

物理化学学报

ACTA PHYSICO-CHIMICA SINICA

第29卷 第8期 Vol.29 No.8 2013



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

物理化学学报(Wuli Huaxue Xuebao)
第 29 卷第 8 期(2013 年 8 月)

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第十三届全国均相催化学术讨论会第一轮通知 (1690)

第十七次全国电化学大会第二轮通知 (1704)

本期责任编辑: 於秀芝

COVER



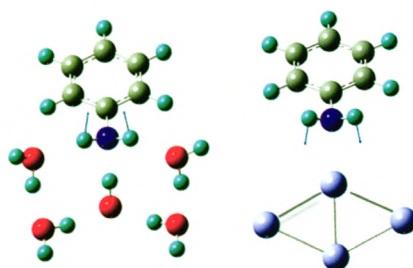
The cover image presents the fabrication of four enzyme electrodes and relevant microscopic pictures. On page 1727, YANG *et al.* demonstrate that glucose oxidase adsorbed on bare, Au-electroplated, multiwalled carbon nanotube (MWCNT)-modified, and Au-electrodeposited MWCNT-modified Au electrodes displays different adsorption amounts, bioactivities, and electroactivities, and these quantitative results obtained from quartz crystal microbalance and electrochemical studies have some significance for optimization of enzymatic immobilization on nanomaterials.

CONTENTS

THERMODYNAMICS, KINETICS, AND STRUCTURE CHEMISTRY

Raman Spectra of Amino Wagging
Vibrational Modes in p - π -Conjugated
Molecules

TAO Sha YU Li-Juan
WU De-Yin TIAN Zhong-Qun

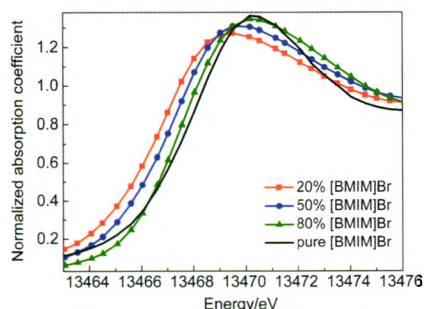


The Raman signal of the ω_{NH_2} peak in p - π -conjugated molecules displays considerable changes because of weak binding interactions.

Acta Phys. -Chim. Sin. 2013, 29 (8), 1609–1617

Effect of the Ratio between Ionic Liquids
[BMIM]Br and [BMIM][BF₄] on the
Charge Transfer of Br⁻

MA Jing-Yuan ZOU Yang
JIANG Zheng HUANG Yu-Ying



As the content of [BMIM][BF₄] added to [BMIM]Br increases, more negative charge is transferred to Br⁻.

Acta Phys. -Chim. Sin. 2013, 29 (8), 1618–1622

Method to Determine the Kinetic Parameters
of the Autocatalytic Decomposition Reaction
and Critical Rate of Temperature Rise of
Thermal Explosion of Energetic Materials
from DSC Curves

HU Rong-Zu ZHAO Feng-Qi
GAO Hong-Xu YAO Er-Gang
ZHANG Hai WANG Yao
CHANG Xiang-Yu ZHAO Hong-An

$$\min_{E, A} \sum_{i=2}^N \left\{ \left(\frac{d\alpha}{dt} \right)_i - A \exp \left(-\frac{E}{RT_i} \right) \alpha_i (1 - \alpha_i) \right\}^2$$

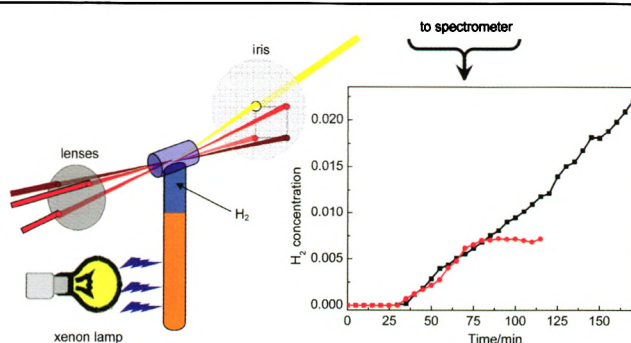
$$\left(\frac{dT}{dt} \right)_{T_b} = \frac{RT_b^2 (T_b - T_{e0}) \left[A \exp \left(-\frac{E}{RT_b} \right) (1 - 2\alpha)_b \right]}{RT_b^2 - (T_b - T_{e0})E}$$

