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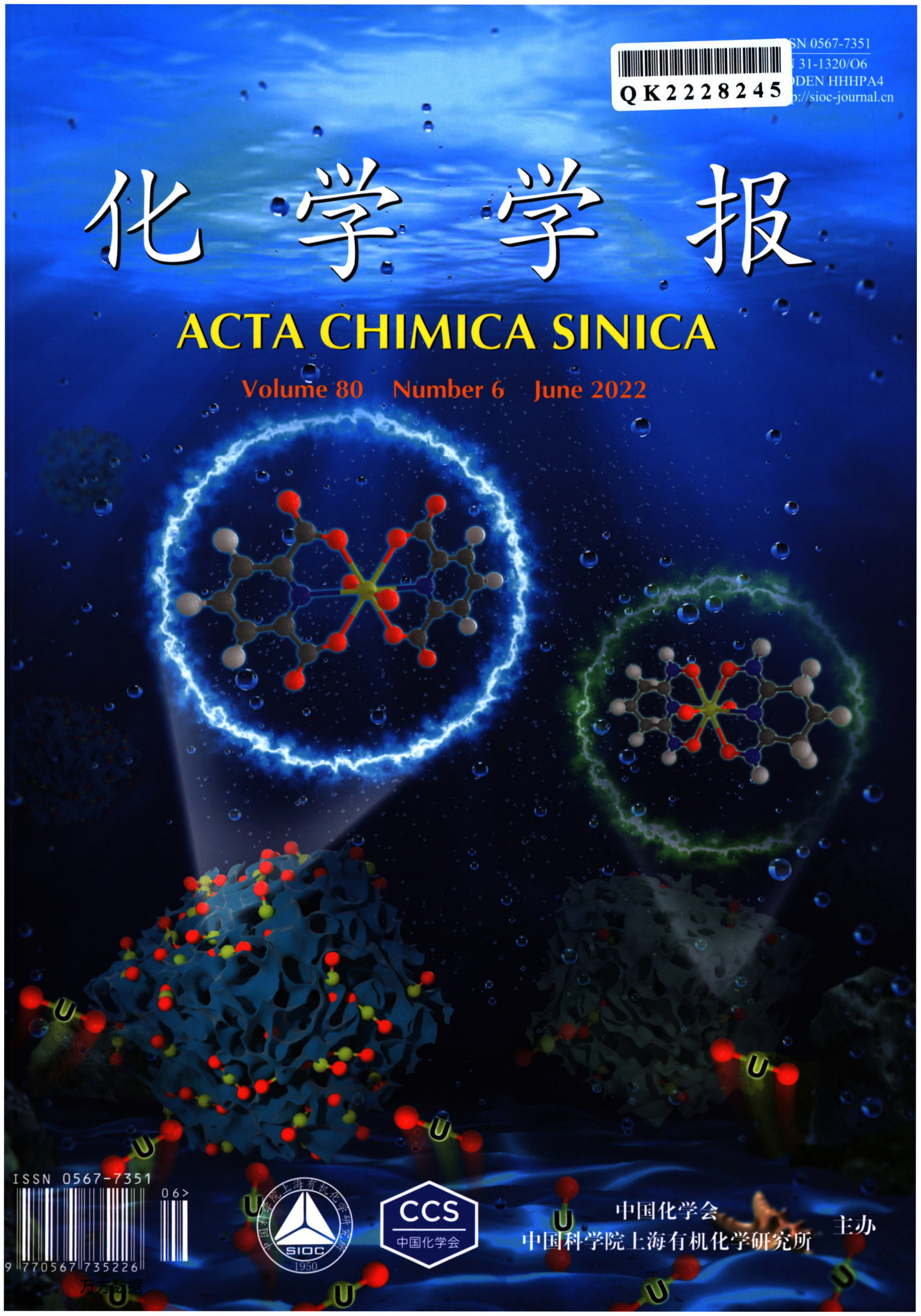
化学学报

ACTA CHIMICA SINICA

Volume 80 Number 6 June 2022



ISSN 0567-7351
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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

化 学 学 报

Acta Chimica Sinica

(Huaxue Xuebao)

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* 通信联系人.

