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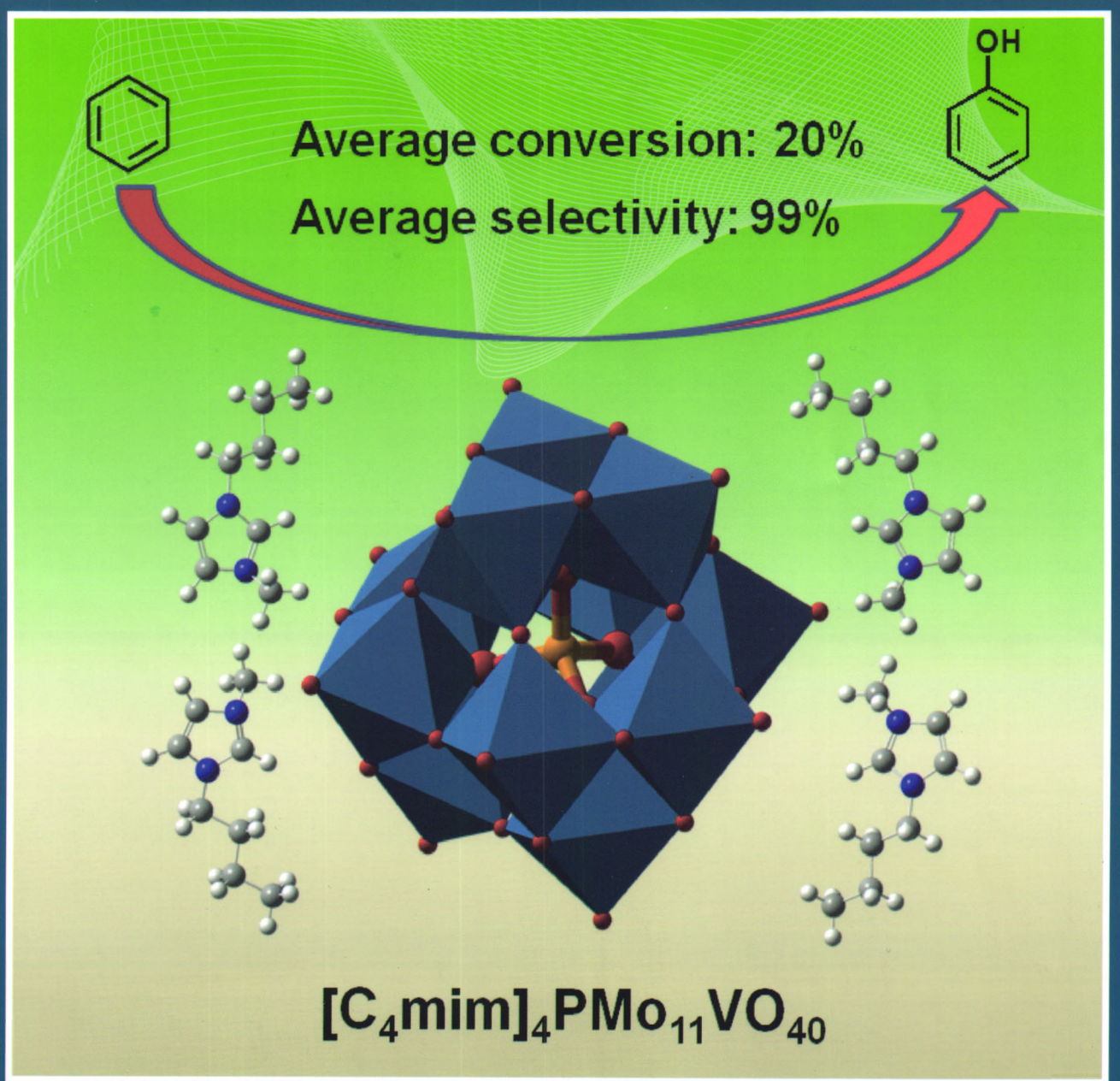
物理化学学报

ACTA PHYSICO-CHIMICA SINICA



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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