A method was presented to determine the kinetic parameters of the autocatalytic decomposition reaction of Au, CnB, Bna, first order/apparent empiric-order, simple first order and n th order and apparent empiric-order of $m=0$, $n=0$, $p=1$ and $m=0$, $n=1$, $p=1$ of energetic materials (EMs) and the critical rate of temperature rise of thermal explosion in EMs when autocatalytic decomposition converts into thermal explosion from DSC curves at different heating rates.

Acta Phys. -Chim. Sin. 2013, 29 (8), 1623–1631

Application of Time-Resolved Coherent Anti-Stokes Raman Scattering Technique on the Study of Photocatalytic Hydrogen Production Kinetics

LÜ Yong-Gang LI Zhi-Jun
WU Li-Zhu WANG Peng
FU Li-Min ZHANG Jian-Ping



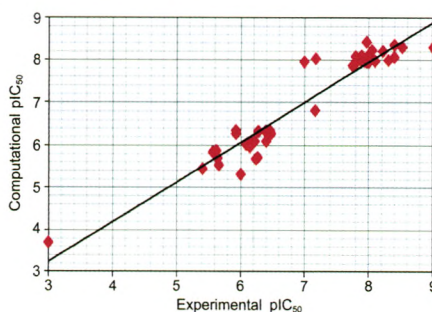
High sensitivity, *in situ* hydrogen concentration monitoring apparatus based on coherent anti-Stokes Raman scattering was constructed. Using this setup, the hydrogen production kinetics of an artificial system was studied.

Acta Phys. -Chim. Sin. **2013**, 29 (8), 1632–1638

THEORETICAL AND COMPUTATIONAL CHEMISTRY

Quantitative Structure–Activity Relationship Study of the Non-Nucleoside Inhibitors of HCV NS5B Polymerase by Machine Learning Methods

CONG Yong XUE Ying

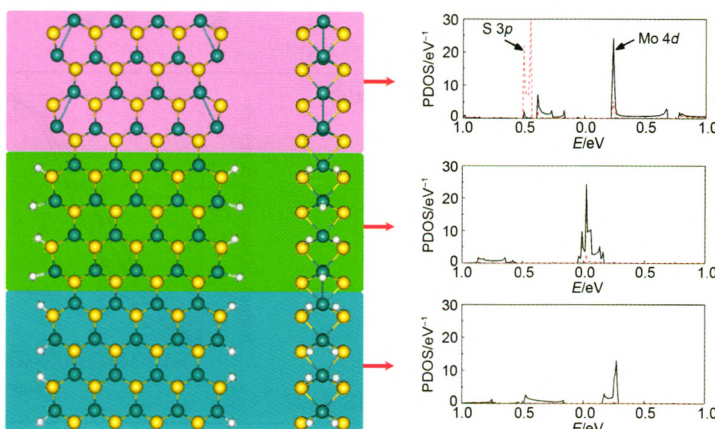


HCV NS5B inhibitors were investigated in a quantitative structure-activity relationship (QSAR) study. Linear stepwise regression analysis and genetic algorithm-partial least squares approaches were used to select descriptors for genetic algorithm-support vector machine modeling. These models achieved satisfactory prediction results and can be extended to other QSAR studies.

Acta Phys. -Chim. Sin. **2013**, 29 (8), 1639–1647

Electronic Structure and Edge Modification of Armchair MoS₂ Nanoribbons

YANG Zhi-Xiong YANG Jin-Xin
LIU Qi XIE Yu-Xin
XIONG Xiang OUYANG Fang-Ping

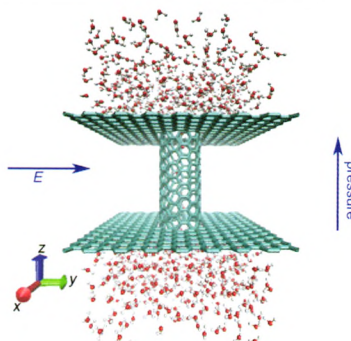


Edge modification plays an important role in the stability and electronic properties of armchair MoS₂ nanoribbons.

