

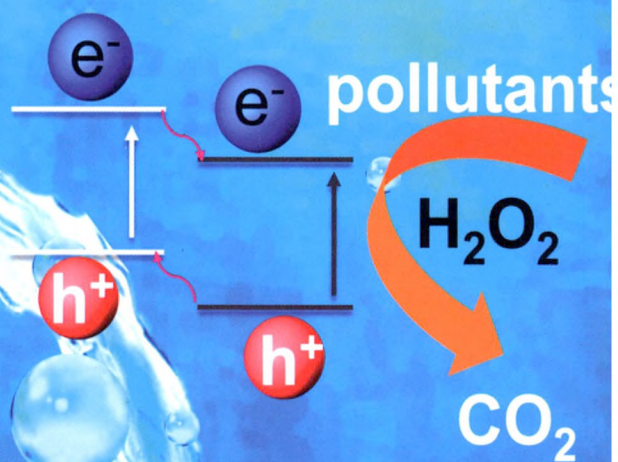
ISSN 0567-7351
CN 31-1320/O6
CODEN HHHPA4
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化学学报

ACTA CHIMICA SINICA

Volume 78 Number 9 September 2020



ISSN 0567-7351

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770567735202
万方数据

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)

第 78 卷 第 9 期 2020 年 9 月 15 日

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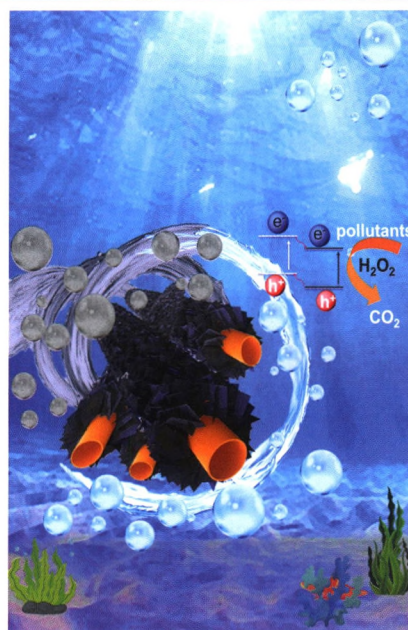
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无序随机多肽组分相关的结构转变的蒙特卡洛模拟: 以赖氨酸、谷氨酸和异亮氨酸组成的随机多肽为例 张鹏程, 郭佳, 朱根, 方文玉, 唐乾元*, 鲍磊*, 康文斌*, 化学学报, 2020, 78(9), 994-1000
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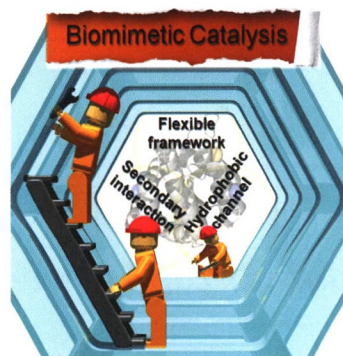
* 通信联系人.

On the cover: The multi-layer structure of CuS@MoS₂ core-shell nanotubes not only improves the utilization of light, but also promotes the rapid transfer of photogenerated electrons. On this basis, in the presence of hydrogen peroxide, CuS@MoS₂ exhibits excellent pollutant degradation ability in photocatalysis and Fenton-like reaction systems, which may offer a new way for the treatment of water pollution. [Li, Hexing *et al.* on page 961-967.]



Account

Exploration of Porous Organic Polymers as a Platform for Biomimetic Catalysis

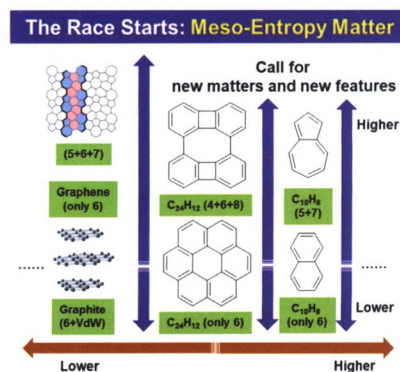


Sun, Qi; Xiao, Feng-Shou*

Acta Chim. Sinica **2020**, 78(9), 827-832

Based on the concepts of secondary interaction modification, flexible framework design, and wettability control commonly adopted in nature, numerous efficient catalytic systems have been developed using porous organic polymers as a designer platform.