2016
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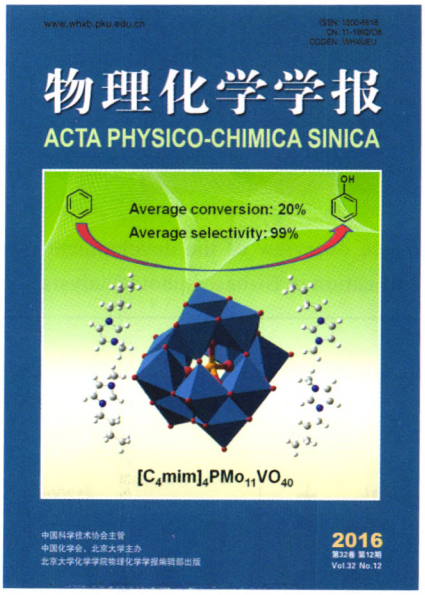
Vol.32 No.12

物理化学学报 (WULI HUAXUE XUEBAO) 第 32 卷第 12 期
ACTA PHYSICO-CHIMICA SINICA, Vol.32, No.12

COVER



The cover image presents the illustration of hydroxylation of benzene catalyzed by hybrids of polyoxometalate/ionic liquid. On page 2961, MA *et al.* demonstrate that benzene can nearly be quantitatively hydroxylated by H_2O_2 using hybrid materials based on V-substituted phosphomolybdic acid $H_{3+x}PMo_{12-x}V_xO_{40}$ (x = 0, 1, 2) and ionic liquid 1-butyl-3-methyl imidazolium bromide ([C_4mim]Br) as catalysts. The catalysts also exhibit good reusability and have been reused five runs without much decrease in conversion and selectivity.

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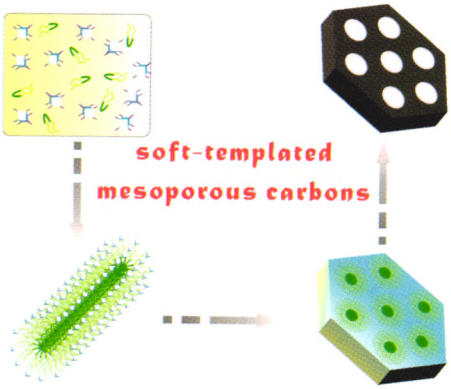
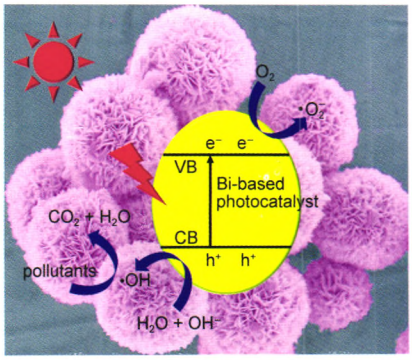


This review summarizes recent advances in synthesis, structural modification and functionalization of soft-templated ordered mesoporous carbon materials.

Acta Phys. -Chim. Sin. **2016,** *32* (12), 2826–2840

铋系光催化剂的形貌调控与表面改性研究进展

赫荣安　曹少文　余家国



Recent Advances in Morphology Control and Surface Modification of Bi-Based Photocatalysts

HE Rong-An　CAO Shao-Wen
YU Jia-Guo

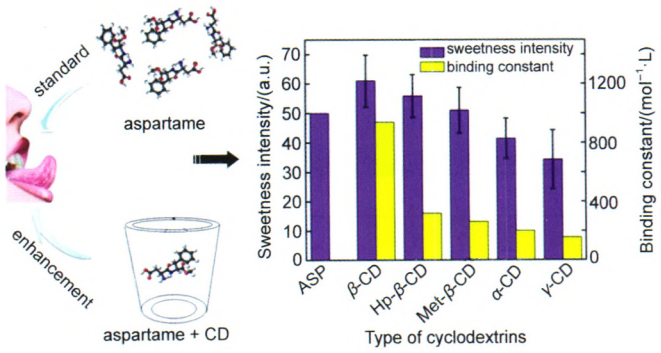
Acta Phys. -Chim. Sin. **2016,** *32* (12), 2841−2870

This review gives a comprehensive overview of the development of morphology control and surface modification in Bi-based photocatalysts.