Acta Phys. -Chim. Sin. **2013**, 29 (8), 1648–1654

Effects of Orthogonal Electric Field on Water Flux through a Carbon Nanotube

GE Zhen-Peng SHI Yan-Chao
LI Xiao-Yi

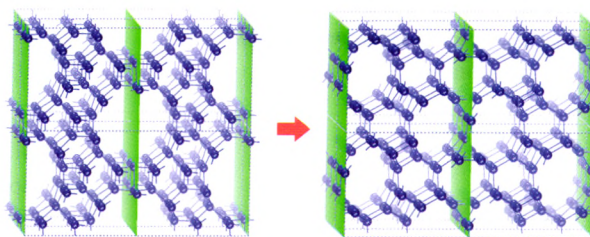


An orthogonal electric field can be used to control the flux of water molecules through a carbon nanotube.

Acta Phys. -Chim. Sin. **2013**, 29 (8), 1655–1660

Predicting Hypothetical Zeolite Frameworks Using Program FraGen

LU Jun-Ran LI Yi
YU Ji-Hong LU Ying

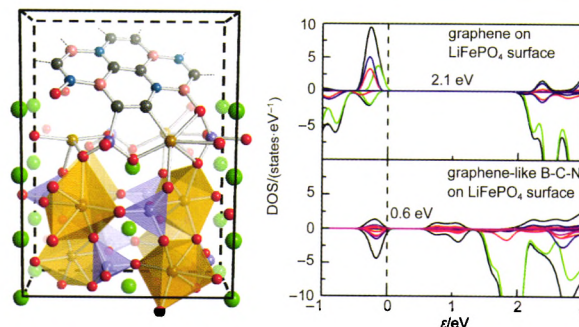


New zeolite frameworks are predicted by the program FraGen by fixing the Wyckoff site symmetry of each atom.

Acta Phys. -Chim. Sin. **2013**, 29 (8), 1661–1665

Improvement of Surface Structure and Enhancement of Conductivity of LiFePO₄ Surface by Graphene and Graphene-Like B-C-N Coating

SUN Chao YAN Liu-Ming
YUE Bao-Hua

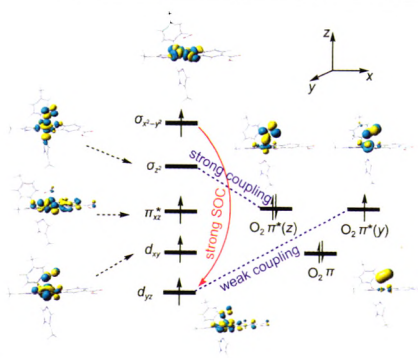


Density functional theory calculations revealed that the electric conductivity of LiFePO₄ surface could be improved by coating with graphene-like B-C-N.

Acta Phys. -Chim. Sin. **2013**, 29 (8), 1666–1672

Spin-Orbit Coupling and Zero-Field Splitting in Dioxygen Activation by Non-Heme Iron(III)

LÜ Ling-Ling WANG Xiao-Fang
ZHU Yuan-Cheng LIU Xin-Wen
YUAN Kun WANG Yong-Cheng



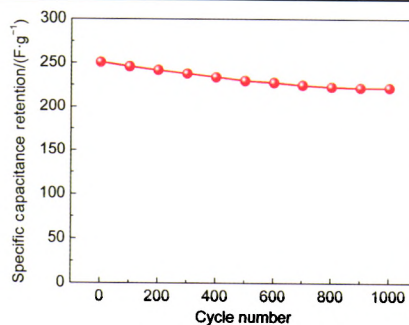
Two coexisting effects cause formation of the quartet state ⁴1, namely electron spin exchange coupling and spin-orbit coupling (SOC); the latter is the dominant factor because of the larger SOC constant (353.16 cm⁻¹).

