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# 化学学报

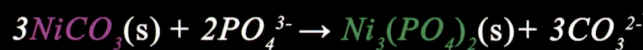
## ACTA CHIMICA SINICA

Volume 78 Number 12 December 2020

$(\text{Mn}_x\text{Co}_y\text{Ni}_z)\text{CO}_3$

$\text{Ni}_3(\text{PO}_4)_2$  coated  $(\text{Mn}_x\text{Co}_y\text{Ni}_z)\text{CO}_3$

serves as the precursor of Li-rich Mn-based cathode  
for advanced Li-ion batteries



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中国化学会  
中国科学院上海有机化学研究所

主办

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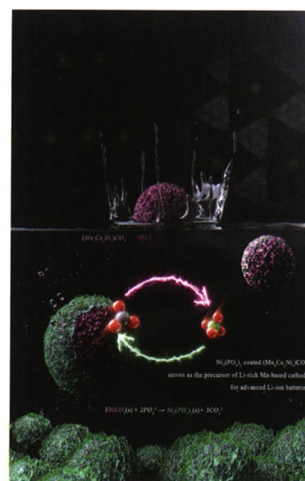
$Co_9S_9/MoS_2$  异质结构的构筑及电催化析氢性能研究..... 张宇, 王世兴, 杨蕊, 戴腾远, 张楠, 席聘贤\*, 严纯华, 化学学报, 2020, 78(12), 1455-1460

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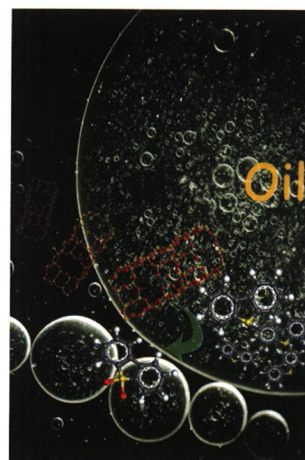
\* 通信联系人.



**On the cover:** A facile approach is developed to synthesize  $\text{Li}_3\text{PO}_4$ -coated Li-rich Mn-based oxides (LRMO) as cathode materials for rechargeable lithium-ion batteries. The synthesis involves *in-situ* carbonate-phosphate precipitate conversion, which ensures homogenous coating of  $\text{Ni}_3(\text{PO}_4)_2$  layer on precursor surface and formation of  $\text{Li}_3\text{PO}_4$  layer during subsequent calcination. The  $\text{Li}_3\text{PO}_4$ -coated LRMO exhibits improved electrochemical performance due to suppressed side reactions and transition metal dissolution. [Cheng, Fangyi *et al.* on page 1426-1433.]

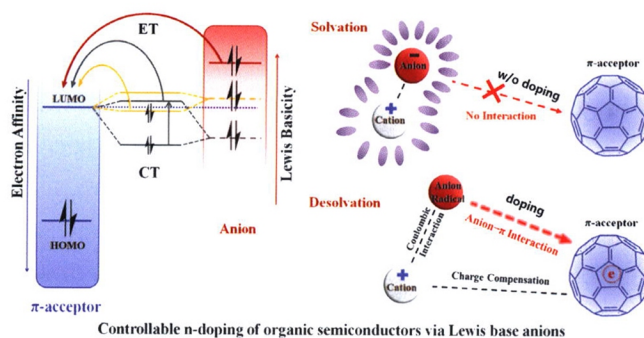


**On the back cover:** Mo/Beta zeolites containing dioxo  $(\text{Si-O})_2\text{Mo}(=\text{O})_2$  species efficiently catalyze the oxidative desulfurization of model oil. [Li, Landong *et al.* on page 1404-1410.]