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多孔离子液体的构筑及应用 …… 李晓倩, 张靖, 苏芳芳, 王德超, 姚东东*, 郑亚萍*, 化学学报, **2022**, *80*(6), 848-860

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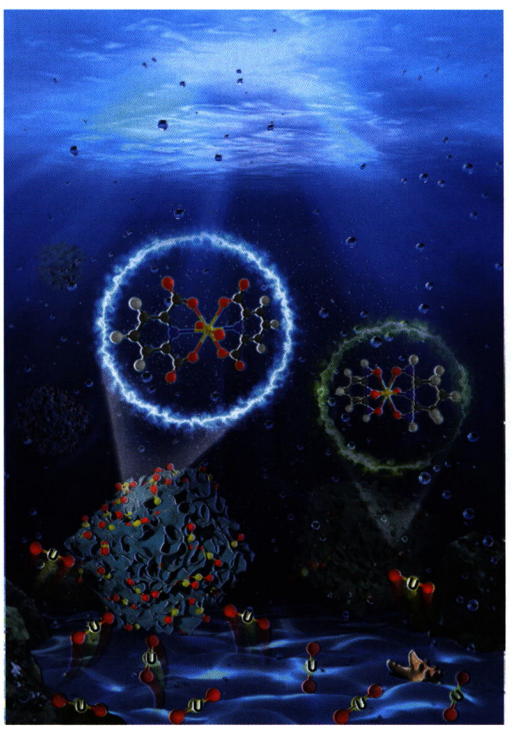
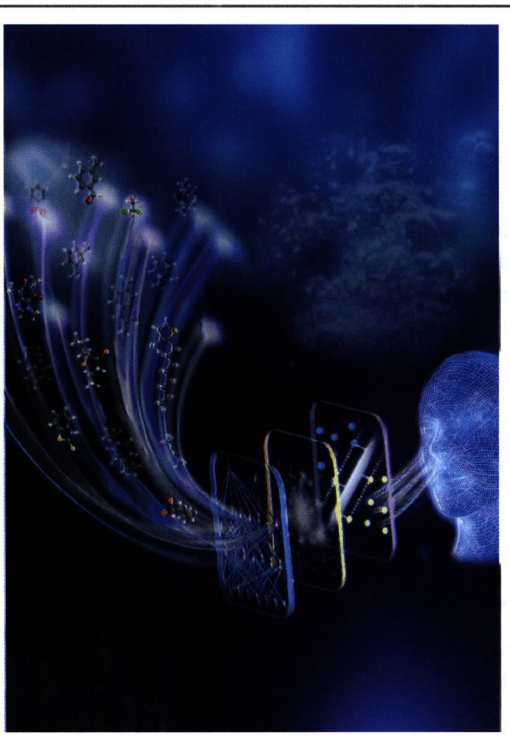


On the cover: In-depth understanding of the complexation behavior of functional groups with uranyl ion is essential for development of high-efficient seawater uranium adsorbents. Density functional theory (DFT) calculations demonstrated that owing to the high proton rearrangement energy and dissociation energy of the glutarimidedioxime group (H_2A), the pyridine-2,6-dicarboxylic acid group (H_2DPA) is more prone to substitution reactions with $[UO_2(CO_3)_3]^{4-}$, and H_2DPA is a potential effective ligand for uranium extraction from seawater. [Shi, Weiqun *et al.* on page 708-713.]



On the back cover: We developed an ensemble machine learning method by integrating three heterogeneous models: ANN (artificial neural networks) based on interpretable descriptors, ANN based on correlated descriptors, and SVM (support vector machines) based on hybrid molecular fingerprints, and realized the boiling point prediction of high accuracy in wide structure space. This multi-component heterogeneous learning model can also be well generalized to the prediction of many physical chemical properties beyond boiling point. [Yu, Xi *et al.* on page 714-723.]

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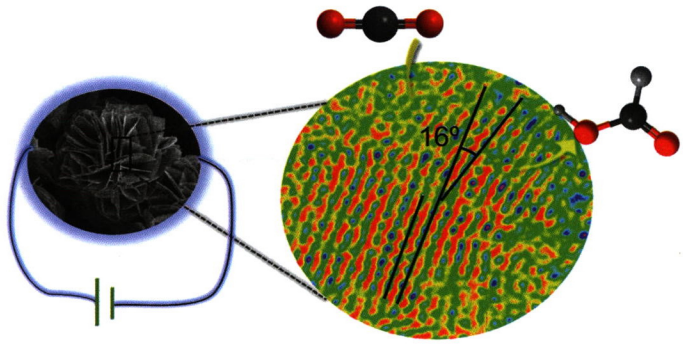
Communication