Acta Phys. -Chim. Sin. **2013**, 29 (8), 1673–1680

ELECTROCHEMISTRY AND NEW ENERGY

Hydrothermal Synthesis of Partially Reduced Graphene Oxide-K₂Mn₂O₈ Nanocomposites as Supercapacitors

LI Le HE Yun-Qiu
CHU Xiao-Fei LI Yi-Ming
SUN Fang-Fang HUANG He-Zhou

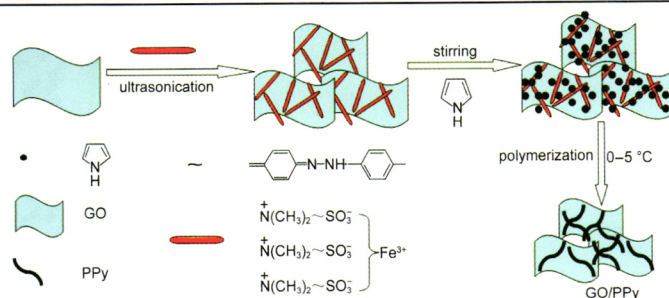


Graphene oxide (GO) to act as heterophase boundaries was combined with a Mn precursor to synthesize reduced graphene oxide (rGO)-MnO₂ nanocomposites for use as supercapacitors.

Acta Phys. -Chim. Sin. **2013**, 29 (8), 1681–1690

Preparation and Electrochemical Capacitance Properties of Graphene Oxide/Polypyrrole Intercalation Composite

SHI Qin MEN Chun-Yan
LI Juan

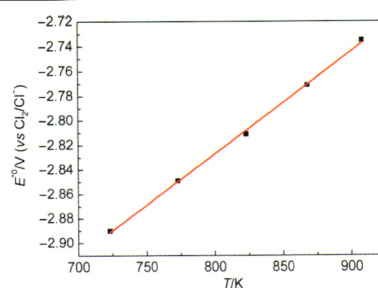


Graphene oxide/polypyrrole (GO/PPy) intercalation composite was prepared by using the fibrillar complex (FeCl₃-methyl orange) as a reactive self-degradation template and the composite exhibited excellent electrochemical capacitance properties.

Acta Phys. -Chim. Sin. **2013**, 29 (8), 1691-1697

Electrochemistry of MgCl₂ in LiCl-KCl Eutectic Melts

TANG Hao YAN Yong-De
ZHANG Mi-Lin XUE Yun
ZHANG Zhi-Jian DU Wei-Chao
HE Hui

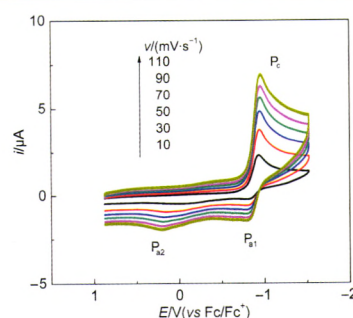


The diffusion coefficient and standard potential of MgCl₂ in LiCl-KCl eutectic melts were determined by different electrochemical techniques.

Acta Phys. -Chim. Sin. **2013**, 29 (8), 1698-1704

Electrochemical Behavior of the System of Uranium(VI) Extraction with CMPO-Ionic Liquid

WU Jing-Ke SHEN Xing-Hai
CHEN Qing-De

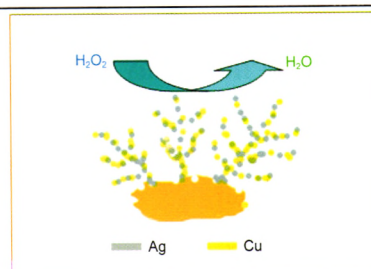


The electrochemical behavior of a U(VI)-CMPO complex and the electrodeposition of U(VI) in an extraction system using the ionic liquid C₄mimNTf₂ as the solvent were studied.