### Perspective

#### Doping of Organic Semiconductors with Lewis Base Anions: Mechanism, Applications and Perspectives



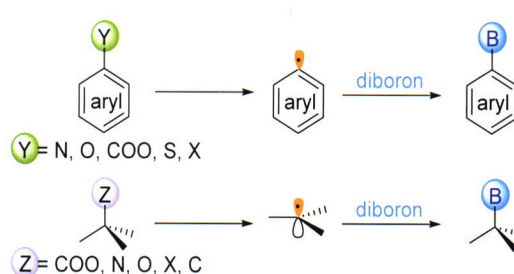
Jiang, Dan-Ni; Yan, Kang-Rong; Li, Chang-Zhi\*

*Acta Chim. Sinica* **2020**, 78(12), 1287-1296

Effective n-doping of organic semiconductors is achieved via Lewis base anion-induced electron transfer in controllable fashion.

Review

Organic Borylation Reactions via Radical Mechanism

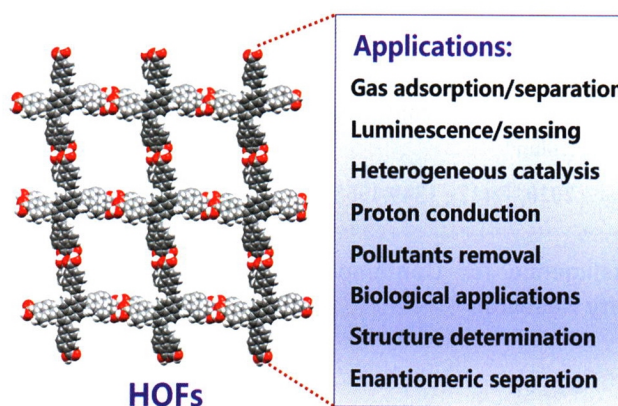


Liu, Qianyi; Zhang, Lei; Mo, Fanyang\*

*Acta Chim. Sinica* **2020**, 78(12), 1297-1308

The development of borylation reactions via radical mechanism, including aryl and alkyl radical borylation via activation of C—N, C—O, C—X, C—S, C—C bonds and decarboxylation of carboxylic acids in the last 10 years is summarized in this review.

Porous Hydrogen-bonded Organic Frameworks (HOFs): Status and Challenges

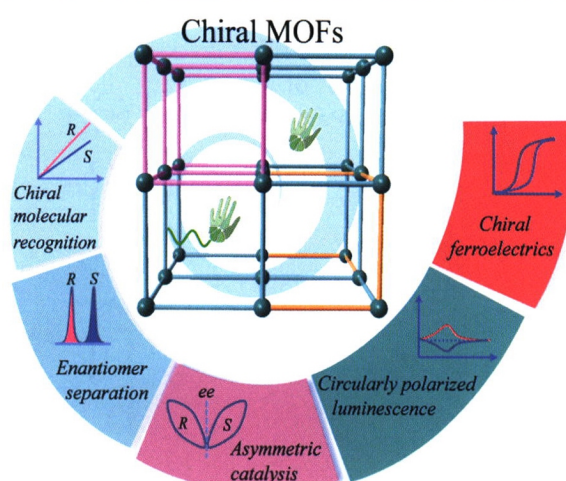


Lin, Zu-Jin\*; Cao, Rong\*

*Acta Chim. Sinica* **2020**, 78(12), 1309-1335

Hydrogen-bonded organic frameworks (HOFs) are becoming a unique type of porous material. HOF design was usually based on supramolecular synthons and scaffolds. This review first elucidates the basic rules to design porous HOFs, and then summarizes the common supramolecular synthons and scaffolds used to build them. Emphasis is put on the potential applications of HOFs.