Carbon-Enriched meso-Entropy Materials: from Theory to Cases



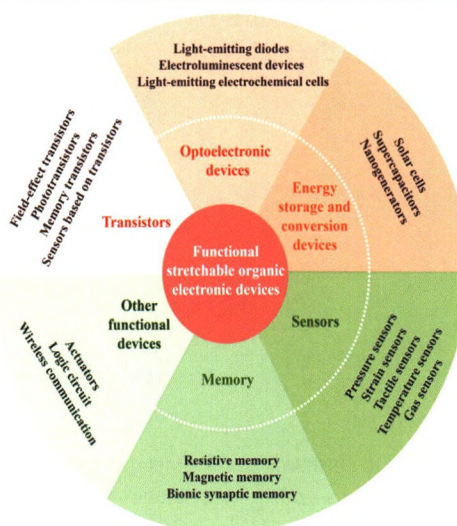
Feng, Boxu; Zhuang, Xiaodong*

Acta Chim. Sinica **2020**, 78(9), 833-847

Meso-entropy concept defined relationship for carbon-enriched materials is proposed for fundamental understanding and development of new carbon-enriched materials.

Review

Research Progress in Functional Stretchable Organic Electronic Devices

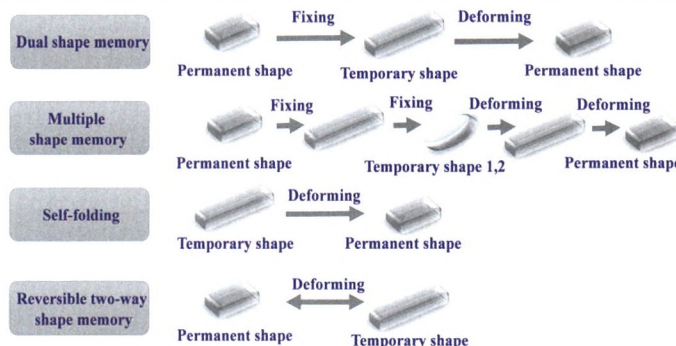


Bian, Yangshuang; Liu, Kai; Guo, Yunlong*; Liu, Yunqi

Acta Chim. Sinica 2020, 78(9), 848-864

Research advances in functional stretchable organic electronic devices are discussed, including transistors, optoelectronic devices, energy storage and conversion devices, sensors, memory and other functional electronic devices.

Research Progress of Shape Memory Polymer Deformation Mode

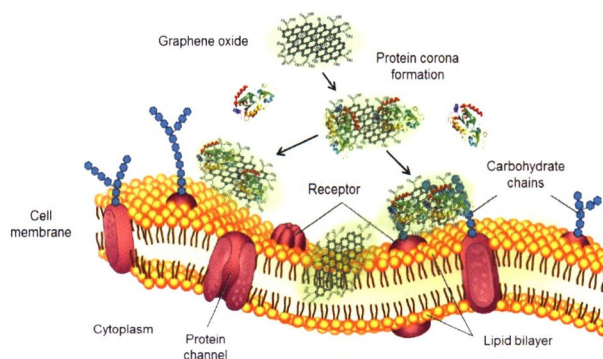


Zhang, Lan; Ma, Suqian; Wang, Hanbing; Liang, Yunhong*; Zhang, Zhihui

Acta Chim. Sinica 2020, 78(9), 865-876

Shape memory polymers are the most widely studied smart deformable materials at present. In this paper, the deformation modes of shape memory polymers are divided into four categories, including the dual shape memory, the multiple shape memory, the self-folding, and the reversible two-way shape memory. In this review, the different deformation modes of shape memory polymers and the progress of their related applications, as well as the challenges faced by different deformation modes and their potential research directions are discussed.

