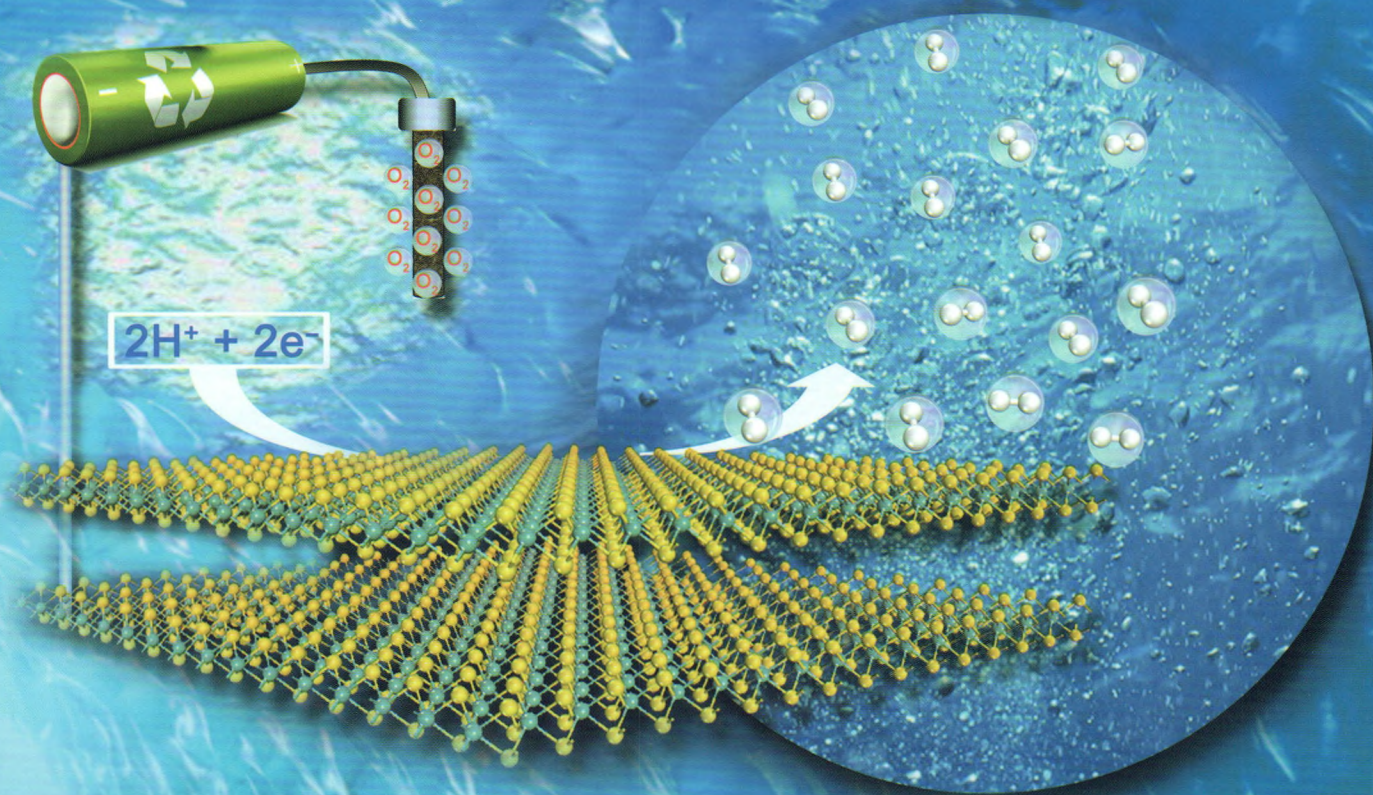


物理化学学报

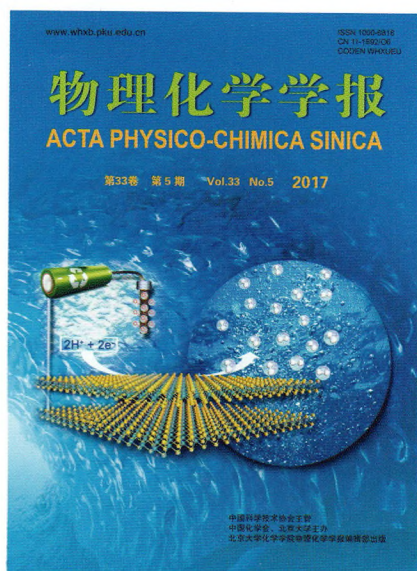
ACTA PHYSICO-CHIMICA SINICA

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中国科学技术协会主管
中国化学会、北京大学主办
北京大学化学学院物理化学学报编辑部出版

COVER



The cover image presents the schematic diagram of hydrogen production from water electrolysis. On page 869, LING and WANG review several two-dimensional materials, including MoS_2 , MXenes and boron monolayer, for electrocatalytic hydrogen evolution reactions, the strategies of performance improvement and the structure – catalytic activity relationship are mainly emphasized, the challenges and prospective for future development of electrocatalysts for hydrogen evolution are also summarized.