Design, Synthesis and Applications of Chiral Metal-Organic Frameworks



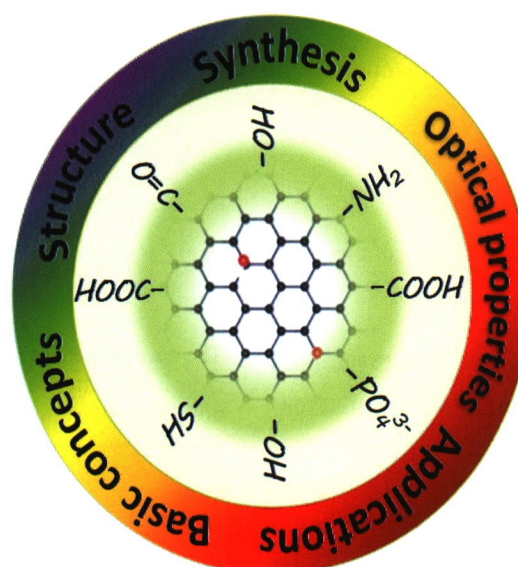
Chen, Zhonghang; Han, Zongsu; Shi, Wei\*; Cheng, Peng

*Acta Chim. Sinica* **2020**, 78(12), 1336-1348

The synthetic strategies of chiral metal-organic frameworks and their applications in several fields including chiral molecular recognition, enantiomer separation, asymmetric catalysis, circularly polarized luminescence and chiral ferroelectrics are summarized in this review.



## Progress in Carbon Dots from the Perspective of Quantum Dots

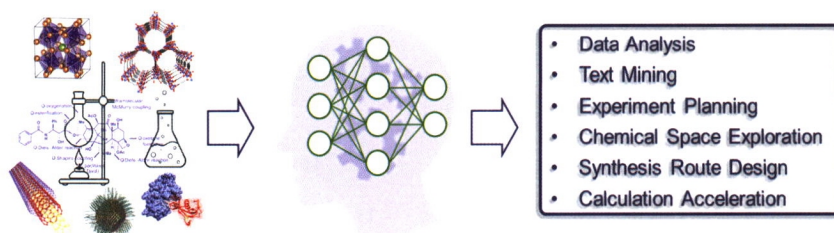


Liu, Yanhong; Zhang, Dongxu; Mao, Baodong\*; Huang, Hui\*; Liu, Yang\*; Tan, Huaqiao; Kang, Zhenhui\*

*Acta Chim. Sinica* **2020**, 78(12), 1349-1365

This review focuses on the four aspects of basic structure, synthetic chemistry, optical properties and application research, and reexamine the research progress and challenges in the field of carbon dots from the view of basic concepts of traditional quantum dots.

## Artificial Intelligence for Contemporary Chemistry Research

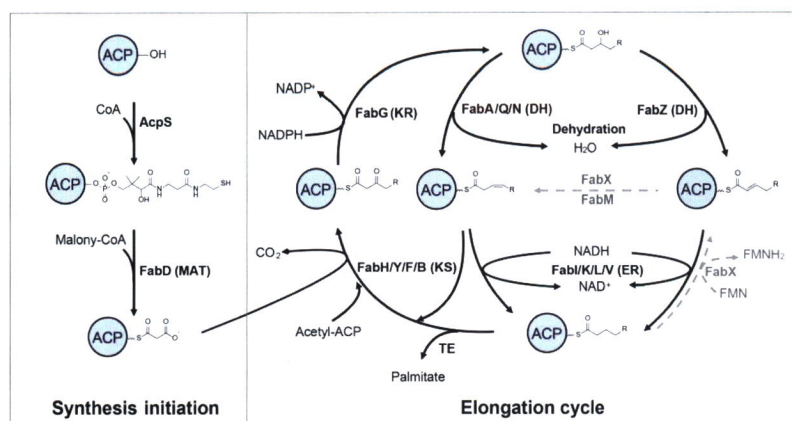


Zhu, Boyang\*; Wu, Ruilong; Yu, Xi\*

*Acta Chim. Sinica* **2020**, 78(12), 1366-1382

Contemporary artificial intelligence methods and the basic principles using machine learning to solve chemical problems are discussed in this review. Methods of artificial intelligence assisted solutions to different chemical research and corresponding machine learning algorithms through specific cases are demonstrated.