Surface Chemical Modifications of Graphene Oxide and Interaction Mechanisms at the Nano-Bio Interface



Ma, Minghao; Xu, Ming*; Liu, Sijin

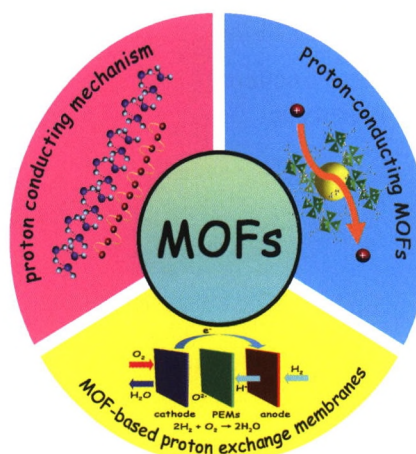
Acta Chim. Sinica 2020, 78(9), 877-887

As a two-dimensional nanomaterial, graphene oxide (GO) has been widely applied in material chemistry, biomedical science and life science, but how to maximize the advantages of GO and overcome the deleterious effects caused by its inherent physico-chemical properties remains to be answered. To update the latest knowledge of surface chemical modifications of GO, the recent progress in this aspect and potential biological effects of surface-modified GO, as well as interaction mechanisms at the nano-bio interface is reviewed. Furthermore, the knowledge gaps and challenges in this research field are detailedly discussed.

Recent Progress on Proton-Conductive Metal-Organic Frameworks and Their Proton Exchange Membranes

Sun, Lian; Wang, Honglei; Yu, Jinshan; Zhou, Xingui*

Acta Chim. Sinica 2020, 78(9), 888-900

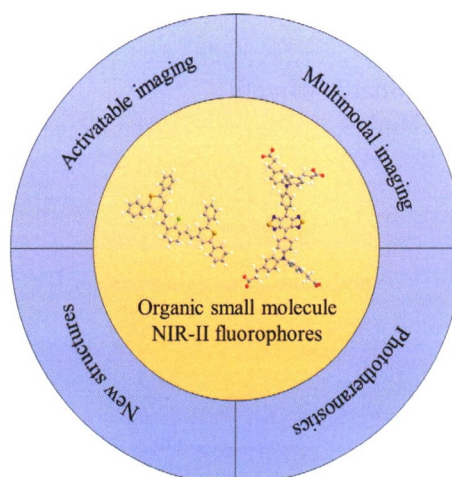


Metal organic frameworks (MOF) are attractive candidates for proton exchange membranes due to their high porosity, crystallinity and designability. This review focuses on the recent progress on proton-conductive MOF structures and their proton exchange membranes.

Near-Infrared-II Fluorescence Probes Based on Organic Small Molecules

Sang, Ruoyu; Xu, Xingpeng; Wang, Qi*; Fan, Quli*; Huang, Wei

Acta Chim. Sinica 2020, 78(9), 901-915

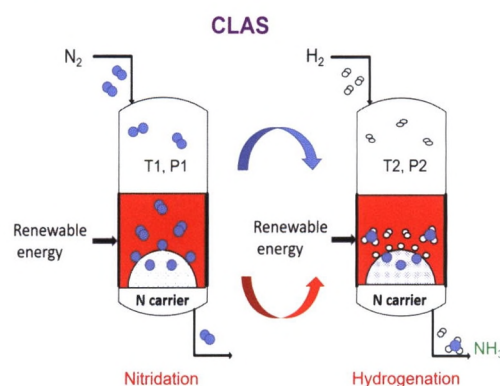


Fluorescence imaging in the near-infrared II (NIR-II) region has been gaining prominence because it can provide higher imaging quality, macroscopic ultra-sensitivity, as well as higher penetration depth compared with fluorescence imaging in the NIR-I region.