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- 自下而上法制备硫掺杂石墨烯薄膜应用于微型超级电容器(Bottom-Up Fabrication of Sulfur-Doped Graphene Films for Micro-Supercapacitors) 刘忠范(LIU Zhong-Fan)(853)
- 多孔三维寡层类石墨烯: 超高功率超级电容器碳材料(Porous 3D Few-Layer Graphene-Like Carbon for Ultrahigh-Power Supercapacitors) 刘忠范(LIU Zhong-Fan)(855)
- MOFs限域Cu/ZnO_x超小纳米粒子催化CO₂选择加氢制甲醇(Catalytic Hydrogenation of CO₂ to Methanol via MOF-Confined Ultrasmall Cu/ZnO_x Nanoparticles) 王 野(WANG Ye)(857)
- 低结晶性羟基氧化铁纳米颗粒: 电化学性能优异的超级电容器负极材料(Low-Crystalline Iron Oxide Hydroxide Nanoparticles: High-Performance Anode for Supercapacitors) 庄 林(ZHUANG Lin)(859)
- 高效CO₂还原至CO催化剂: 核/壳结构Cu/SnO₂纳米粒子(High-Efficient Electrocatalysts for CO₂ Reduction to CO: Core/Shell Cu/SnO₂ Nanoparticles) 庄 林(ZHUANG Lin)(861)
- 提升二氧化碳光催化转化选择性的催化位点晶格工程策略(Lattice Engineering on Catalytic Sites for Achieving Highly Selective Photocatalytic CO₂ Conversion) 张铁锐(ZHANG Tie-Rui)(863)
- 耐高温赤铁矿($\alpha\text{-Fe}_2\text{O}_3$)型氧化铁纳米管阵列的可控制备(Controllable Fabrication of High-Temperature Resistant $\alpha\text{-Fe}_2\text{O}_3$ Nanotube Arrays) 韩布兴(HAN Bu-Xing)(865)
- 化学战剂降解的双功能高效催化剂——双阴离子多金属氧簇(A Polyoxoniobate-Polyoxovanadate Double-Anion Catalyst for Simultaneous Oxidative and Hydrolytic Decontamination of Chemical Warfare Agent Simulants) 吴 凯(WU Kai)(867)

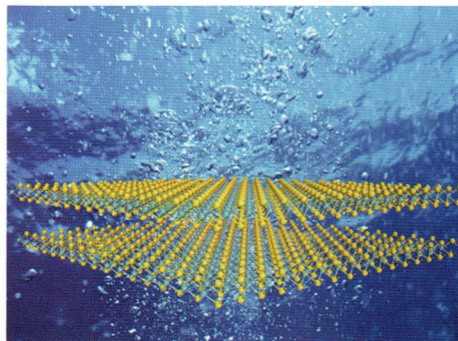
基于类石墨烯二维材料的析氢反应电催化剂的研究进展

凌崇益 王金兰

Recent Advances in Electrocatalysts for the Hydrogen Evolution Reaction Based on Graphene-Like Two-Dimensional Materials

LING Chong-Yi WANG Jin-Lan

Acta Phys. -Chim. Sin. **2017**, 33 (5), 869–885



We highlight research efforts towards developing electrocatalysts for the hydrogen evolution reaction in this review based on 2D materials including transition metal disulfides, MXenes, and boron monolayers, and we summarize the challenges and perspectives for the future development of electrocatalysts for the HER.