Acta Phys. -Chim. Sin. **2013**, 29 (8), 1705-1711

Synthesis and Application of Ag-Cu Bimetallic Dendrites

KANG Ya-Rong CHEN Fu-Yi

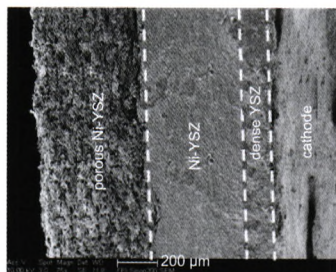


Ag-Cu dendrites synthesized by electrodeposition of Cu foam and subsequent galvanic displacement reaction are a good catalyst for reduction of H₂O₂.

Acta Phys. -Chim. Sin. **2013**, 29 (8), 1712-1718

Preparation and Properties of Direct-Methane Solid Oxide Fuel Cell Based on a Graded Cu-CeO₂-Ni-YSZ Composite Anode

MENG Xiu-Xia GONG Xun
YANG Nai-Tao TAN Xiao-Yao
MA Zi-Feng

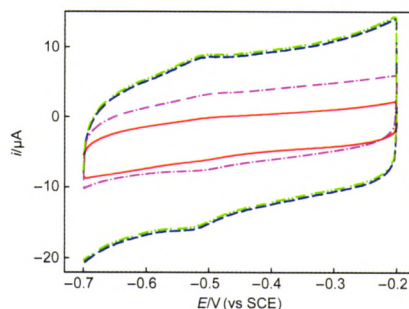


A graded anode-supported solid oxide fuel cell (SOFC) was fabricated by a combined trilayer co-pressing-sintering and coating method.

Acta Phys.-Chim. Sin. **2013**, 29 (8), 1719–1726

Comparison of Enzymatic Activities and Electroactivities of Adsorbed Glucose Oxidase on Several Nanomaterial-Modified Electrodes

YANG Da-Wei CHEN Chao
XIE Qing-Ji YAO Shou-Zhuo

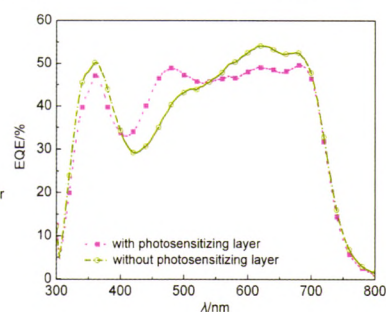
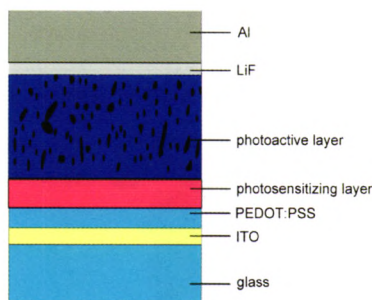


The bioactivities and electroactivities of glucose oxidase adsorbed on bare, Au-electrodeposited, multi-walled carbon nanotube (MWCNT)-modified, and Au-electrodeposited MWCNT-modified Au electrodes were quantitatively studied and compared using a quartz-crystal microbalance and electrochemical techniques.

Acta Phys.-Chim. Sin. **2013**, 29 (8), 1727–1734

Spectrum Response Enhancement of Organic Solar Cell Using a Poly(3-hexylthiophene) Photosensitizing Layer

WU Zhen-Wu LIU Yang
WEI Shang-Jiang HUANG Xun
ZHANG Dong-Yu ZHOU Ming
CHEN Li-Wei MA Chang-Qi
WANG Hua

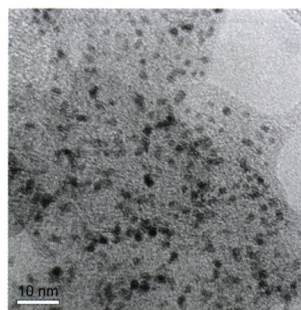


Introducing a thin layer of poly(3-hexylthiophene) (P3HT) between the photoactive layer and anode of an organic solar cell enhanced its spectral response over the 450–600 nm range, and consequently increased its short-circuit current density, revealing the promise of using a conjugated polymer as a photosensitizing layer in solar cells.