论文　ARTICLE

环糊精对阿斯巴甜的甜感增强作用及二者相互作用热力学

朱甜甜　徐淑臻　葛炳强　陈忠秀



Sweetness Enhancement of Aspartame in the Presence of Cyclodextrins and the Thermodynamics in Binding

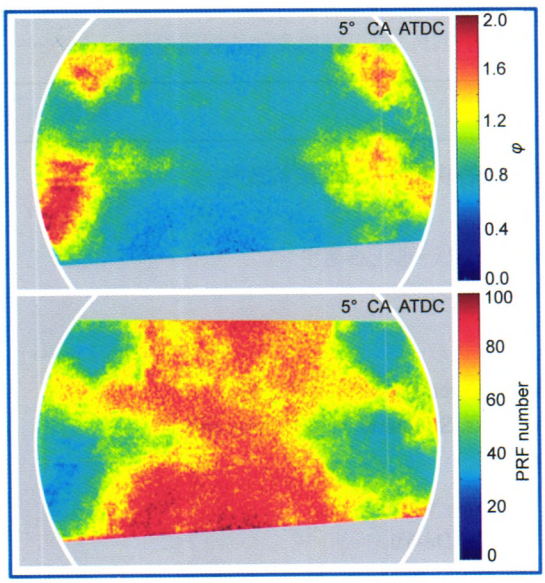
ZHU Tian-Tian　XU Shu-Zhen
GE Bing-Qiang　CHEN Zhong-Xiu

Acta Phys. -Chim. Sin. **2016,** *32* (12), 2871−2878

The cyclodextrin that had the largest binding constant was the best flavor-retention agent, and resulted in an enhanced sweetness intensity of aspartame.

双燃料发动机缸内分层激光诱导荧光实验及化学动力学模拟研究

唐青龙　刘海峰　李明坤　尧命发



Study on In-Cylinder Charge Stratification of a Dual-Fuel Engine Using Fuel-Tracer Laser-Induced Fluorescence and Chemical Kinetic Simulation

TANG Qing-Long　LIU Hai-Feng
LI Ming-Kun　YAO Ming-Fa

Acta Phys. -Chim. Sin. **2016,** *32* (12), 2879−2890

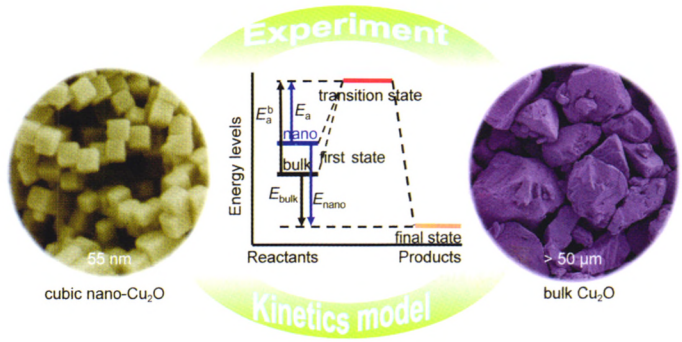
The equivalence ratio and primary reference fuel (PRF) number in an optical engine were determined quantitatively using a fuel-tracer laser-induced fluorescence (PLIF) technique.

立方体纳米氧化亚铜反应动力学的理论及实验研究

汤焕丰　黄在银　肖　明　梁　敏　陈栎莹

An Investigation into the Reaction Kinetics of Cubic Nano-Cu_2O in Theory and Experiment

TANG Huan-Feng　HUANG Zai-Yin
XIAO Ming　LIANG Min
CHEN Li-Ying



Acta Phys. -Chim. Sin. **2016,** *32* (12), 2891−2897

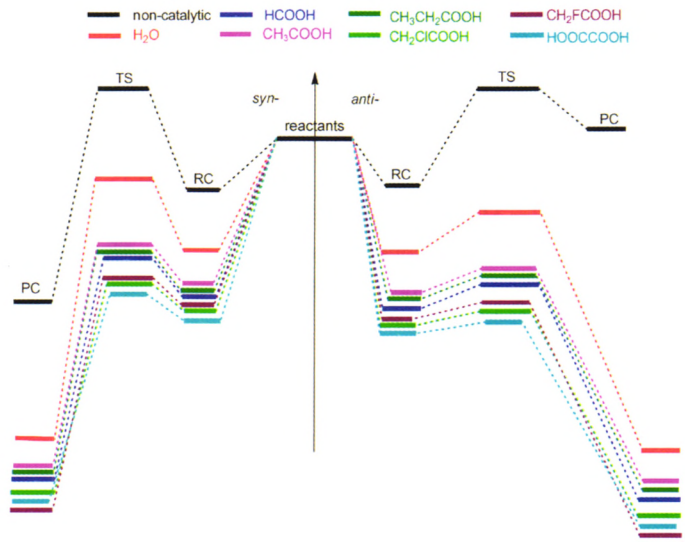
In-situ microcalorimetry and cube kinetic models were applied for investigating the different reaction kinetic behaviors between nano-Cu_2O and bulk Cu_2O.