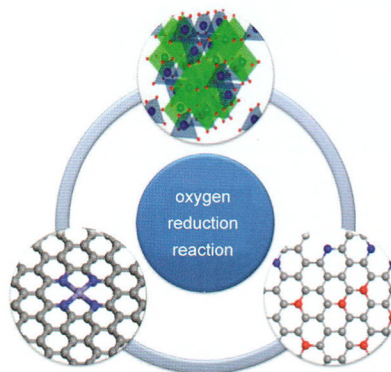
非贵金属氧还原催化剂的研究进展

王 俊 魏子栋

Recent Progress in Non-Precious Metal Catalyst for Oxygen Reduction Reaction

WANG Jun WEI Zi-Dong

Acta Phys. -Chim. Sin. **2017**, 33 (5), 886–902



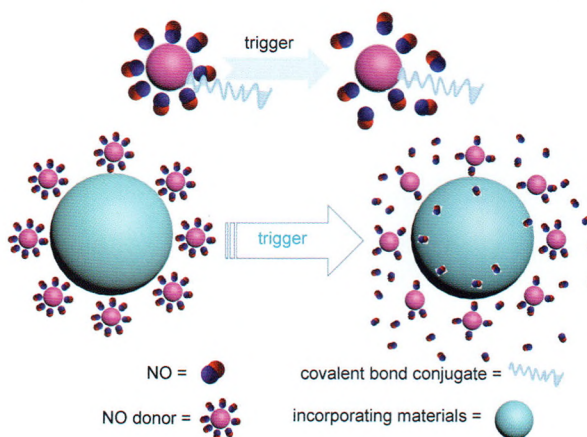
This review summarizes the recent development of non-precious metal catalysts for oxygen reduction reaction and highlights the existing problems in different kinds of catalysts, then further providing corresponding research directions.

可释放一氧化氮纳米材料的研究进展

向慧静 刘劲刚 赵彦利

Recent Research Advancements in NO-Releasing Nanomaterials

XIANG Hui-Jing LIU Jin-Gang
ZHAO Yanli

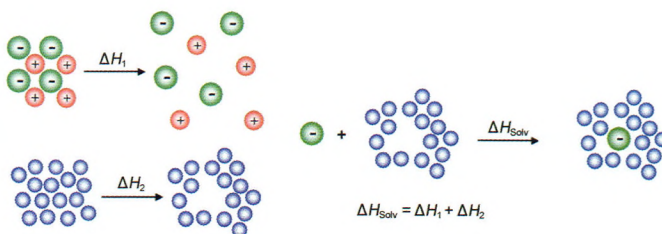


This review describes recent major research advances in the integration of nitric oxide with various nanoplatforms for the controlled delivery of nitric oxide.

Acta Phys. -Chim. Sin. **2017**, 33 (5), 903–917

Developing a Support Vector Machine Based QSPR Model to Predict Gas-to-Benzene Solvation Enthalpy of Organic Compounds

GOLMOHAMMADI Hassan
DASHTBOZORGI Zahra
KHOOSHECHIN Sajad

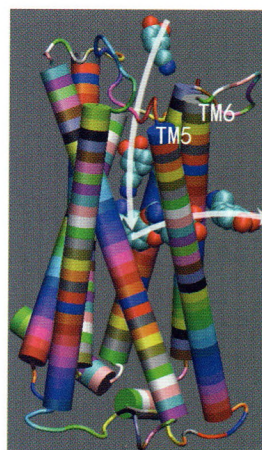


In this paper, quantitative structure – property relationship QSPR models were developed for predicting the gas-to-benzene solvation enthalpy ΔH_{Solv} of organic compounds based on molecular descriptors.

Acta Phys. -Chim. Sin. **2017**, 33 (5), 918–926

多巴胺在其第三受体蛋白结构中的分子通道上传输动力学

李爱静 谢 炜 王 明 徐四川



Molecular Dynamics of Dopamine to Transmit through Molecular Channels within D₃R

LI Ai-Jing XIE Wei
WANG Ming XU Si-Chuan

We have studied the molecular channels for the transmission of dopamine from the intercellular spaces to inside the space region of D₃R to act as a neurotransmitter, followed by escape from the internal structure to maintain a normal physiological balance of dopamine.