Porous Bismuth Nanoflowers Enriched with Lattice Dislocations for Highly Efficient Electrocatalytic Reduction of Carbon Dioxide to Formate



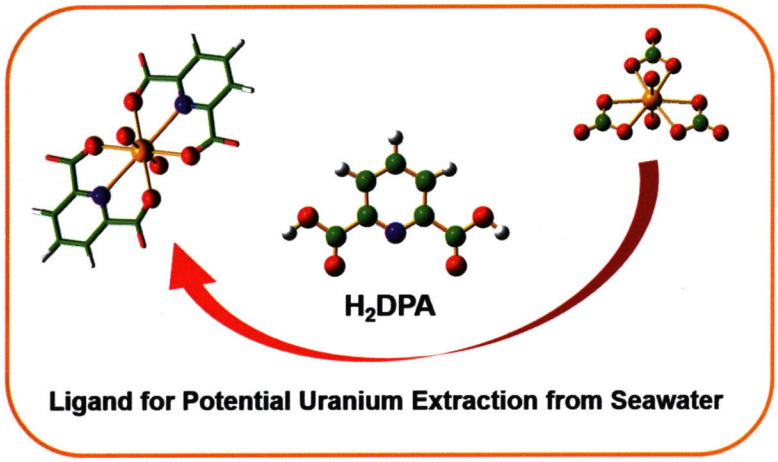
Jiang, Yinlong; Li, Guochao; Chen, Qingsong*; Xu, Zhongning; Lin, Shanshan; Guo, Guocong*

Acta Chim. Sinica **2022**, *80*(6), 703-707

In this paper, the layered bismuth oxide formate nanoflowers synthesized by simple solvothermal method were *in situ* electrochemically reduced to porous bismuth nanoflowers with high intrinsic activity sites such as a large number of lattice dislocations and defects, which exhibit excellent performance towards electrochemical reduction of carbon dioxide to formate.

Article

Theoretical Studies on the Interaction of Uranyl with Carboxylic Acids and Oxime Ligands

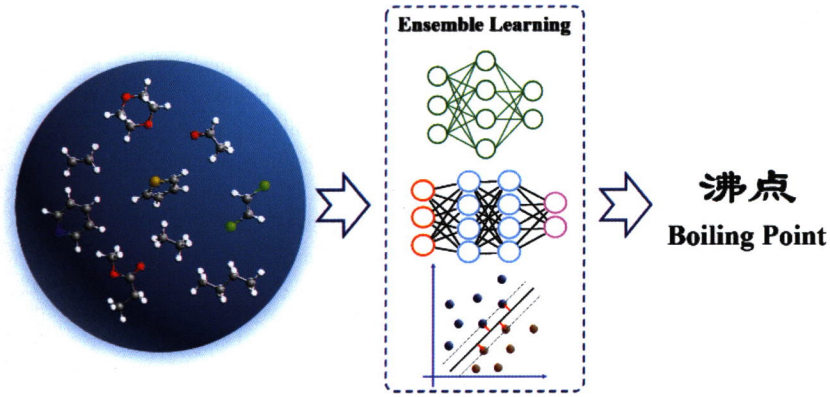


Luan, Xuefei; Wang, Congzhi; Xia, Liangshu*; Shi, Weiqun*

Acta Chim. Sinica **2022**, *80*(6), 708-713

H_2DPA (pyridine-2,6-dicarboxylic acid) ligand is a potential effective ligand for uranium extraction from seawater.

Accurate Prediction of the Boiling Point of Organic Molecules by Multi-Component Heterogeneous Learning Model



Liu, Yuze; Li, Kunhua; Huang, Jiaxing; Yu, Xi*; Hu, Wenping*

Acta Chim. Sinica **2022**, *80*(6), 714-723

An ensemble machine learning model based on three heterogeneous learners exhibited high accuracy in boiling point prediction and good generalization with low overfitting.