Criegee 中间体 CH_3CHOO 与 H_2O 反应机理及酸催化效应

高志芳　周丽婷　王渭娜　刘峰毅　王文亮

Reaction Mechanism of Criegee Intermediate CH_3CHOO with H_2O and the Acid Catalytic Effect

GAO Zhi-Fang　ZHOU Li-Ting
WANG Wei-Na　LIU Feng-Yi
WANG Wen-Liang



Acta Phys. -Chim. Sin. **2016,** *32* (12), 2898−2904

Theoretical investigations show that different catalysts play an important role in the reaction of Criegee intermediate (CH_3CHOO) with water (H_2O).

Se 掺杂对单层 MoS_2 电子能带结构和光吸收性质的影响

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桑胜波　侯静静

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LI Gang　CHEN Min-Qiang
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HU Jie　SANG Sheng-Bo
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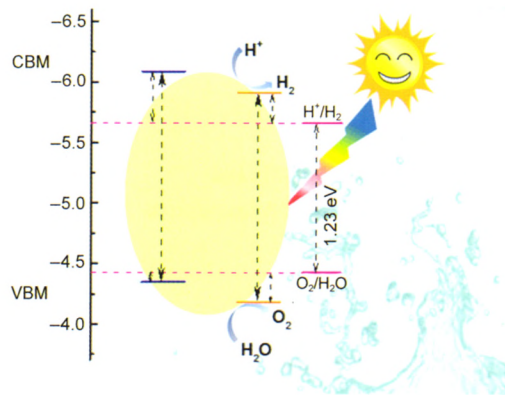
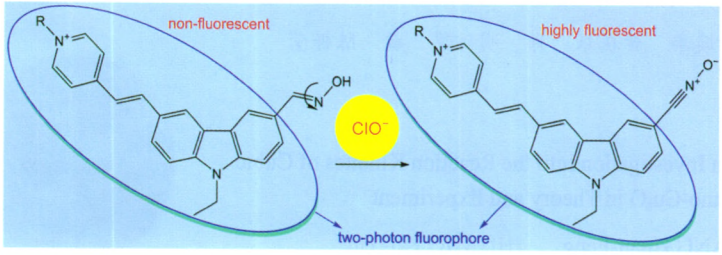


Acta Phys. -Chim. Sin. **2016,** *32* (12), 2905−2912

Photocatalytic water splitting using sunlight is a promising strategy for the energy crisis.

基于咔唑的双光子荧光次氯酸根探针光学性质及响应机理

王　昕　张玉瑾　王传奎



Optical Properties and Responsive Mechanism of Carbazole-Based Two-Photon Fluorescent Probes for the Detection of Hypochlorite

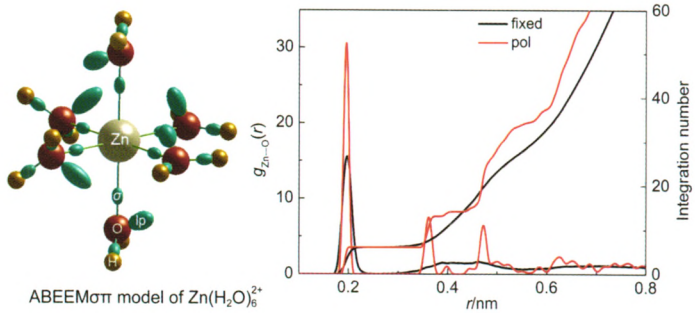
WANG Xin　ZHANG Yu-Jin
WANG Chuan-Kui

Acta Phys. -Chim. Sin. **2016,** *32* (12), 2913−2920

Two-photon fluorescent probes for the detection of hypochlorite in living biological organelles were investigated and found to undergo C=N isomerization.