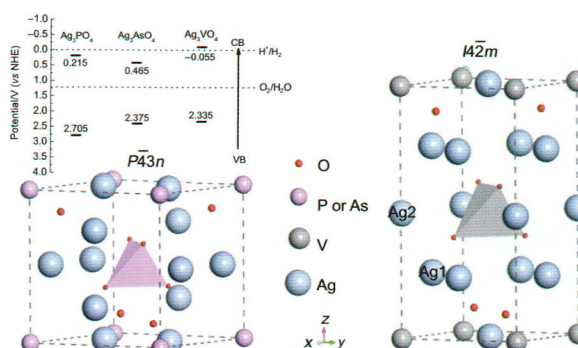
Acta Phys. -Chim. Sin. **2017**, 33 (5), 927–940

Ag₃XO₄ (X = P, As, V)电子结构及光催化性质的第一性原理计算

李 蛟 陈 忠

First-Principles Study on the Electronic and Photocatalytic Properties of Ag₃XO₄ (X = P, As, V)

LI Jiao CHEN Zhong



Electronic structures and photocatalytic properties of Ag₃XO₄ (X = P, As, V) are investigated using the first principles based on the density functional theory.

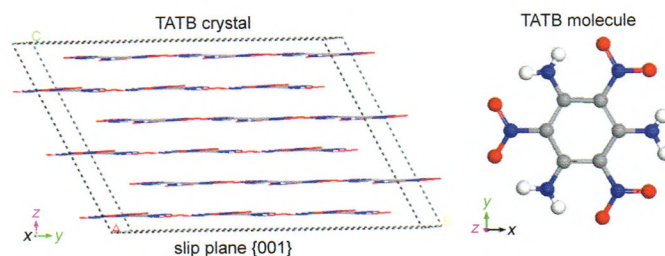
Acta Phys. -Chim. Sin. **2017**, 33 (5), 941–948

冲击载荷下 TATB 晶体滑移和各向异性的分子动力学研究

周婷婷 宋华杰 黄风雷

The Slip and Anisotropy of TATB Crystal under Shock Loading via Molecular Dynamics Simulation

ZHOU Ting-Ting SONG Hua-Jie
HUANG Feng-Lei



For TATB, the slip systems that are likely to be activated are on the {001} plane under shock loading along various orientations, which is consistent with the layered structure of TATB crystal along the c axis and the planar structure of TATB molecule.

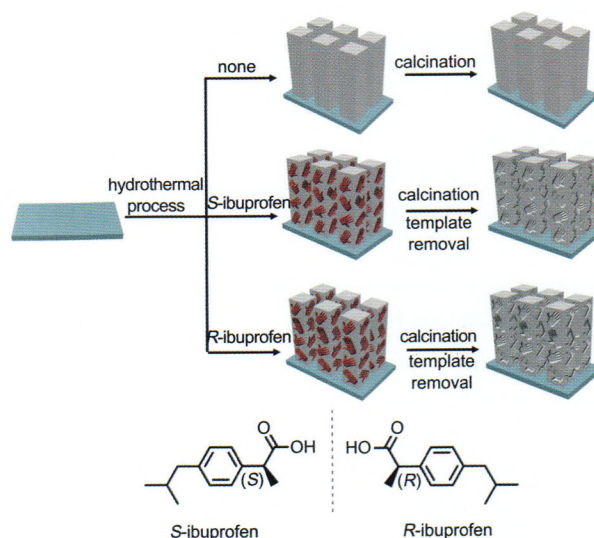
Acta Phys. -Chim. Sin. **2017**, 33 (5), 949–959

手性布洛芬对映体的选择性光电化学氧化

代卫国 何丹农

Selective Photoelectrochemical Oxidation of Chiral Ibuprofen Enantiomers

DAI Wei-Guo HE Dan-Nong



S -ibuprofen and R -ibuprofen molecular imprinting sites were constructed on the surfaces of monocrystalline TiO_2 nanorods, which have the ability to selectively recognize and catalytically oxidize S -ibuprofen and R -ibuprofen.

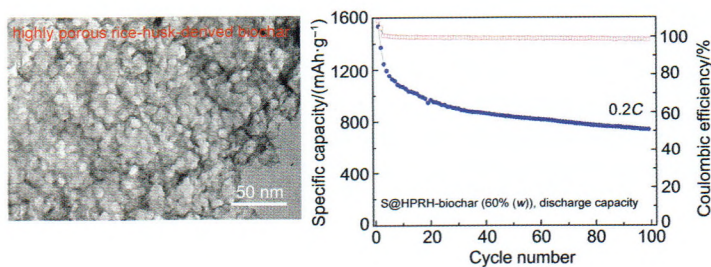
Acta Phys. -Chim. Sin. **2017**, 33 (5), 960–967

不同生物炭材料的制备及其在 Li-S 电池中的应用

李君涛 吴娇红 张涛 黄令

Preparation of Biochar from Different Biomasses and Their Application in Li-S Battery

LI Jun-Tao WU Jiao-Hong
ZHANG Tao HUANG Ling



Biochar derived from reproducible massive biomasses was used as the host matrix materials for the Li-S battery.