Acta Phys.-Chim. Sin. **2013**, 29 (8), 1735–1744

Effects of Pt Content on the Catalytic Performance of Co@Pt/C Core-Shell Structured Electrocatalysts

ZHAO Tian-Tian LIN Rui
ZHANG Lu CAO Chui-Hui
MA Jian-Xin



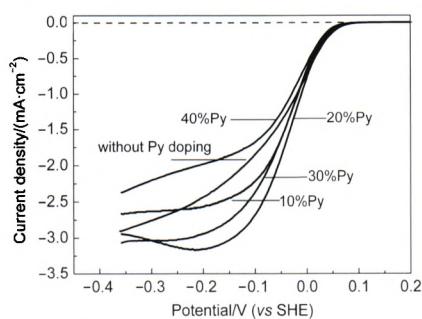
Co@Pt/C electrocatalysts with metal particles well dispersed on the carbon support were successfully synthesized and their performances were investigated.

Acta Phys.-Chim. Sin. **2013**, 29 (8), 1745–1752

Electrochemical Behavior of Pyridine-Doped Carbon-Supported Co-Phthalocyanine (Py-CoPc/C) for Oxygen Reduction Reaction and Its Application to Fuel Cell

DAI Xian-Feng ZHENG Ming-Fu
XU Pan SHI Jing-Jing
MA Cheng-Yu QIAO Jin-Li

Acta Phys. -Chim. Sin. **2013**, 29 (8), 1753–1761



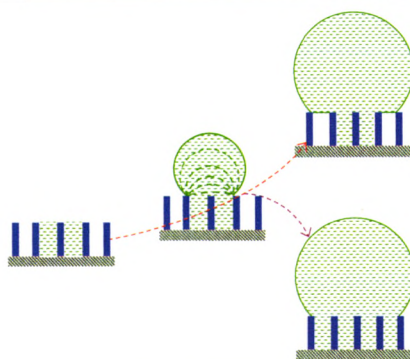
Novel non-precious catalysts based on pyridine-doped carbon-supported Co-phthalocyanine (Py-CoPc/C) nanoparticles were synthesized. Py doping significantly improves the catalytic activity of CoPc/C in the oxygen reduction reaction.

SOFT MATTER

Growth Modes of Condensates on Nanotextured Surfaces and Mechanism of Partially Wetted Droplet Formation

LIU Tian-Qing SUN Wei
LI Xiang-Qin SUN Xiang-Yu
AI Hong-Ru

Acta Phys. -Chim. Sin. **2013**, 29 (8), 1762–1770



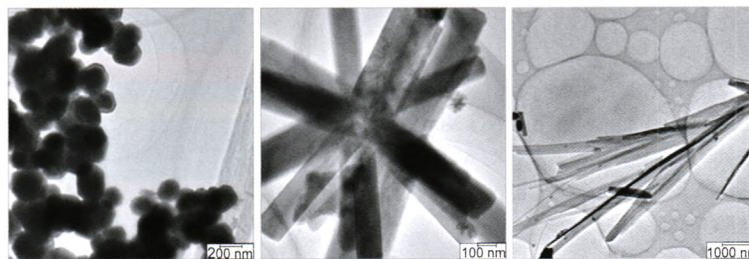
The growth modes of condensed droplets on nanotextured surfaces were analyzed by considering the energy increasing rate of the droplets.

CATALYSIS AND SURFACE SCIENCE

Controllable Synthesis and Photocatalytic Activity of Spherical, Flowerlike and Threadlike Bismuth Vanadates

LIN Xue YU Li-Li
YAN Li-Na GUAN Qing-Feng
YAN Yong-Sheng ZHAO Han

Acta Phys. -Chim. Sin. **2013**, 29 (8), 1771–1777

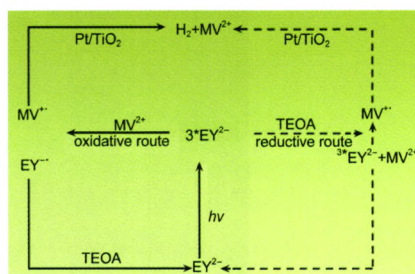


BiVO₄ particles with different morphologies that exhibited excellent visible-light-induced photocatalytic performance were fabricated. BiVO₄ microspheres showed the highest photocatalytic activity of the different morphologies produced.