Advances in the Chemical Looping Ammonia Synthesis

Feng, Sheng; Gao, Wenbo; Cao, Hujun; Guo, Jianping*; Chen, Ping

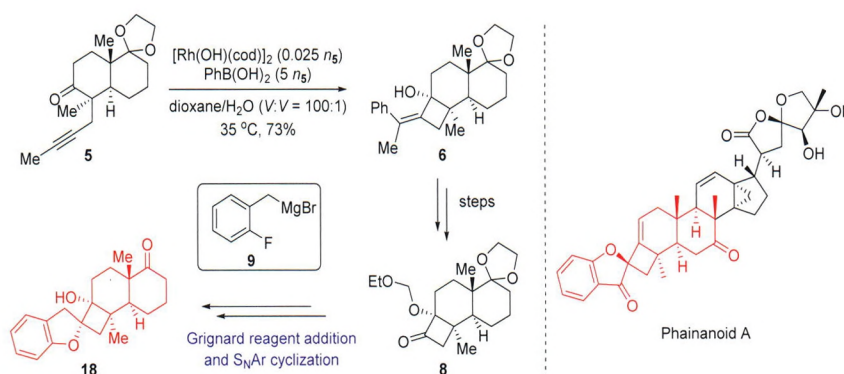
Acta Chim. Sinica 2020, 78(9), 916-927



The recent progress in chemical looping ammonia synthesis driven by renewable energy is reviewed, with the focuses on the materials development and optimization of nitrogen carriers.

Communication

Synthetic Study Toward the 4,5-Spirocycle Skeleton of Phainanoids



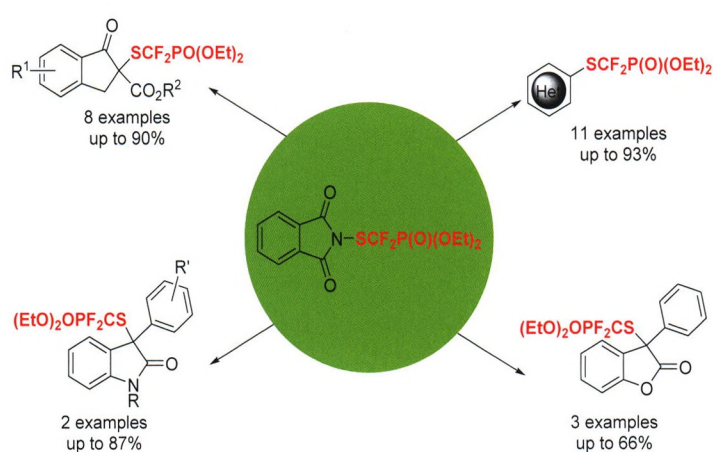
Jiang, Chongguo; Chen, Sijia; Gong, Jianxian*; Yang, Zhen*

Acta Chim. Sinica 2020, 78(9), 928-932

Attempts to synthesize 4,5-spirocycle skeleton of Phainanoids through rhodium-catalyzed arylation, Grignard reagent addition and intramolecular $\text{S}_{\text{N}}\text{Ar}$ cyclization is described.

Article

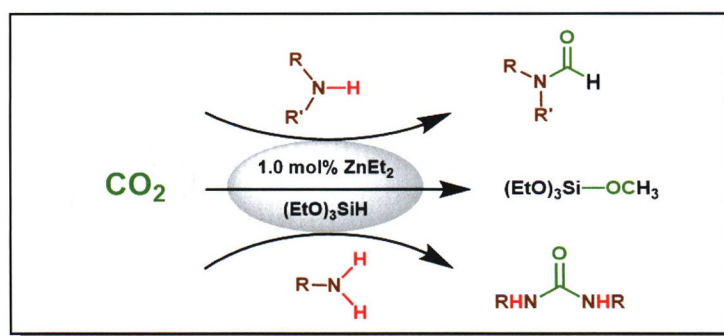
N-[(Diethoxyphosphoryl)difluoromethylthio]phthalimide: A New Electrophilic Fluoroalkylthiolating Reagent



Shen, Feng; Lu, Long*; Shen, Qilong*

Acta Chim. Sinica 2020, 78(9), 933-937

A shelf-stable reagent for the preparation of fluoroalkylthiolated compounds, [(diethylphosphonate)difluoromethylthio]phthalimide **1**, was successfully developed, which could react with electron-rich heteroarenes, β -ketoesters, oxindoles and benzofuranones respectively in high yield.

