIP) Z-scheme heterojunction is successfully constructed to realize high-flux charge transfer and efficient photocatalytic overall water splitting. A giant internal electric field in the Z-scheme junction is built, enabling the charge separation efficiency to be enhanced dramatically by 8.5 times. Thus, g-C3N4/rGO/PDIP presents an efficient and stable photocatalytic overall water splitting activity with H-2 and O-2 evolution rate of 15.80 and 7.80 mu mol h(-1), respectively, approximate to 12.1 times higher than g-C3N4 nanosheets. Meanwhile, a notable quantum efficiency of 4.94% at 420 nm and solar-to-hydrogen energy-conversion efficiency of 0.30% are achieved, prominently surpassing many reported g-C3N4-based photocatalysts. Briefly, this work throws light on enhancing the internal electric field by interface control to dramatically improve the photocatalytic performance.

## Keywords

## **Author Keywords**

graphitic carbon nitrideoverall water splittingperylene diimide polymerphotocatalysisZ-scheme heterostructures



Water Keywords Plus: <u>VISIBLE-LIGHT-DRIVENHYDROGEN-PRODUCTIONNANOPARTICLESG-</u> <u>C3N4COCATALYSTSURFACEH-2</u>



## 54- Climate change impact on yields and water use of wheat and maize in the North China Plain under future climate change scenarios

By:

Xiao, DP (Xiao, Dengpan) [1], [2]; Liu, DL (Liu, De Li) [2], [3]; Wang, B (Wang, Bin) [2], [4]; Feng, PY (Feng, Puyu) [2], [4]; Bai, HZ (Bai, Huizi) [1]; Tang, JZ (Tang, Jianzhao) [1] (provided by Clarivate) Volume 238 Article Number 106238 DOI 10.1016/j.agwat.2020.106238 Published AUG 1 2020 Indexed 2020-06-10 Document Type Article

## Abstract

Climate change has already and will continue to exert a vital impact on crop yield and water use in the North China Plain (NCP). Currently, this plain is facing a dilemma between groundwater depletion and grain production demand. It is urgent to identify the impact of future climate change on crop yield and water consumption and then develop efficient adaptation strategies in the region. In this study, we used statistically downscaled daily climate data from 33 global climate models (GCMs) and two Representative Concentration Pathways (RCP4.5 and RCP8.5) for 61 stations distributed across the NCP and drove the well-validated APSIM model to simulate crop yield and water use for two future periods of 2031-2060 (2040s) and 2071-2100 (2080s). Data from all 33 GCMs show an increase in annual mean temperature and almost all the GCMs also show increases in annual mean solar radiation and annual total precipitation across the NCP. Future climate warming led to an advance in phenology for both winter wheat and summer maize, two typical crops in the NCP. However, the length of the reproductive growth period (RGP) of winter wheat was prolonged while that of summer maize was shortened under future climate scenarios across the NCP. Our simulated results show that future climate change had negative impacts on maize yield but positive impacts on wheat yield across the NCP. Mainly due to the shortening of the whole growth period, crop water consumption was largely decreased under future climate scenarios. The amount of irrigation required was also reduced mainly due to increased precipitation and decreased ET. Although future climate change would likely mitigate groundwater overdraft in most part of NCP, some areas in the northern NCP still had groundwater over-pumping in the future. Therefore, we suggest that it might be a good choice to change cropping system for reducing planting area of water-consuming crop (e.g. winter wheat) in those over-pumping areas to balance groundwater use and crop yield.