Highly Active and Stable Catalyst for Visible Light Hydrogen Production Based on Oxidative Quenching of Eosin Y

LI Bo LÜ Gong-Xuan

Acta Phys. -Chim. Sin. **2013**, 29 (8), 1778–1784

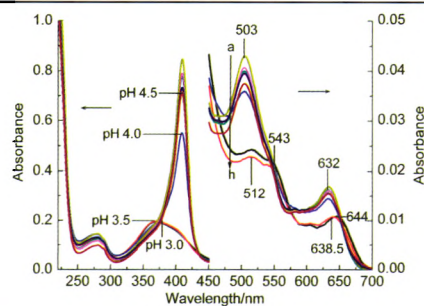


Methyl viologen (MV²⁺) promoted electron transfer from excited states of eosin Y (EY) to Pt/TiO₂ and effectively improved the activity and stability of photocatalytic hydrogen production by an EY-sensitized Pt/TiO₂ system based on an oxidative and reductive quenching mechanism.

Acid-Induced Unfolding Process of Myoglobin and Its Mutant under Macromolecular Crowding Conditions

ZHANG Yu-Jiao TANG Qian
CAO Hong-Yu ZHENG Xue-Fang

Acta Phys. -Chim. Sin. **2013**, 29 (8), 1785–1792

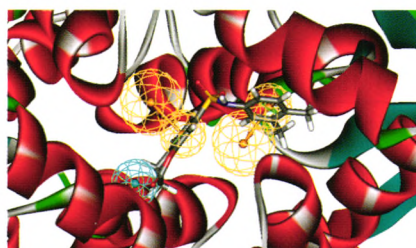


The unfolding process of myoglobin and its mutant induced by acid under macromolecular crowding conditions was investigated by a range of spectroscopic techniques.

Multicomplex-Based Pharmacophore and QSAR of Aryl-Sulfamides as Pyruvate Kinase M2 Activators

CHEN Zheng-Jun JIANG Qing-Lin
HE Gu HAN Bo
GUO Li

Acta Phys. -Chim. Sin. **2013**, 29 (8), 1793–1803

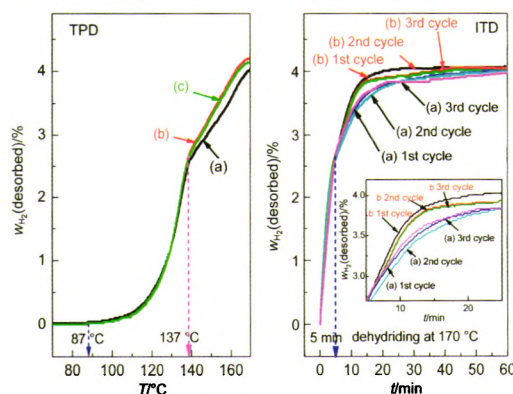


Multicomplex-based pharmacophore (MCBP) and MCBP-guided 3D-QSAR models are generated from a series of structurally diverse aryl-sulfamide PKM2 activators.

PHYSICAL CHEMISTRY OF MATERIALS

Influence of KH on Reversible Dehydrodring Performance of Na-Al-H Complex Hydride

WANG Shun-Kui LI Zhi-Jie
XIAO Xue-Zhang FAN Xiu-Lin
CHEN Zhi-Wen LI Shou-Quan
GE Hong-Wei CHEN Li-Xin



The addition of KH can improve the second step dehydrogenation kinetics of the Na-Al-H composite system. The enhanced dehydrogenation kinetics is mainly ascribed to the lattice volume expansion of Na_3AlH_6 that resulted from the addition of KH, which decreases the activation energy of the second step decomposition of NaAlH_4 .