ZnEt₂ Promoted Hydrosilylation of CO₂ and Formylation or Ureolation of Amines with CO₂ as a C1 Building Block

Du, Chongyang; Chen, Yaofeng*

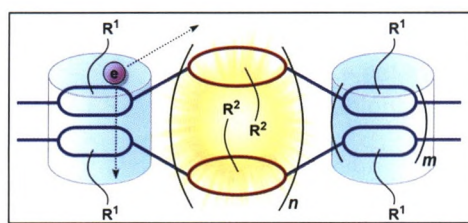
Acta Chim. Sinica 2020, 78(9), 938-944

In the presence of 1.0 mol% ZnEt_2 , hydrosilylation of CO_2 with $(\text{EtO})_3\text{SiH}$ occurs to give methoxysilane ($\text{CH}_3\text{OSi}(\text{OEt})_3$) in high yield. When organic amine is added to the above reaction system, formamide or urea derivative is generated. The secondary amine provides the formamide while the primary amine affords the urea derivative.

Synthesis and Property Study of Field-effect Emissive Conjugated Polymers Based on Styrene and Benzothiadiazole

Liu, Qingqing; Zhang, Yihan; Gao, Can; Wang, Tianyu; Hu, Wenping; Dong, Huanli*

Acta Chim. Sinica 2020, 78(9), 945-953

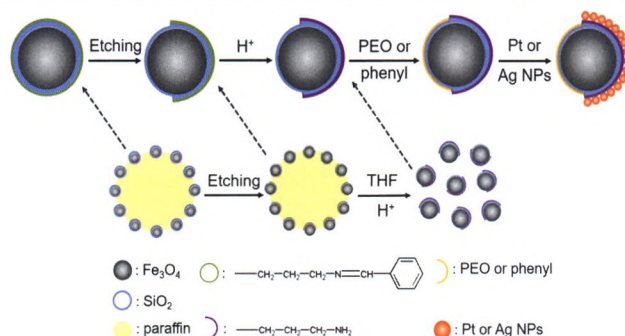


In this work, we synthesized two new conjugated polymers, PVBT and nPVBT based on copolymerized emitting unit of styrene and electron withdrawing unit of benzothiadiazole where styrene is used for modulating the emission characteristics and BTz used for tuning charge transport property to achieve integrated optoelectronic performances. Results demonstrate that both of PVBT and nPVBT are field-effect emissive conjugated polymers with maximum luminous wavelength at 590~605 nm and high photoluminescence quantum yields of 23%~35% in dichloromethane solution ($1 \times 10^{-5} \text{ mol} \cdot \text{L}^{-1}$), and 12%~20% in solid films. This work provides valuable guideline for developing high mobility emissive conjugated polymers towards solution-processed optoelectronic device applications.

Multifunctional $\text{Fe}_3\text{O}_4@/\text{SiO}_2$ Janus Particles

Zhao, Ruotong; Han, Tianhao; Sun, Dayin; Shan, Dan; Liu, Zhengping*; Liang, Fuxin*

Acta Chim. Sinica 2020, 78(9), 954-960

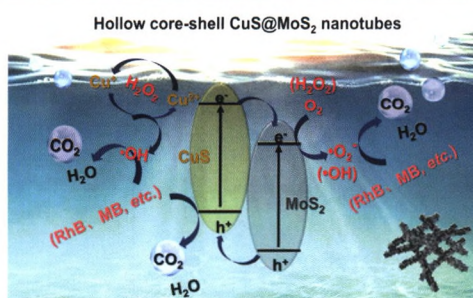


The Janus particles as a solid emulsifier were emulsified in paraffin/water to obtain an oil-in-water Pickering emulsion. The particles were etched in ammonium fluoride aqueous solution. Via the *in situ* growth of metal Pt or Ag nanoparticles, $\text{Fe}_3\text{O}_4@/\text{SiO}_2$ -Pt or $\text{Fe}_3\text{O}_4@/\text{SiO}_2$ -Ag Janus particles were obtained.