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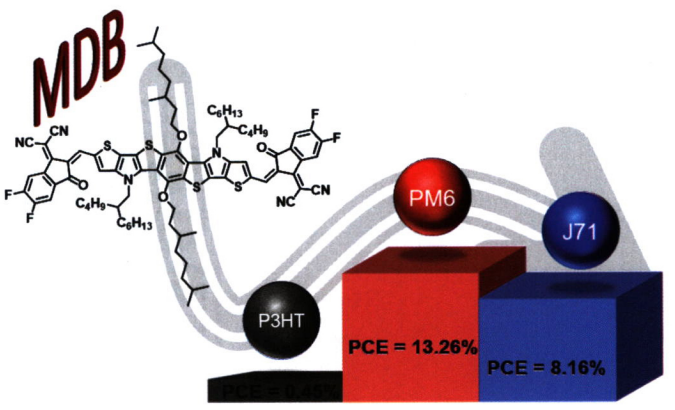
Rationally Tuning Blend Miscibility of Polymer Donor and Nonfullerene Acceptor for Constructing Efficient Organic Solar Cells

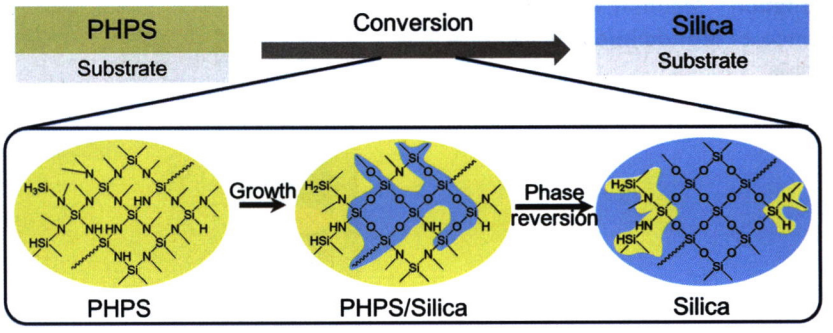


Lin, Wenyuan; Zhu, Qingzhe; Ma, Yunlong*; Wang, Peng; Wan, Shuo; Zheng, Qingdong*

Acta Chim. Sinica **2022**, *80*(6), 724-733

In this work, three wide-bandgap polymer donors (PM6, J71, and P3HT) are used to blend with a newly designed nonfullerene acceptor (MDB), which has a sp^3-hybridized-carbon-free ladder-type skeleton, to fabricate polymer solar cells. Among them, PM6 exhibits the most suitable miscibility and ordered molecular packing with MDB thereby leading to the best efficiency of 13.26%.

Conversion Process of Perhydropolysilazane to Silica

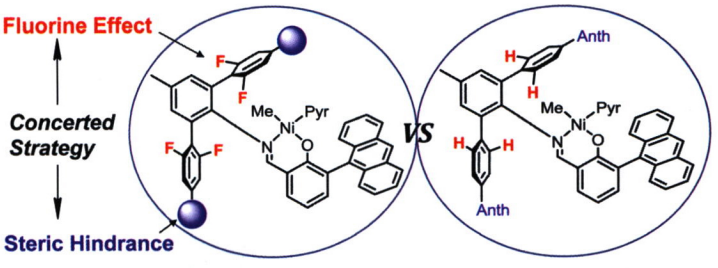


Wang, Dan; Guo, Xiang; Li, Pengfei; Zhang, Yulin; Xu, Caihong; Zhang, Zongbo*

Acta Chim. Sinica **2022**, *80*(6), 734-740

Conversion of perhydropolysilazane (PHPS) to silica via hydrolysis-condensation, and high-temperature oxidation reaction was studied. The PHPS-to-silica conversion undergoes random formation of reaction centers, growth of silica phase, phase reverse between PHPS and silica phase, and finally the formation of continuous silica phase. The volume shrinkage, refractive index, and mechanical properties of the obtained coatings depend on the conversion degree and phases' distribution.

Enhancement on Nickel-Mediated Ethylene Polymerization by Concerted Steric Hindrance and Fluorine Effect



Neutral salicylaldiminato nickel mediated ethylene polymerization

Molecular weight	1124000 g·mol^{-1}	38000 g·mol^{-1}
Catalytic activity	1.5x10^7 g·mol^{-1}·h^{-1}	2.0x10^5 g·mol^{-1}·h^{-1}
Branching density	5 brs/1000C	26 brs/1000C

Wang, Yuyin; Hu, Xiaoqiang; Mu, Hongliang; Xia, Yan*; Chi, Yue*; Jian, Zhongbao*

Acta Chim. Sinica **2022**, *80*(6), 741-747

The concerted strategy of fluorine effect and steric shielding effect enables remarkable enhancement of catalytic activity and polymer molecular weight in neutral and single-component salicylaldiminato nickel promoted ethylene polymerization.