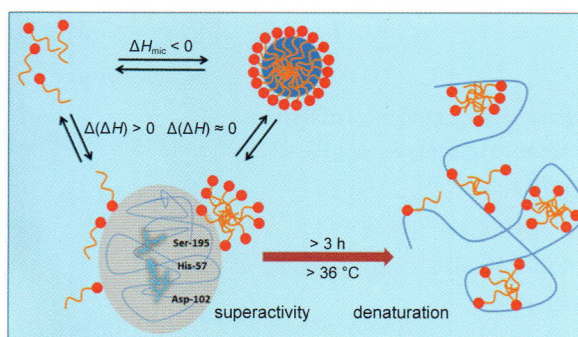
Acta Phys. -Chim. Sin. **2017**, 33 (5), 968–975

阳离子双子表面活性剂诱导的 α -CT超活性和构象变化

白光月 刘君玲 王九霞 王玉洁 李艳娜
赵 扬 姚美焕

Enzymatic Superactivity and Conformational Change of α -CT Induced by Cationic Gemini Surfactant

BAI Guang-Yue LIU Jun-Ling
WANG Jiu-Xia WANG Yu-Jie
LI Yan-Na ZHAO Yang
YAO Mei-Huan



Acta Phys. -Chim. Sin. **2017**, 33 (5), 976–983

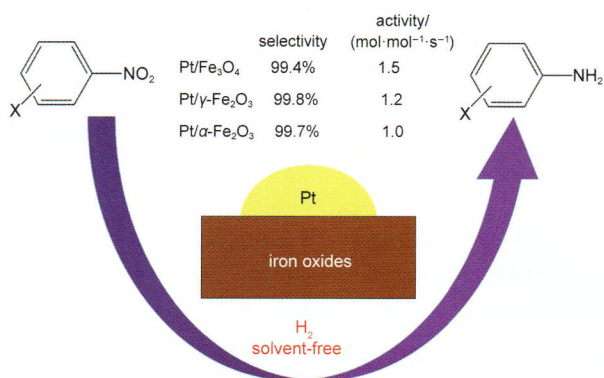
Cationic gemini surfactants can induce superactivity and instability of α -CT.

氧化铁负载铂纳米簇催化卤代硝基苯本体氢化性质研究

连 超 张 垚 王 远

Catalytic Properties of Platinum Nanoclusters Supported on Iron Oxides for the Solvent-Free Hydrogenation of Halonitrobenzene

LIAN Chao ZHANG Kai
WANG Yuan



Acta Phys. -Chim. Sin. **2017**, 33 (5), 984–992

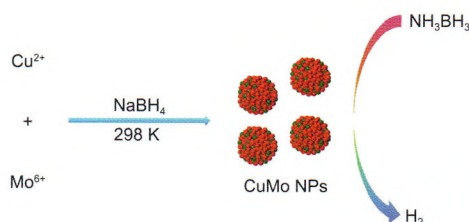
The effects of iron oxide crystal structure on the catalytic properties for the selective hydrogenation of halonitrobenzene over Pt/iron-oxide nanocomposites in the absence of a solvent were investigated, which is helpful to understand the enhanced catalytic properties over the catalysts of interest.

快速合成廉价CuMo纳米粒子高效催化氨硼烷水解产氢

杨 昆 姚淇露 卢章辉 康志兵 陈祥树

Facile Synthesis of CuMo Nanoparticles as Highly Active and Cost-Effective Catalysts for the Hydrolysis of Ammonia Borane

YANG Kun YAO Qi-Lu
LU Zhang-Hui KANG Zhi-Bing
CHEN Xiang-Shu



Acta Phys. -Chim. Sin. **2017**, 33 (5), 993–1000

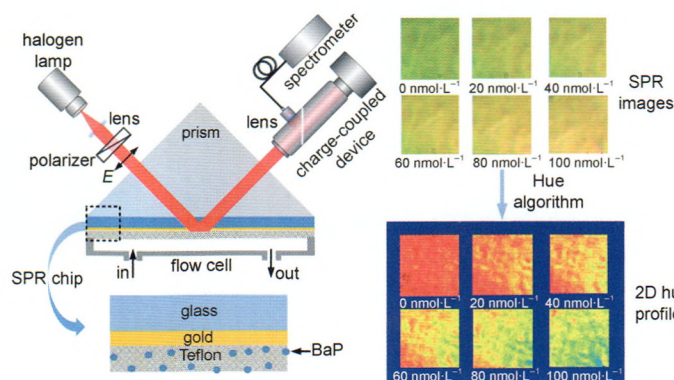
Noble-metal-free CuMo NPs that exhibited excellent catalytic activity for the hydrolysis of ammonia borane have been facilely prepared.