## Mechanism and Drug Discovery of Type-II Fatty Acid Biosynthesis Pathway



Zhou, Jiashen; Zhang, Lin; Zhang, Liang\*

*Acta Chim. Sinica* **2020**, 78(12), 1383-1398

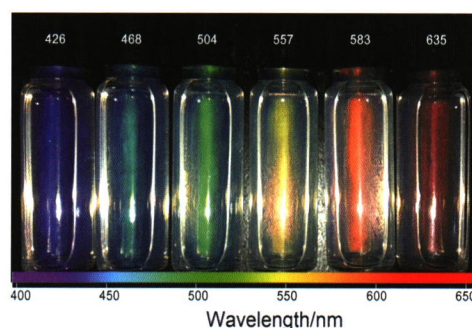
Type-II fatty acid biosynthesis pathway (FAS-II) plays an indispensable role in bacteria. Elucidating the catalytic regulation mechanism of the FAS-II and developing antibacterial drug targeting FAS-II enzyme system is the focus of research in this field. Investigating FAS-II may potentially facilitate further understanding of FAS-II biological functions as well as antibacterial drug discovery for infectious diseases.

## Communication

Dispersions of  $\alpha$ -Zirconium Phosphate/organic Solvent with Structural Colors

Zhang, Chao; Zhang, Baoqing; Liu, Chenyang\*

*Acta Chim. Sinica* **2020**, 78(12), 1399-1403



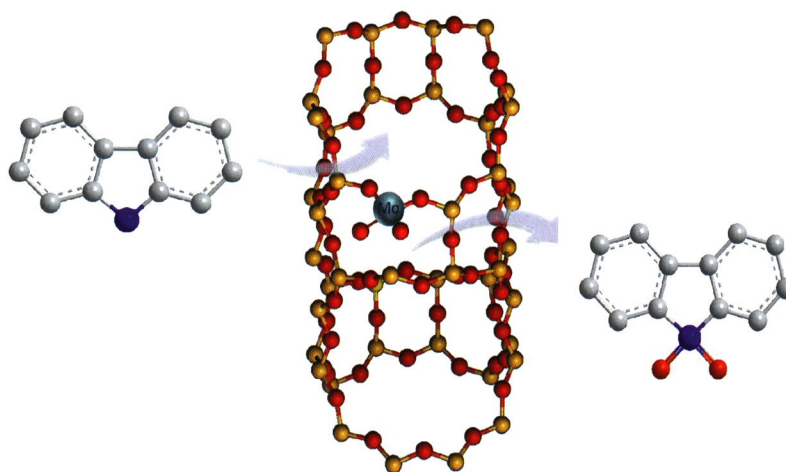
With acetone as the solvent,  $\alpha$ -zirconium phosphate ( $\alpha$ -ZrP) dispersions could reflect visible light in the range of 426 nm to 635 nm when the mass fraction of  $\alpha$ -ZrP was between 0.76% and 1.86%, thus showing the corresponding structural colors.