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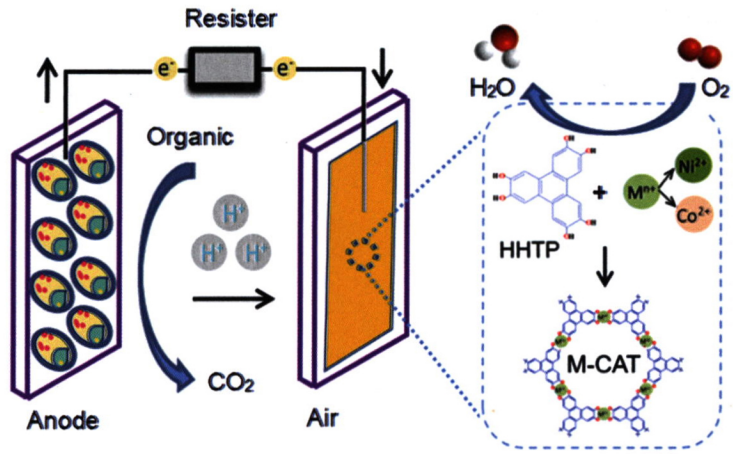
Preparation of Bimetallic Conductive Metal-organic Framework Material Ni/Co-CAT for Electrocatalytic Oxygen Reduction

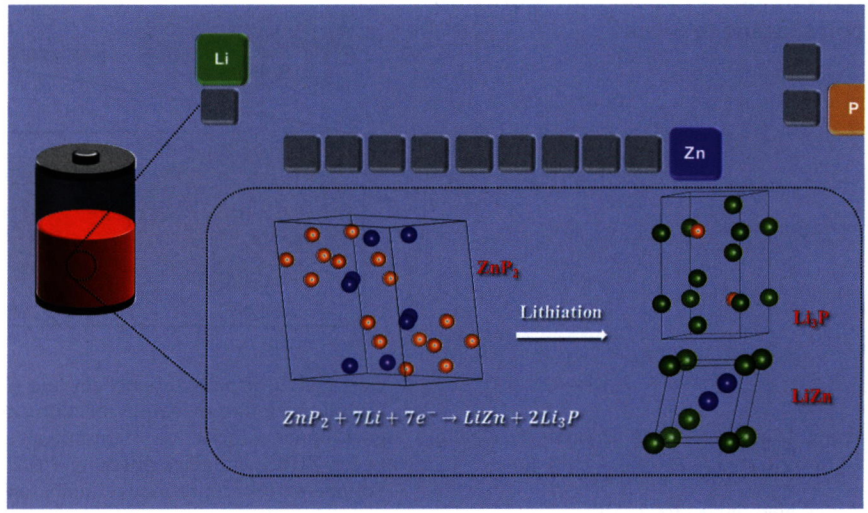


Geng, Yuanhao; Lin, Xiaoqiu; Sun, Yaxin; Li, Huiyu; Qin, Yue; Li, Congju*

Acta Chim. Sinica **2022**, *80*(6), 748-755

Ni-catecholate (Ni-CAT) and Ni-Co-catecholate (Ni-Co-CAT) were prepared by hydrothermal method and applied to microbial fuel cell (MFC) cathode. At the anode, microorganisms decompose organic pollutants into carbon dioxide. At the cathode, oxygen is reduced to water.

Lithiation Mechanism and Performance of Monoclinic ZnP_2 Anode Materials

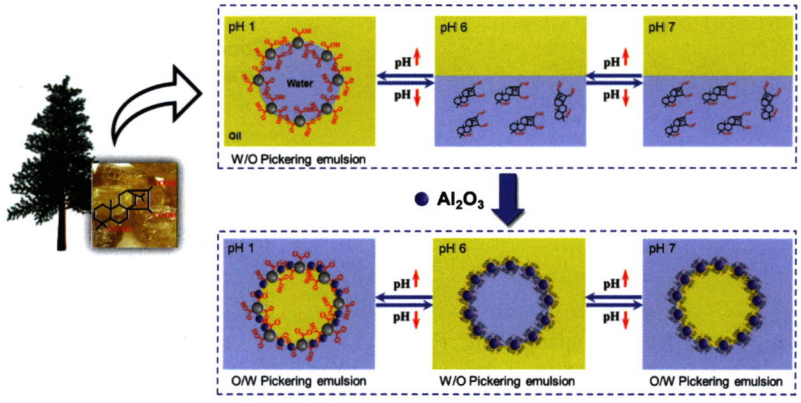


Bi, Wenchao; Zhang, Linfeng; Chen, Jian; Tian, Ruixue; Huang, Hao*; Yao, Man*

Acta Chim. Sinica **2022**, *80*(6), 756-764

The lithiation mechanism and electrochemical properties of ZnP_2, which is a double active transition metal phosphide with high phosphorus ratio, were investigated by first-principles calculations and experimental methods.