应用ABEEMσπ极化力场对Zn^{2+}水溶液配位微结构和水交换反应进行分子动力学模拟研究

赫兰兰　郭　宇　赵　健　姜新蕊　杨忠志
赵东霞



Study on Coordination Microstructure and Water Exchange Reaction of Zn^{2+} Aqueous Solutions through Molecular Dynamics Simulations Using the ABEEMσπ Polarizable Force Field

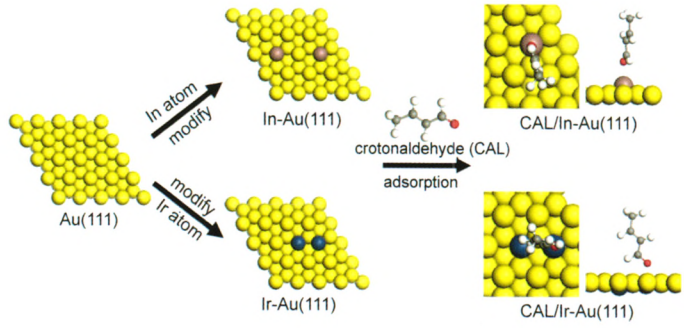
HE Lan-Lan　GUO Yu
ZHAO Jian　JIANG Xin-Rui
YANG Zhong-Zhi　ZHAO Dong-Xia

Acta Phys. -Chim. Sin. **2016,** *32* (12), 2921−2931

The coordination microstructure and water exchange of Zn^{2+} aqueous solution based on the ABEEMσπ polarizable field were studied.

In-Au(111)和Ir-Au(111)合金表面的性质及其对巴豆醛的吸附比较

蒋军辉　钱梦丹　薛继龙　夏盛杰　倪哲明
邵蒙蒙



Comparison of Properties of In-Au(111) and Ir-Au(111) Alloy Surfaces, and Their Adsorption to Crotonaldehyde

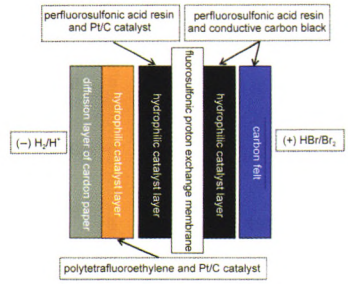
JIANG Jun-Hui　QIAN Meng-Dan
XUE Ji-Long　XIA Sheng-Jie
NI Zhe-Ming　SHAO Meng-Meng

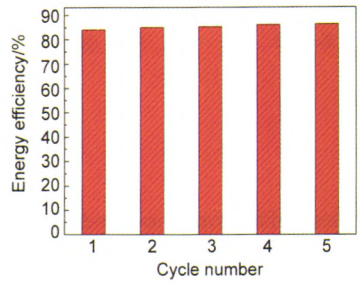
Acta Phys. -Chim. Sin. **2016,** *32* (12), 2932−2940

The geometrical parameters and adsorption capacity of crotonaldehyde towards In-Au(111) and Ir-Au(111) alloy surfaces were examined using density functional theory.

氢溴储能电池结构的优化和运行条件对电池性能的影响

史继诚　徐洪峰　卢　璐　高　俊





Hydrogen Bromine Battery Structure Optimization and the Operation Condition Effects on Battery Performance

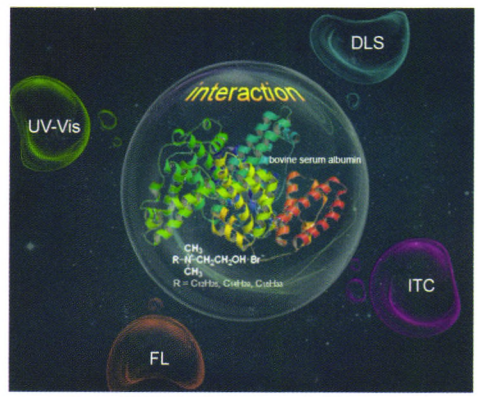
SHI Ji-Cheng　XU Hong-Feng
LU Lu　GAO Jun

The structure of the hydrogen bromine battery can solve acid permeation problems from the bromine electrode to the hydrogen electrode and improve the bromine electrode electrochemical reaction speed. With this structure, the energy efficiency of the hydrogen bromine battery is 85.3% and the Coulombic efficiency is 100% at the 200 mA·cm^{-2} current density with five cycles.