## Article

## Zeolite Stabilized Isolated Molybdenum Species for Catalytic Oxidative Desulfurization

Zhang, Mengting; Yan, Tingting; Dai, Weili; Guan, Naijia; Li, Landong\*

*Acta Chim. Sinica* **2020**, 78(12), 1404-1410

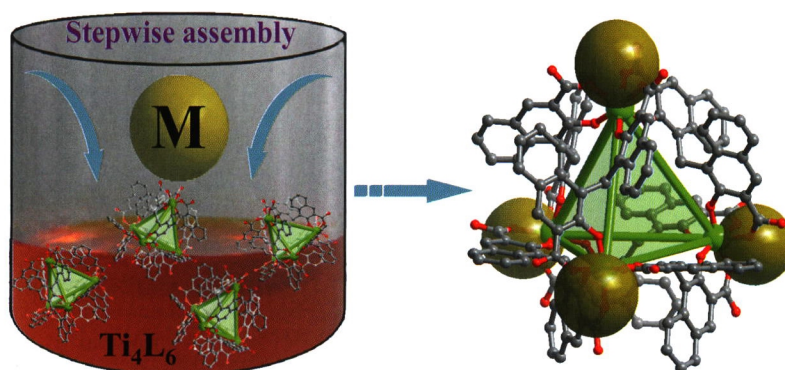


A series of Mo/beta zeolite samples with different Mo loadings were prepared via a two-step post-synthesis strategy. The Mo/beta samples were thoroughly characterized by several spectroscopic techniques and dioxo  $(\text{Si-O})_2\text{Mo}(=\text{O})_2$  species were determined to be the dominant Mo species stabilized and confined in BEA zeolite structure. The as-prepared Mo/beta samples were applied as possible catalysts in the reaction of oxidative desulfurization (ODS) from model fuel. Mo/beta exhibited remarkable oxidative desulfurization efficiency in the removal of heterocyclic sulfur compounds like dibenzothiophene (DBT) from model fuel and might be developed as efficient and stable ODS catalysts for future applications.

Syntheses and Structural Studies of a Series of  $\text{Ti}_4(\text{embonate})_6$ -based Complexes

Chen, Guanghui; He, Yanping\*; Zhang, Lei; Zhang, Jian\*

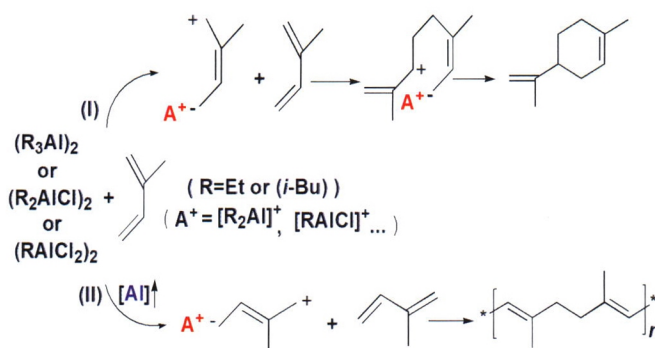
*Acta Chim. Sinica* **2020**, 78(12), 1411-1417



By employing the  $\text{Ti}_4\text{L}_6$  cages to assemble with  $\text{Mn}^{2+}$ ,  $\text{Nd}^{3+}$ ,  $\text{Ba}^{2+}$  and  $\text{Ca}^{2+}$  ions, respectively, a series of  $\text{Ti}_4\text{L}_6$ -based complexes have been synthesized through two-step reaction.



### Oligomerization and Polymerization of Isoprene Catalyzed by Alkylaluminium with Different Structures

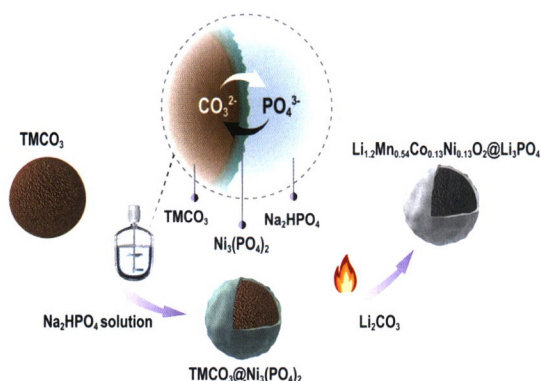


Peng, Wei; Qi, Peiyao; Dong, Kaixuan; He, Aihua\*

*Acta Chim. Sinica* **2020**, 78(12), 1418-1425

Alkylaluminium could catalyze both oligomerization and cationic polymerization of isoprene.  $AlEtCl_2$  had higher catalytic activity at high alkylaluminium concentration ( $n(Al)/n(M)=1050 \times 10^{-5}$ ). Too low and too high alkylaluminium concentration were not beneficial to obtain polyisoprene with high molecular weight.

