

物理化学学报

ACTA PHYSICO-CHIMICA SINICA

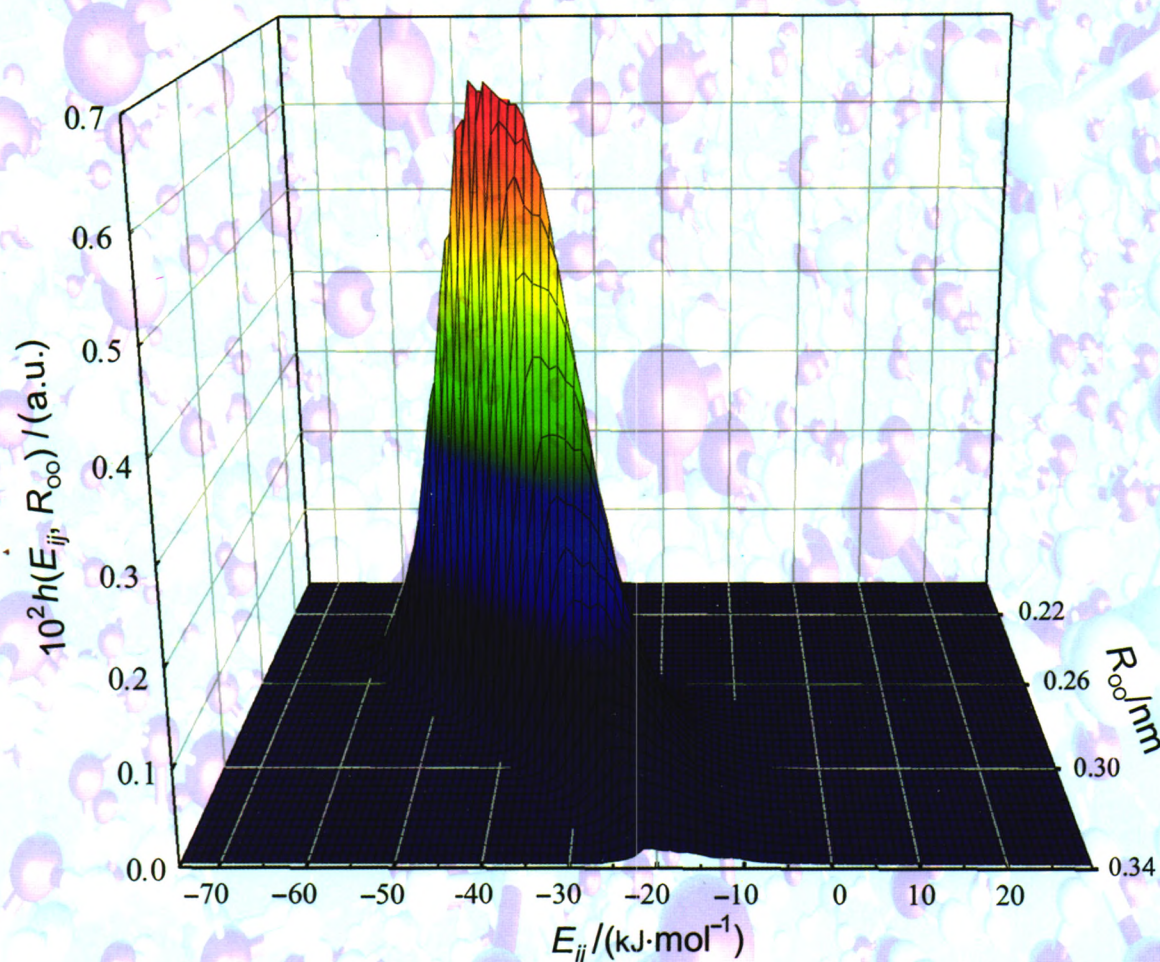
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中国化学会、北京大学主办
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..... 乔荫颇 殷海荣 张燕斌 潘云娟 乔 璐 刘 婷(2056)

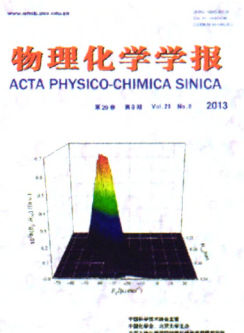
材料物理化学

微波水热合成 Zn₂GeO₄ 纳米带及其光催化活性 杜书青 袁宇峰 涂伟霞(2062)

第十七次全国电化学大会第二轮通知 (2026)