基于色相算法的表面等离子体共振成像传感器对苯并芘的敏感特性

范智博 龚晓庆 逯丹凤 高 然 祁志美

Benzo[a]pyrene Sensing Properties of Surface Plasmon Resonance Imaging Sensor Based on the Hue Algorithm

FAN Zhi-Bo GONG Xiao-Qing
LU Dan-Feng GAO Ran
QI Zhi-Mei

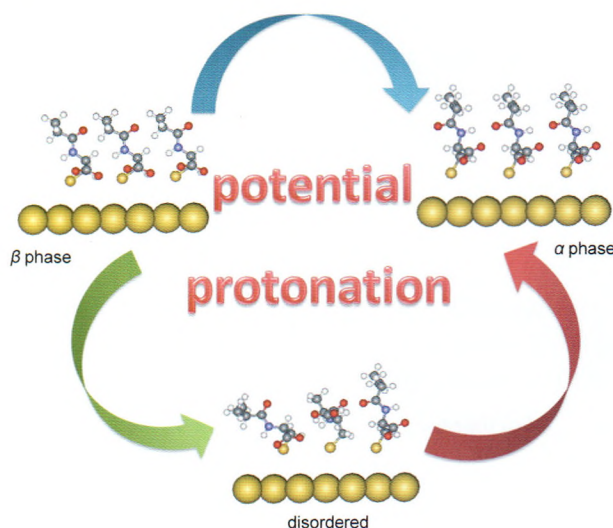


The surface plasmon resonance imaging (SPRI) sensor can provide intuitive image information and can quantitatively analyze the concentration and adsorption/desorption processes of an analyte by combining the hue algorithm.

Acta Phys.-Chim. Sin. **2017**, 33 (5), 1001–1009

电势诱导的*N*-异丁酰基-L-半胱氨酸分子在金(111)表面的相转变

陈爱喜 汪 宏 段 赛 张海明 徐 昕
迟力峰



Potential-Induced Phase Transition of *N*-Isobutyryl-L-cysteine Monolayers on Au(111) Surfaces

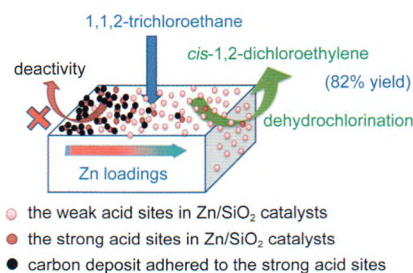
CHEN Ai-Xi WANG Hong
DUAN Sai ZHANG Hai-Ming
XU Xin CHI Li-Feng

The potential-induced phase transition of chemisorbed *N*-isobutyryl-L-cysteine monolayers is investigated by *in-situ* electrochemical scanning tunneling microscopy in 0.1 mol·L⁻¹ H₂SO₄ aqueous solutions.

Acta Phys.-Chim. Sin. **2017**, 33 (5), 1010–1016

Zn/SiO₂气相催化裂解1,1,2-三氯乙烷脱HCl: 酸性与失活

胡益浩 宋通洋 王月娟 胡庚申 谢冠群
罗孟飞



Gas Phase Dehydrochlorination of 1,1,2-Trichloroethane over Zn/SiO₂ Catalysts: Acidity and Deactivation

HU Yi-Hao SONG Tong-Yang
WANG Yue-Juan HU Geng-Sheng
XIE Guan-Qun LUO Meng-Fei

During the gas-phase dehydrochlorination of 1,1,2-trichloroethane (TCE), Zn/SiO₂ had high TCE conversion (98%) and excellent selectivity to *cis*-1,2-dichloroethylene (82%). The weak acid centers of Zn/SiO₂ were catalytic active sites for the dehydrochlorination of TCE while the strong acid sites on the catalyst surface were responsible for coke deposition and deactivation of the Zn/SiO₂ catalysts.