Keywords Author Keywords Crop yieldGroundwater overdraftFuture climate change scenarioAPSIM modelNorth China Plain Keywords Plus ALTERNATIVE CROPPING SYSTEMSNEXT-GENERATIONGRAIN-YIELDMANAGEMENTRESPONSESLEVELMODELCMIP5



## 55- Water use indicators and economic analysis for on-farm irrigation decision: A case study of a super high density olive tree orchard By: Fernandez, JE (Fernandez, J. E.) [1]; Alcon, F (Alcon, F.) [2]; Diaz-Espejo, A (Diaz-Espejo, A.) [1] ; Hernandez-Santana, V (Hernandez-Santana, V) [1]; Cuevas, MV (Cuevas, M., V) [1] (provided by Clarivate) Volume 237 **Article Number** 106074 DOI 10.1016/j.agwat.2020.106074 Published JUL 1 2020 Indexed 2020-05-22 **Document Type** Article

#### Abstract

Increasing the efficiency of on-farm water use requires wise decisions on the irrigation system, the irrigation strategy and the method to schedule irrigation, among other factors related to water management. Since the early 2000s, the water productivity approach has been widely used to address this issue. It provides useful indicators to both the biophysical water productivity and the economic performance of irrigation. Analysis of the literature, however, shows both confusion on the use of terms and lack of agreement on the equations. We have addressed the rational use of the water productivity approach for the irrigator to improve both biophysical and economic water productivity at the field scale. We also addressed the increasing use of the water footprint approach at the field scale. The literature shows a lack of consensus on the reliability of the conceptual framework behind that approach. We focused on its potential for irrigation decision making, and concluded that it is not advantageous, as compared to the water productivity approach, for assessing on-farm water use. In addition, we show a case study of a super high density olive orchard which analyses the joint use of economic water productivity indicators and both production and profit functions to improve decision making.

#### Keywords

#### Author Keywords

<u>Water use efficiencyCrop water productivityEconomic water productivityMarginal profitProduction</u> <u>functionProfit function</u> **Keywords Plus** 



REGULATED DEFICIT IRRIGATIONVIRTUAL WATEROIL QUALITYPRODUCTIVITYFOOTPRINTSYIELDMANAGEMENTCROPSIMPROVEMENTPERFORMANCE



56- Green sonochemical synthesis of BaDy2NiO5/Dy2O3 and BaDy2NiO5/NiO nanocomposites in the presence of core almond as a capping agent and their application as photocatalysts for the removal of organic dyes in water

#### By:

<u>Yousefi, SR</u> (Yousefi, Seyede Raheleh) [1]; <u>Sobhani, A</u> (Sobhani, Azam) [2]; <u>Alshamsi, HA</u> (Alshamsi, Hassan Abbas) [3]; <u>Salavati-Niasari, M</u> (Salavati-Niasari, Masoud) [1] (provided by Clarivate)

Volume 11 Issue 19 Page 11500-11512 DOI 10.1039/d0ra10288a Published MAR 31 2021 Indexed 2021-04-03 Document Type Article

## Abstract

The present work reports the sonochemical synthesis of DBNO NC (dysprosium nickelate nanocomposite) using metal nitrates and core almond as a capping agent. In addition, the effects of the power of ultrasound irradiation were investigated. The BaDy2NiO5/Dy2O3 and BaDy2NiO5/NiO nanocomposites were synthesized with sonication powers of 50 and 30 W, respectively. The agglomerated nanoparticles were obtained using different sonication powers, including 15, 30, and 50 W. The results showed that upon increasing the sonication power, the particle size decreased. After characterization, the optical, electrical, magnetic, and photocatalytic properties of the NC were studied. The nanocomposites showed an antiferromagnetic behavior. In this study, the photocatalytic degradations of two dyes, AR14 and AB92, were investigated in the presence of DBNO NC. Furthermore, the effects of the amount of photocatalyst, the concentration of the dye solution, the type of organic dye, and light irradiation on the photocatalytic activity of the nanocomposite were studied. The results showed that with an increasing amount of catalyst and decreasing concentration of dye, the photocatalytic activity of the nanocomposite was increased. This activity for the degradation of AR14 is higher than that of AB92. Both AR14 and AB92 dyes show higher photocatalytic degradation.

Keywords Keywords Plus



 Water

 STRUCTURAL-CHARACTERIZATIONOPTICAL SPECTROSCOPYCARBON NITRIDER2BANIO5

 RCHAINDEGRADATIONREDUCTIONPOLYMORPHISMTIO2GAP