本期责任编辑: 黄 路

COVER



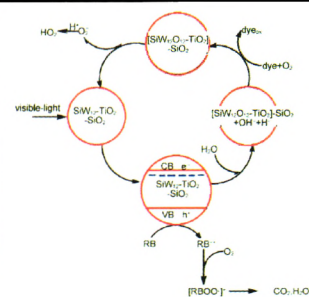
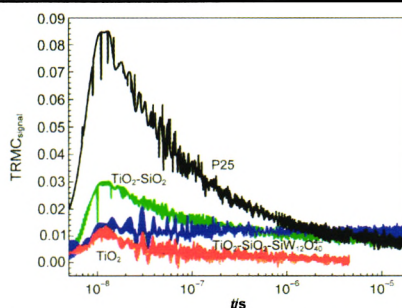
The cover image presents the three-dimensional normalized statistical distribution of the hydrogen bonded molecules as a function of pair interaction energy and acceptor-donor distance. On page 1891, ZHANG *et al.* demonstrate that both geometric and energetic criteria have deficiencies in determining hydrogen bonds, and extended criterion involving both geometric and energetic thresholds is recommended for hydrogen bonding analysis.

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COMMUNICATION

Synthesis of Ternary Hybrid $\text{TiO}_2\text{-SiO}_2\text{-POM}$ Catalysts and Its Application in Degrading Rhodamine B under Visible Light Illumination

WANG Xiao-Xia XU Hua-Long
SHEN Wei RUHLMANN Laurent
QIN Feng SORGUES Sébastien
COLBEAU-JUSTIN Christophe



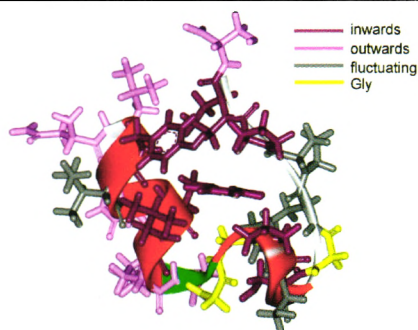
The high photocatalytic activity of $\text{TiO}_2\text{-SiO}_2\text{-SiW}_{12}\text{O}_{40}$ under visible light illumination results from the synergistic effect among the three components.

Acta Phys. -Chim. Sin. **2013**, 29 (9), 1837–1841

REVIEWS

Research Progress of the Trp-Cage Formation and Its Folding Mechanism

WU Xiao-Min YUAN Xiao-Hui
XUE Shu-Lei ZHA Ling-Sheng
WANG Guang-Li ZHANG Hai-Jun

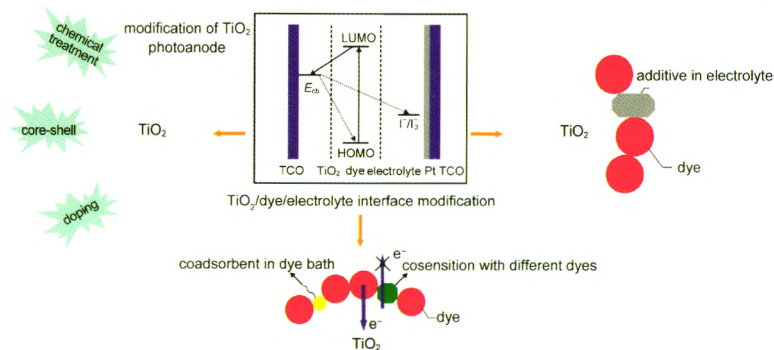


A few key residues (inwards) cooperated with special effects of “non-key residues” (outwards or with fluctuating orientation) as the driving force for the folding of the Trp-cage mini-protein.

Acta Phys. -Chim. Sin. **2013**, 29 (9), 1842–1850

TiO₂/Dye/Electrolyte Interface Modification for Dye-Sensitized Solar Cells

LI Jing-Zhe KONG Fan-Tai
WU Guo-Hua HUANG Yang
CHEN Wang-Chao DAI Song-Yuan

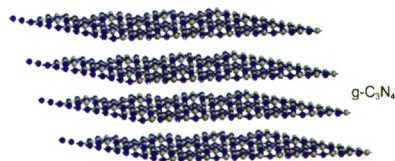


Acta Phys. -Chim. Sin. **2013**, 29 (9), 1851–1864

Chemical Synthesis and Applications of Graphitic Carbon Nitride

ZHANG Jin-Shui WANG Bo
WANG Xin-Chen

Different methods of TiO₂/dye/electrolyte interface modification (by modifying TiO₂, the dye bath, or the electrolyte solution) are reviewed in detail.