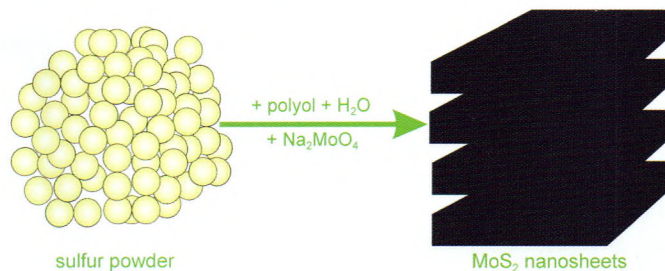
Acta Phys.-Chim. Sin. **2017**, 33 (5), 1017–1026

硫粉为硫源,多元醇辅助合成硫化钼纳米片

王 辉 邹德春

Polyol-Mediated Synthesis of MoS₂ Nanosheets Using Sulfur Powder as the Sulfur Source

WANG Hui ZOU De-Chun

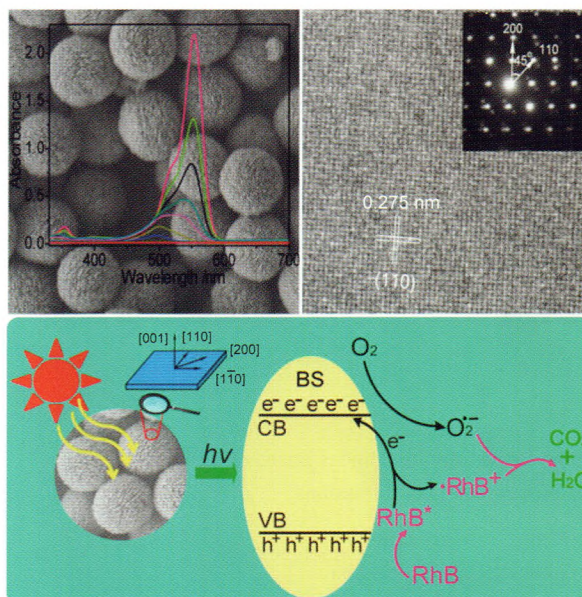


MoS₂ nanosheets are prepared with sulfur powder as the sulfur source at 170–200 °C for 8 h.

Acta Phys. -Chim. Sin. **2017**, 33 (5), 1027–1032

纳米片自组装的(BiO)₂CO₃单分散微米绒球的绿色可控合成及其光催化性能

阮毛毛 宋乐新 王青山 夏 娟 杨 尊
滕 越 许哲远



Facile Green Synthesis of Highly Monodisperse Bismuth Subcarbonate Micropompons Self-assembled by Nanosheets: Improved Photocatalytic Performance

RUAN Mao-Mao SONG Le-Xin
WANG Qing-Shan XIA Juan
YANG Zun TENG Yue
XU Zhe-Yuan

This study developed a green hydrothermal method for the synthesis of highly monodisperse hierarchical (BiO)₂CO₃ micropompons self-assembled by single-crystalline nanosheets with exposed {001} facets. Urea played multiple roles in the formation of the (BiO)₂CO₃ crystals. The self-assembled (BiO)₂CO₃ micropompons presented improved photocatalytic activity relative to other reported values.

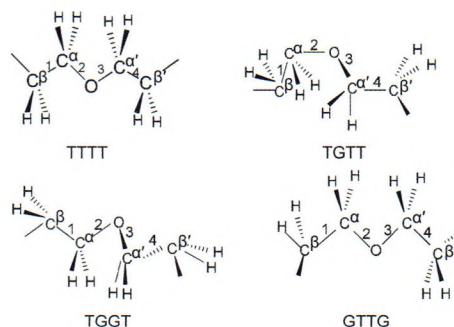
Acta Phys. -Chim. Sin. **2017**, 33 (5), 1033–1042

液态聚乙二醇CH₂剪切振动和扭转振动——拉曼光谱和密度泛函理论计算

韩 磊 彭 丽 蔡凌云 郑旭明 张富山

CH₂ Scissor and Twist Vibrations of Liquid Polyethylene Glycol ——Raman Spectra and Density Functional Theory Calculations

HAN Lei PENG Li
CAI Ling-Yun ZHENG Xu-Ming
ZHANG Fu-Shan



The relationships between the conformation (TTTT, TGTT, TGGT, and GTTG) of the CH₂CH₂—O—CH₂CH₂ segment, the CH₂ scissor and twist vibrational modes, and frequencies of various conformers of liquid polyethylene oxide (PEO) are determined.