Microwave-induced Assembly of $\text{CuS}@/\text{MoS}_2$ Core-shell Nanotubes and Study on Their Photocatalytic Fenton-like Reactions

Zhao, Jingjing; Zhang, Zhengzhong; Chen, Xiaolang; Wang, Bei; Deng, Jinyuan; Zhang, Dieqing*; Li, Hexing*

Acta Chim. Sinica 2020, 78(9), 961-967

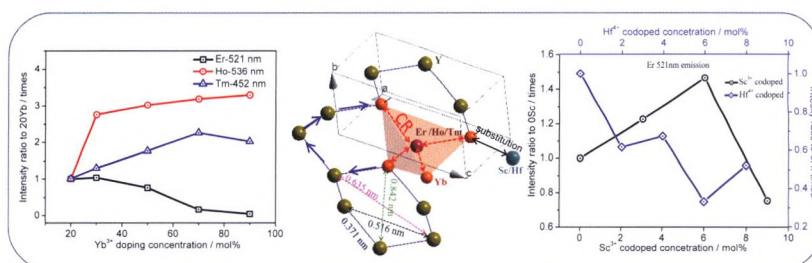


Under the synergistic of photocatalysis and Fenton-like reaction, large amounts of $\cdot\text{OH}$ and $\cdot\text{O}_2^-$ are produced to degrade pollutants together.

Study on the Upconversion Luminescence Mechanism of Tetragonal $\text{LiYF}_4:\text{RE}$ with Sublattice Energy Cluster Construction and Crystal Field Manipulation

Huang, Qingming*

Acta Chim. Sinica 2020, 78(9), 968-979

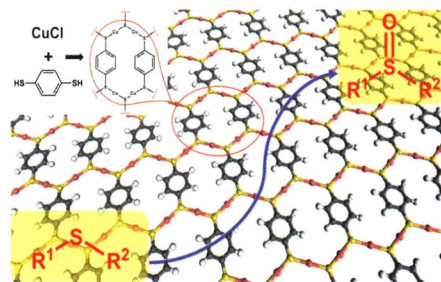


Tetragonal LiYF_4 shows hexagonal sublattice structure of Y^{3+} ions, different sublattice energy clusters of $1\text{Er}-2\text{Yb}$, $1\text{Ho}-2\text{Yb}$ and $1\text{Tm}-4\text{Yb}$ can be constructed, and crystal field asymmetry were successfully manipulated by Sc^{3+} or Hf^{4+} doping. The upconversion luminescence influence mechanism of the construction of sublattice energy clusters and crystal field manipulation with Sc^{3+} or Hf^{4+} as dopant were revealed.

Synthesis of Two-dimensional Hydrophobic Copper-based Nanosheets and Their Application in Catalytic Oxidation of Sulfides

Yang, Zhongjie; Zhang, Xiaofei; Shi, Yanan; Long, Chang; Zhang, Binhao; Yan, Shuhao; Chang, Lin; Tang, Zhiyong*

Acta Chim. Sinica **2020**, 78(9), 980-988

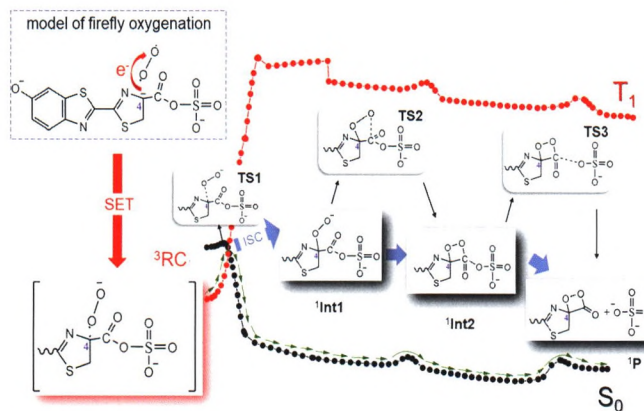


Two-dimensional hydrophobic copper-based nanosheets were constructed by using monovalent copper ion as the metal precursor and 1,4-benzenedithiol as organic ligand, which exhibited high catalytic performance for oxidation of sulfides.