Acta Phys. -Chim. Sin. **2016,** *32* (12), 2941−2950

季铵盐型阳离子表面活性剂与牛血清白蛋白的相互作用

谢湖均　刘程程　孙　强　顾　青　雷群芳
方文军



The Interactions between Quaternary Ammonium Cationic Surfactants and Bovine Serum Albumin

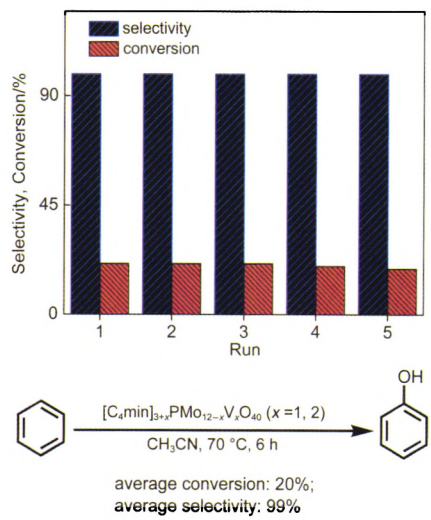
XIE Hu-Jun　LIU Cheng-Cheng
SUN Qiang　GU Qing
LEI Qun-Fang　FANG Wen-Jun

UV-visible (UV-Vis), fluorescence (FL) spectroscopy, dynamic light scattering (DLS) and isothermal titration calorimetry (ITC) were used to investigate the interactions between bovine serum albumin (BSA) and three different quaternary ammonium surfactants.

Acta Phys. -Chim. Sin. **2016,** *32* (12), 2951−2960

杂多酸/离子液体杂化材料催化苯的高选择性羟基化

马　青　童金辉　宿玲弟　王文慧　马文梅
薄丽丽



Highly Selective Hydroxylation of Benzene Catalyzed by Hybrids of Polyoxometalate/Ionic Liquid

MA Qing　TONG Jin-Hui
SU Ling-Di　WANG Wen-Hui
MA Wen-Mei　BO Li-Li

Benzene can be highly effective hydroxylated to produce phenol using H_2O_2 as a green oxidant with 99% selectivity for phenol after five consecutive runs.

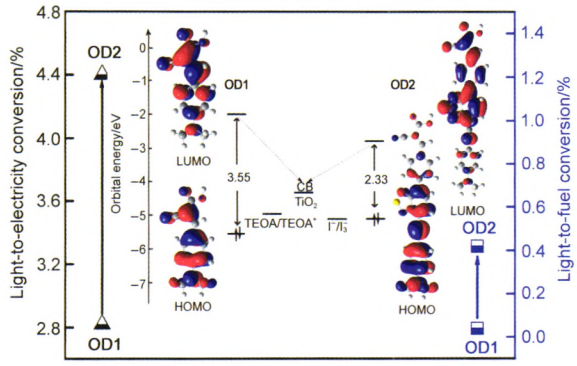
Acta Phys. -Chim. Sin. **2016,** *32* (12), 2961−2967

D-π-A-π-A结构有机光敏染料的合成及其在太阳能光电转化和光解水制氢中的应用

肖　岸　卢　辉　赵　阳　骆耿耿

Synthesis of a Novel D-π-A-π-A Organic Sensitizer and Its Application in a Dye-Sensitized Solar Cell and Dye-Sensitized Photocatalytic H_2 Production

XIAO An　　LU Hui
ZHAO Yang　　LUO Geng-Geng

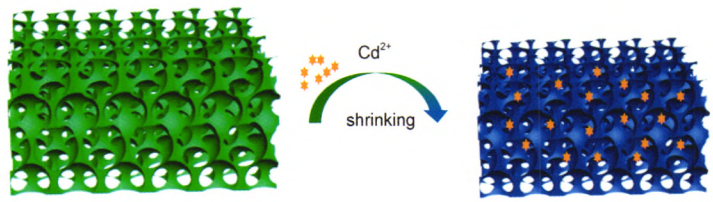


Acta Phys. -Chim. Sin. **2016,** *32* (12), 2968−2975

Compared with the traditional D-π-A sensitizer (**OD1**), a novel metal-free D-π-A-π-A-based sensitizer (**OD2**) exhibited multifunctional properties with improved efficiency in light-to-electricity and light-to-fuel conversions.

镉离子响应性凝胶光子晶体传感膜的构建

张晓栋　秦立彦　陈明清　刘士荣



Fabrication of a Responsive Hydrogel Photonic Crystal Sensing Film for Cadmium Ions

ZHANG Xiao-Dong　　QIN Li-Yan
CHEN Ming-Qing　　LIU Shi-Rong

Acta Phys. -Chim. Sin. **2016,** *32* (12), 2976−2982

A hydrogel photonic crystal that was modified using 1-allyl-2-thiourea exhibited an inverse opal structure and was used to detect Cd^{2+} by a simple color change.

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