Acta Phys. -Chim. Sin. **2013**, 29 (8), 1804–1808

Synthesis of Plate Like Silicalite-1 with Controlled Thickness

YAO Xiao-Qiang XU Xiang-Yu
LÜ Zhi JIAO Kun
SONG Jia-Qing LI Zhao-Fei
WANG Qian YAN Li-Jun
HE Ming-Yuan

Acta Phys. -Chim. Sin. **2013**, 29 (8), 1809–1813

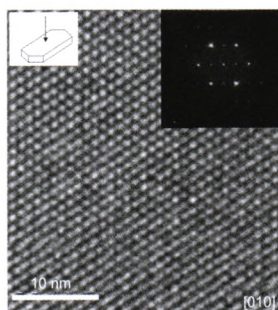
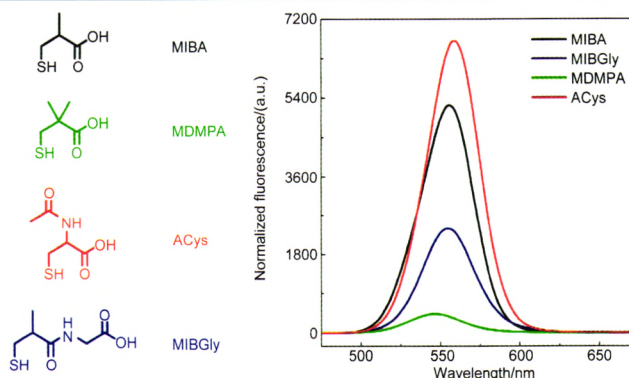


Plate like Silicalite-1 can be prepared by addition of NH_4F , and the plate thickness was controlled by modifying the molar ratio of NH_4F to SiO_2 .

Effects of Derivatives of 3-Mercaptoisobutyric Acid on the Aqueous Synthesis of CdTe Quantum Dots

MA Kai-Guo FANG Tan
BAI Jin-Yi GUO Hai-Qing

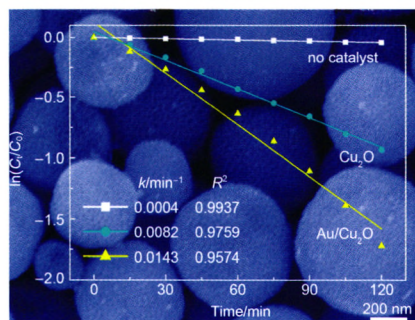


N-Acetylcysteine (ACys), a 3-mercaptoisobutyric acid derivative with a hydrophilic side-chain, can be used to produce CdTe quantum dots (QDs) with strong fluorescence.

Acta Phys.-Chim. Sin. **2013**, 29 (8), 1814–1818

Synthesis and Visible Light Photocatalytic Activities of Au/Cu₂O Heterogeneous Nanospheres

SHANG Yang CHEN Yang
SHI Zhan-Bin ZHANG Dong-Feng
GUO Lin

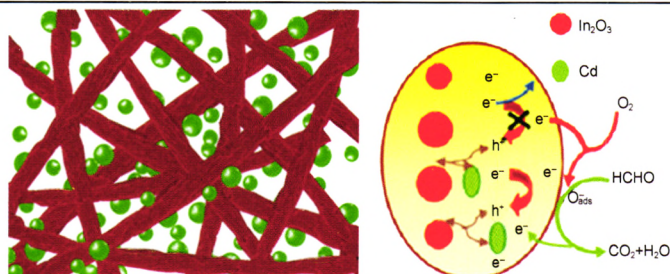


Au/Cu₂O heterogeneous nanospheres with high photocatalytic activity are prepared by an *in-situ* reduction process.

Acta Phys.-Chim. Sin. **2013**, 29 (8), 1819–1826

Preparation of Electrospun In₂O₃/CdO Composite and Its Formaldehyde-Sensing Properties

CHEN Peng-Peng WANG Jing
ZHANG Chun-Li HAO Yu-Wen
DU Hai-Ying



Sensors based on In₂O₃/CdO composite nanofibers possessed excellent sensing properties to formaldehyde and the sensing mechanism was analyzed.

Acta Phys.-Chim. Sin. **2013**, 29 (8), 1827–1836