Mechanistic Study of Oxygenation Reaction in Firefly Bioluminescence

Yu, Mohan; Cheng, Yuanyuan; Liu, Yajun*

Acta Chim. Sinica **2020**, 78(9), 989-993

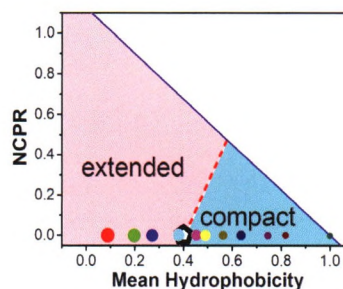


The single electron transfer (SET) oxygenation mechanism of firefly bioluminescence is studied by M06-2X method in dimethyl sulfoxide (DMSO) solvent model.

Monte Carlo Simulations of Composition-Related Structural Transition of Disordered Peptides: The Case Study of Random Peptides Composed of Lysine, Glutamic Acids and Isoleucine

Zhang, Pengcheng; Guo, Jia; Zhu, Gen; Fang, Wenyu; Tang, Qianyan*; Bao, Lei*; Kang, Wenbin*

Acta Chim. Sinica **2020**, 78(9), 994-1000

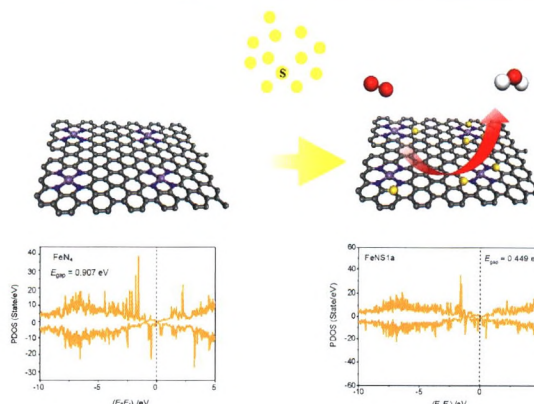


With the ABSINTH (self-Assembly of Biomolecules Studied by an Implicit, Novel, and Tunable Hamiltonian) implicit solvation model, our all-atom Markov Chain Monte Carlo simulations clearly show a transition between the extended conformations to compact structures for each peptide.

Investigation on Oxygen Reduction Reaction Mechanism on S Doped Fe-NC Isolated Single Atoms Catalyst

Lu, Xiaoqing*; Cao, Shoufu; Wei, Xiaofei; Li, Shaoren; Wei, Shuxian*

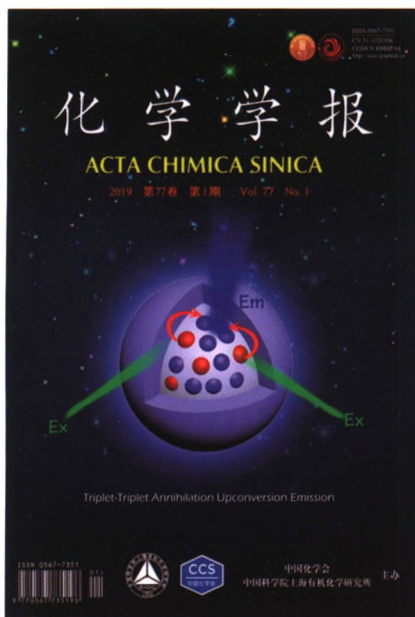
Acta Chim. Sinica **2020**, 78(9), 1001-1006



The doping of sulfur atoms on FeN₄ catalysts would reduce the band gap of the catalyst, thus improves the conductivity of the catalyst, which is beneficial to electrocatalytic oxygen reduction reactions.

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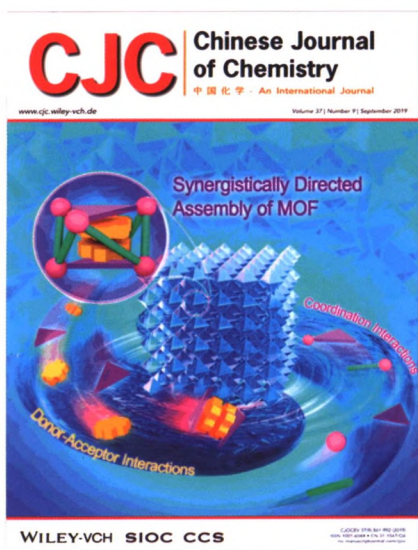
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- 1983年创刊(原名*Acta Chimica Sinica English Edition*)
- 与Wiley-VCH合作出版
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