### In-situ $Li_3PO_4$ Coating of Li-Rich Mn-Based Cathode Materials for Lithium-ion Batteries

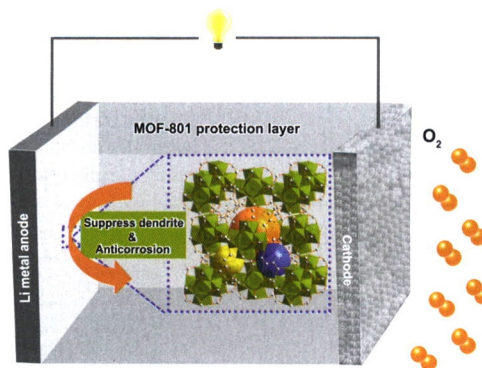


Liu, Jiuding; Zhang, Yudong; Liu, Junxiang; Li, Jinhan; Qiu, Xiaoguang; Cheng, Fangyi\*

*Acta Chim. Sinica* **2020**, 78(12), 1426-1433

A  $Li_3PO_4$  coating layer *in-situ* formed by precipitate conversion and solid state reaction improves the performance of lithium-rich manganese-based oxide cathode due to suppression of phase transformation, side reactions and transition metal dissolution.

### Porous Metal-Organic Frameworks Lithium Metal Anode Protection Layer towards Long Life Li-O<sub>2</sub> Batteries



Yu, Yue; Zhang, Xinbo\*

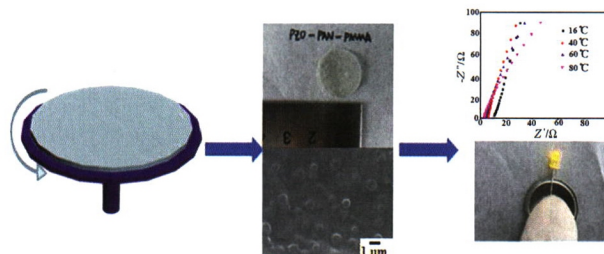
*Acta Chim. Sinica* **2020**, 78(12), 1434-1440

Metal-organic frameworks materials (MOF-801) with high specific surface area and abundant pores act as a protection layer on lithium metal anode in Li-O<sub>2</sub> batteries. The abundant hole-channels can assist uniform  $Li^+$  flux to suppress uncontrollable dendrite growth and the shield effect as well as the water capture function of protection layer can effectively prevent serious corrosion. Consequently, the electrochemical performances have been greatly improved that 800 h plating/stripping cycles and 170 cycles in Li-O<sub>2</sub> batteries have been achieved.

### Blending Based PEO-PAN-PMMA Gel Polymer Electrolyte Prepared by Spaying Casting for Solid-state Lithium Metal Batteries

Kang, Shusen\*; Yang, Chengxiang; Yang, Zelin; Wu, Ningning; Zhao, Shan; Chen, Xiaotao; Liu, Fuliang; Shi, Bin\*