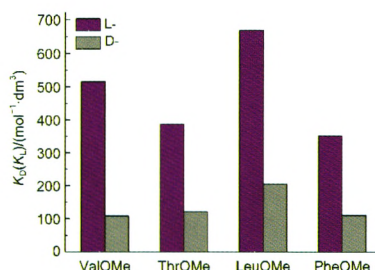
Graphitic carbon nitride (g-C₃N₄), with a layered structure analogous to graphite, has been widely used in fields related to energy and material science, because of its unique electronic structure and excellent chemical inertness. In this review, some recent advances in g-C₃N₄ synthesis and applications are presented. The prospects for the development of g-C₃N₄ in energy- and environment-related fields are also discussed.

Acta Phys. -Chim. Sin. **2013**, 29 (9), 1865–1876

THERMODYNAMICS, KINETICS, AND STRUCTURE CHEMISTRY

Molecular Recognition of Glycoconjugated Porphyrin with Chiral Amino Acid Methyl Ester

YANG Le-Le LIU Jia
LI Yue LIU Kun
RUAN Wen-Juan

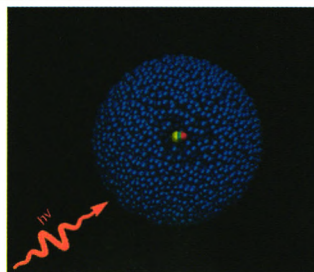


The recognition actions of three atropisomeric tetrasaccharide-substituted zinc porphyrins toward a set of amino acid methyl esters were explored by spectroscopic titration.

Acta Phys. -Chim. Sin. **2013**, 29 (9), 1877–1885

Photodissociation Dynamics of Carbonyl Sulfide in Helium Droplets

ZHANG Cui-Mei ZHANG Zhi-Guo
HUANG Cun-Shun ZHANG Qun
CHEN Yang

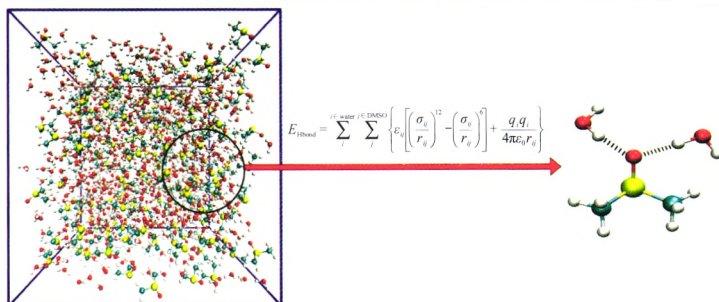


The surrounding helium atoms show cage effects on the photodissociation of carbonyl-sulfide doped helium droplets.

Acta Phys. -Chim. Sin. **2013**, 29 (9), 1886–1890

Evaluation of the Application of Hydrogen Bonding Criteria to DMSO Aqueous Solution

ZHANG Ning LI Wei-Zhong
CHEN Cong ZUO Jian-Guo



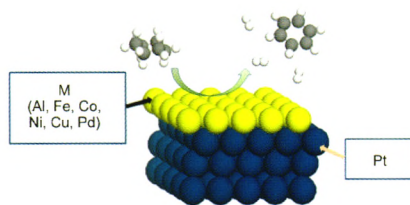
Hydrogen bonding in DMSO/water mixtures is studied by molecular dynamics simulations using geometric and energetic criteria to determine the most suitable criterion.

Acta Phys. -Chim. Sin. **2013**, 29 (9), 1891–1899

THEORETICAL AND COMPUTATIONAL CHEMISTRY

Study of Hydrogen Adsorption on Pt and Pt-Based Bimetallic Surfaces by Density Functional Theory

GAO Zi-Feng CHEN Hao
QI Sui-Tao YI Chun-Hai
YANG Bo-Lun

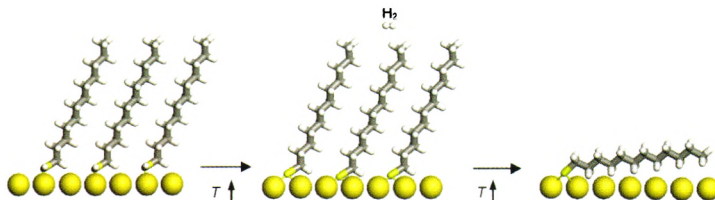


The addition of a 3d metal monolayer on a Pt(111) surface can change the hydrogen adsorption, revealing that 3d-Pt surfaces are likely to have better dehydrogenation activity than Pt.

Acta Phys. -Chim. Sin. **2013**, 29 (9), 1900–1906

Density Functional Theory Study on the Adsorption of Dodecylthiol on Au(111) Surface

FAN Xiao-Li RAN Run-Xin
ZHANG Chao YANG Yong-Liang

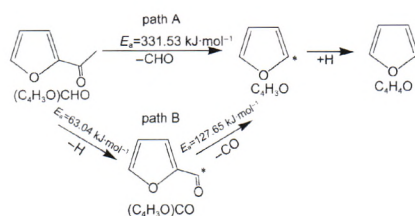


At low temperatures, the $C_{12}H_{25}SH$ molecule prefers to stay on the top site, when the surface temperature is increased, the S–H bond may be cleaved and the H atoms desorb as H_2 , and the lying-down geometry of the $C_{12}H_{25}S$ group adsorption may appear.