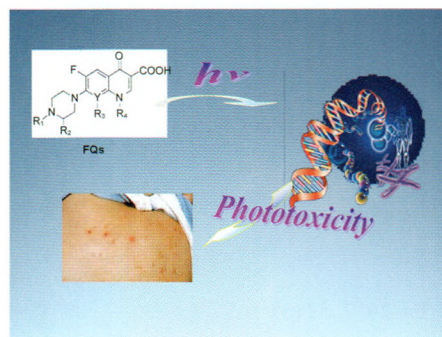
Acta Phys. -Chim. Sin. **2017**, 33 (5), 1043–1050

二氟沙星激发态氧化损伤氨基酸和脱氧鸟苷酸的激光光解研究

李海霞 刘艳成 唐睿智 张 鹏 马六達
魏驰原 王文锋

Reactions of Triplet-State Difloxacin with Amino Acids and dGMP: A Laser Flash Photolysis Study

LI Hai-Xia LIU Yan-Cheng
TANG Rui-Zhi ZHANG Peng
MA Liu-Kui WEI Chi-Yuan
WANG Wen-Feng



The triplet states of DFX can oxidize deoxyguanylic acid and various amino acids. The results suggest that the anti-tumor mechanism of DFX involves both Type I and Type II processes and that the dominant mechanism in biological systems is Type I photochemistry.

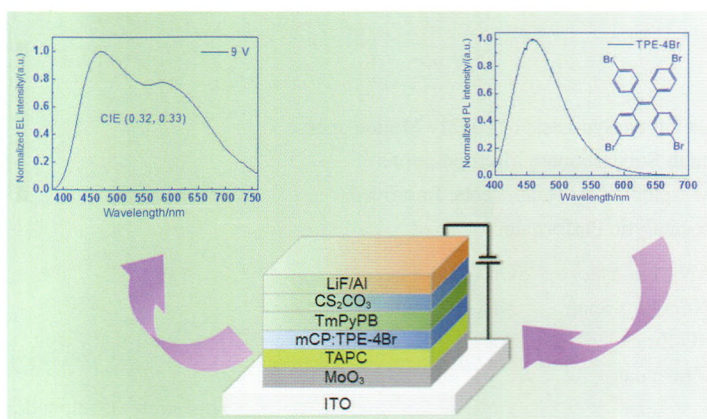
Acta Phys.-Chim. Sin. **2017**, 33 (5), 1051–1056

基于激子和电致激基复合物双重发光的白光 OLED

檀康明 闫敏楠 王英男 解令海 钱 妍
张宏梅 黄 维

White Organic Light-Emitting Diodes Based on Exciton and Electroplex Dual Emissions

TAN Kang-Ming YAN Min-Nan
WANG Ying-Nan XIE Ling-Hai
QIAN Yan ZHANG Hong-Mei
HUANG Wei



White organic light-emitting diode has been designed using local emission and electroplex emission, formed between the light-emitting layer and the carrier transporting layer.

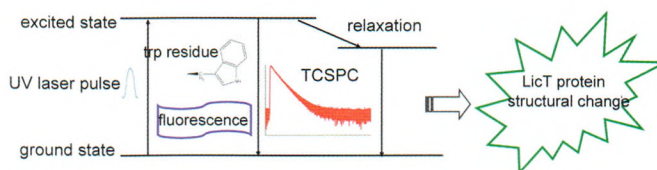
Acta Phys.-Chim. Sin. **2017**, 33 (5), 1057–1064

基于时间分辨方法的LicT蛋白荧光动力学特性

常孟方 李 磊 曹潇丹 贾梦辉 周加胜
陈绍泉 徐建华

Fluorescence Dynamics of LicT Protein by Time-Resolved Spectroscopy

CHANG Meng-Fang LI Lei
CAO Xiao-Dan JIA Meng-Hui
ZHOU Jia-Sheng CHEN Jin-Quan
XU Jian-Hua



In this paper, the fluorescence dynamics of tryptophan residues in the LicT protein were studied by time-resolved spectroscopy to explore the structural changes and microenvironment of the activated LicT, AC 141 as compared to the wild-type protein, Q 22.

Acta Phys.-Chim. Sin. **2017**, 33 (5), 1065–1070

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