*Acta Chim. Sinica* **2020**, 78(12), 1441-1447

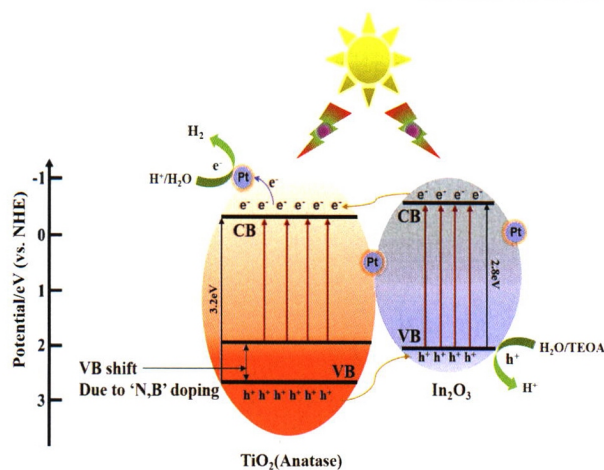


Polymer electrolyte films consisting of polyethylene oxide (PEO), polyacrylonitrile (PAN), polymethyl methacrylate (PMMA) and liquid electrolyte were prepared by spaying casting and examined in order to obtain the best compromise between high conductivity, homogeneity, dimensional and electrochemical stability. The high ionic conductivity of PEO-PAN-PMMA gel polymer electrolyte (GPE) is examined using electrochemical impedance spectroscopy (EIS) and attended due to the high absorption. And the highest ionic conductivity is 0.4 mS/cm at room temperature.

### Preparation and Photocatalytic Hydrogen Production of B, N Co-doped $\text{In}_2\text{O}_3/\text{TiO}_2$

Li, Chen; Chen, Fenghua\*; Ye, Li; Li, Wei; Yu, Han; Zhao, Tong\*

*Acta Chim. Sinica* **2020**, 78(12), 1448-1454

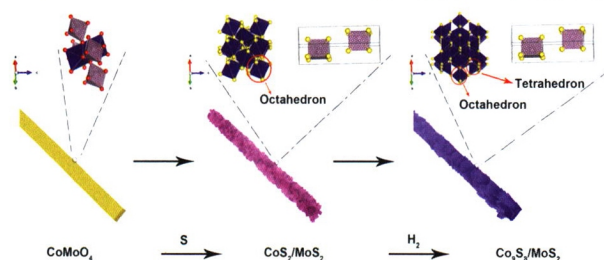


B, N co-doping and heterojunction construction to synergistically prepare the B, N-doped  $\text{In}_2\text{O}_3/\text{TiO}_2$  photocatalyst by using polymer precursor method is presented. Band gap of the pyrolyzed sample is narrowed from 3.09 eV of P25 to 2.71 eV of IT-500 (the modified sample annealed at 500 °C). Visible light absorption range has been greatly broadened. Under the irradiation of visible light ( $>380$  nm), hydrogen production rate of IT-500 reaches  $5961 \mu\text{mol} \cdot \text{g}^{-1} \cdot \text{h}^{-1}$ . When the B, N- $\text{In}_2\text{O}_3/\text{TiO}_2$  polymer precursor is gas sprayed, pyrolyzed at the optimal conditions and used as photocatalyst, hydrogen production rate reaches  $1186 \mu\text{mol} \cdot \text{g}^{-1} \cdot \text{h}^{-1}$  and keeps 97% after 5-cycle test, which shows high potential for commercial use of this material.

### Construction of $\text{Co}_9\text{S}_8/\text{MoS}_2$ Heterostructures for Enhancing Electrocatalytic Hydrogen Evolution Reaction

Zhang, Yu; Wang, Shixing; Yang, Rui; Dai, Tengyuan; Zhang, Nan; Xi, Pinxian\*; Yan, Chun-Hua

*Acta Chim. Sinica* **2020**, 78(12), 1455-1460



$\text{CoMoO}_4$  nanorods were synthesized by hydrothermal method, and then  $\text{CoS}_2/\text{MoS}_2$  heterostructures were formed by vulcanizing the  $\text{CoMoO}_4$  nanorods. Among  $\text{CoS}_2/\text{MoS}_2$  heterostructures, Co possesses octahedral configuration. Finally, the  $\text{CoS}_2/\text{MoS}_2$  heterostructures were calcined in hydrogen atmosphere to generate an activated  $\text{Co}_9\text{S}_8/\text{MoS}_2$  hetero-catalysts with the partial octahedral configuration of Co changing to the tetrahedral configuration. The generation of the new tetrahedral configuration activates the catalyst material, thereby producing excellent activity in the alkaline hydrogen evolution reaction.

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# Oi



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