pH-Responsive Pickering Emulsions Synergistically Stabilized by Maleopimaric Acid and Alumina Nanoparticles



He, Xufa; Jia, Kangle*; Yu, Longfei*; Liu, Mingjie; Zheng, Xiaoshan; Li, Huanling; Xin, Jinlan; Huang, Linjia*

Acta Chim. Sinica **2022**, *80*(6), 765-771

Al_2O_3 nanoparticles induce phase transition of pH-responsive Pickering emulsions based on maleopimaric acid.

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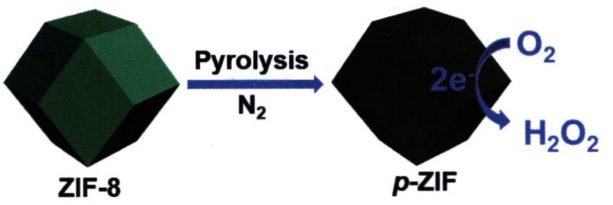
Nitrogen-doped Carbon Pyrolyzed from ZIF-8 for Electrocatalytic Oxygen Reduction to Hydrogen Peroxide

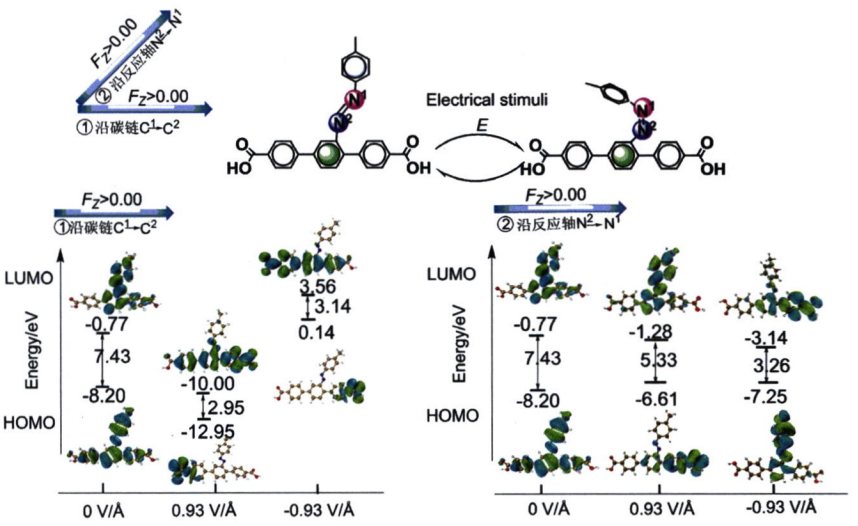


Wang, Dan; Feng, Bo; Zhang, Xiaoxin; Liu, Yanan; Pei, Yan; Qiao, Minghua*; Zong, Baoning*

Acta Chim. Sinica **2022**, *80*(6), 772-780

The pyrolyzed ZIF (*p*-ZIF) catalysts were synthesized by pyrolyzing ZIF-8 at high temperatures, which nicely inherited the regular morphology of ZIF-8. In two-electron oxygen reduction reaction (2e-ORR) in an acidic electrolyte, the *p*-ZIF catalysts displayed low overpotential, low Tafel slope, and high stability. Among them, the *p*-ZIF-950 catalyst displayed the highest H_2O_2 selectivity of 89.2% and constant H_2O_2 production rate of 87 mmol•g_{cat}^{-1}•h^{-1}.

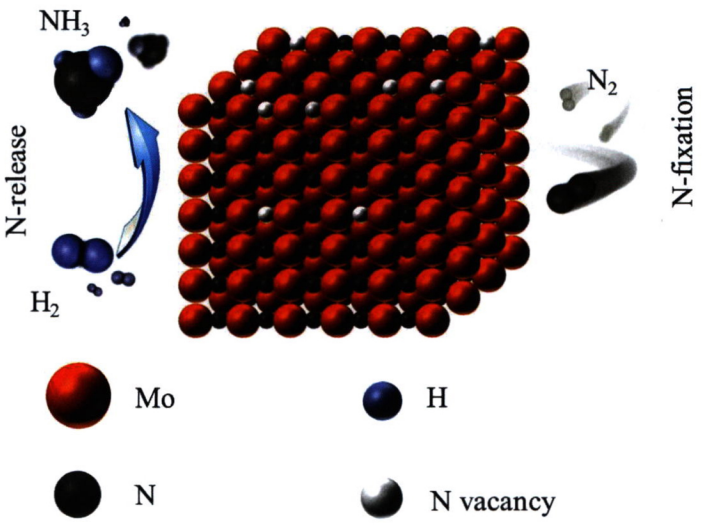
Theoretical Study on the Isomerization Mechanism of Azobenzene Derivatives under Electric Field



Wang, Luocong; Li, Zhewei; Yue, Caiwei; Zhang, Peihuan; Lei, Ming*; Pu, Min*

Acta Chim. Sinica **2022**, *80*(6), 781-787

Chemical Looping Ammonia Synthesis with High Performance Supported Molybdenum-based Nitrogen Carrier



Zhang, Tan; Yu, Zhongliang*; Yu, Jiaqi; Wan, Huining; Bao, Chengyu; Tu, Wenqiang; Yang, Song

Acta Chim. Sinica **2022**, *80*(6), 788-796

The supported molybdenum-based nitrogen carrier can be regarded as a storage medium of activated nitrogen that can be discharged and charged.

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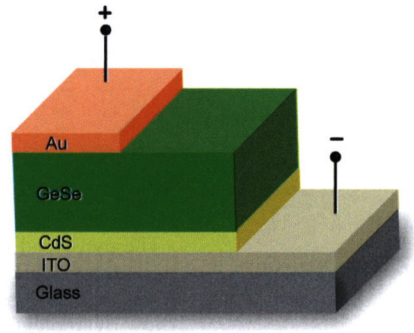
Account

Recent Progress in GeSe Thin-Film Solar Cells



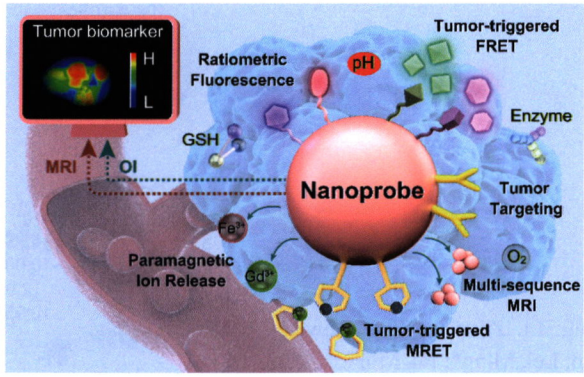
Yan, Bin; Xue, Ding-Jiang*; Hu, Jin-Song

Acta Chim. Sinica **2022**, *80*(6), 797-804

GeSe has recently emerged as a promising photovoltaic absorber material due to its attractive optical and electrical properties as well as earth-abundant and non-toxic constituent elements. The efficiencies of GeSe solar cells have increased from 1.48% in 2017 to a certified 5.2% now. We believe that the efficiency of GeSe thin-film solar cells would be enhanced dramatically by further optimizations.

Review

Nanoprobes for Visualization of Cancer Pathology *in Vivo*

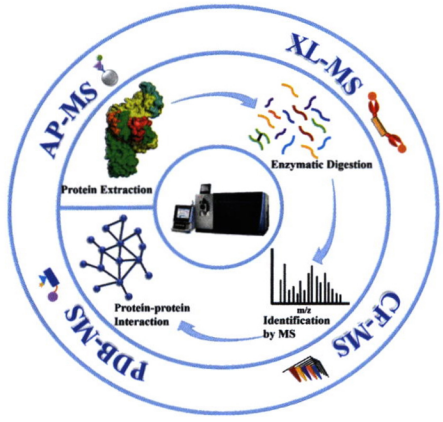


Zhang, Peisen*; Jing, Lihong*

Acta Chim. Sinica **2022**, *80*(6), 805-816

It is necessary to achieve precise diagnosis of tumor at the molecular pathology level. In this review, the development of nanoprobe-based molecular imaging and the *in vivo* visualization of tumor molecular pathology are summarized. The construction of the pathology responsive nanoprobes is highlighted. The challenges and perspectives on the future steps needed to implement this nanotechnology are also discussed.

Research Progress of Protein-Protein Interaction Based on Liquid Chromatography Mass Spectrometry



Chen, Yuwan; Zhou, Wen; Li, Xinwei; Yang, Kaiguang*; Liang, Zhen; Zhang, Lihua*; Zhang, Yukui

Acta Chim. Sinica **2022**, *80*(6), 817-826

Liquid chromatography-mass spectrometry (LC-MS) based methods for studying protein-protein interactions, including affinity purification mass spectrometry (AP-MS), proximity-dependent biotinylation coupled to mass spectrometry (PDB-MS), chemical cross-linking with mass spectrometry (XL-MS) and co-fractionation mass spectrometry (CF-MS) are introduced. This review discusses the mechanism, advantages and applications of these methods for the identification towards the protein-protein interactions in cells.

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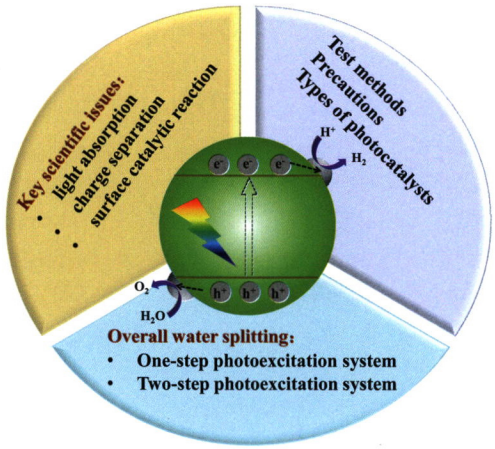
Photocatalytic Water Splitting for Hydrogen Production

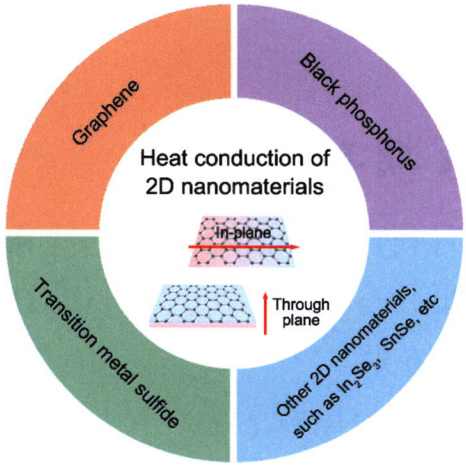


Qi, Yu; Zhang, Fuxiang*

Acta Chim. Sinica **2022**, *80*(6), 827-838

This paper introduces the basic concepts, activity test methods and precautions, types of photocatalytic materials, and summaries the important research progresses from the perspectives of light absorption, photo-generated charge separation and surface catalytic reaction of photocatalytic water splitting for hydrogen production.

Heat Conduction Behavior of Two-Dimensional Nanomaterials and Their Interface Regulation

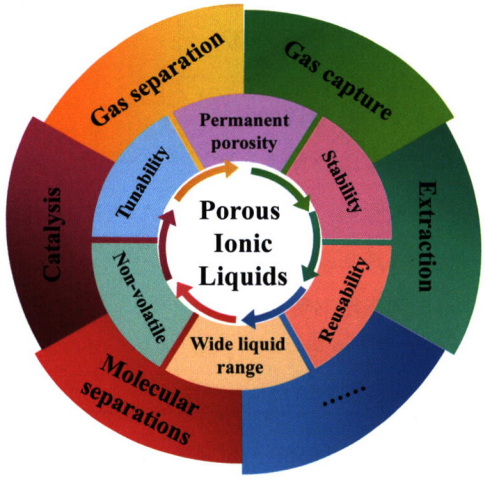


Yuan, Ruilin; Chen, Long; Wu, Changzheng*

Acta Chim. Sinica **2022**, *80*(6), 839-847

This paper is aimed to introduce the heat conduction properties of classical two-dimensional (2D) nanomaterials, such as graphene, black phosphorus, transition metal sulfide, *etc*. Then, we elucidated the effect of interfacial interactions on the thermal conductivity and further expected the prospects of atomic-molecular interface regulation in the field of heat conduction.

Construction and Application of Porous Ionic Liquids



Li, Xiaoqian; Zhang, Jing; Su, Fangfang; Wang, Dechao; Yao, Dongdong*; Zheng, Yaping*

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