Acta Phys. -Chim. Sin. **2013**, 29 (9), 1907–1915

Adsorption and Decarbonylation Reaction of Furfural on Pt(111) Surface

NI Zhe-Ming XIA Ming-Yu
SHI Wei QIAN Ping-Ping

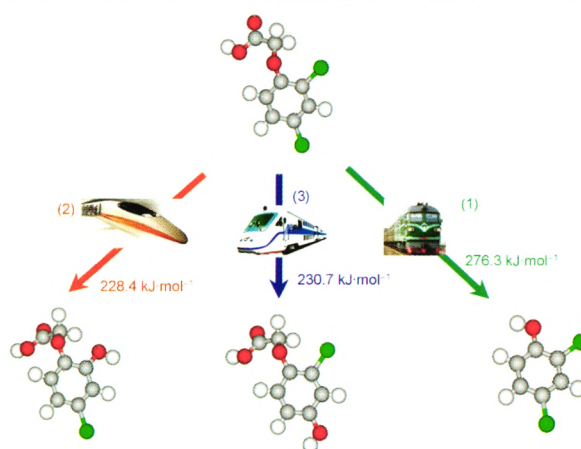


The reaction mechanism for formation of furan from decarbonylation of furfural on the Pt(111) plane was investigated theoretically. Furfural formed an acyl intermediate by losing the H atom from the branched chain rather than direct decarbonylation.

Acta Phys. -Chim. Sin. **2013**, 29 (9), 1916–1922

Hydrolysis Reaction Mechanism of 2,4-Dichlorophenoxy Acetic Acid Metabolism

LI Jia XU Wen-Li
HU Jing LING Min
YAO Jian-Hua

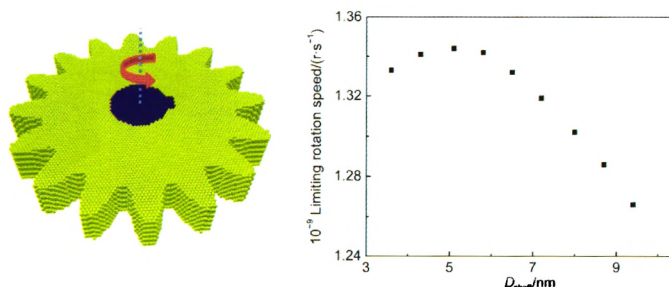


Acta Phys. -Chim. Sin. **2013**, 29 (9), 1923–1930

In the metabolism of 2,4-dichlorophenoxy acetic acid, the energy barrier of the first step reaction determines the priority of metabolism paths.

Molecular Dynamics Simulation of a Nanosized Device

SUN Wei ZHANG Jin-Jiang
ZHAO Jian-Wei

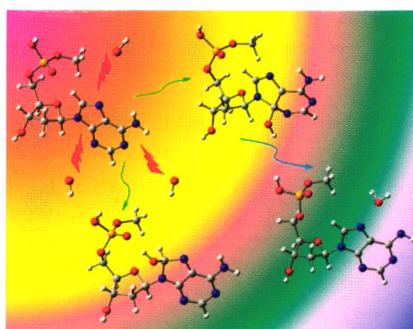


Acta Phys. -Chim. Sin. **2013**, 29 (9), 1931–1936

Molecular dynamics simulations show that a size effect limits the rotation speed of a nanogear.

Radicals Created from the Reactions of 2'-Deoxyadenosine-5'-monophosphate with Hydroxyl Radical

HOU Ruo-Bing TANG Zong-Xiang
FAN You-Jun YI Xiang-Hui
WANG Bei-Bei SUN Yan-Li

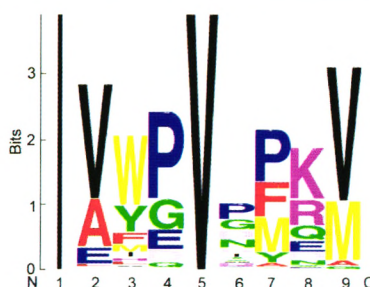


The thermodynamics of the reactions of 2'-deoxyadenosine 5'-monophosphate with a hydroxyl radical depends primarily on the stability of the products and the electrostatic interactions between the reactants.

Acta Phys. -Chim. Sin. **2013**, 29 (9), 1937–1944

Prediction of HLA-A*0201 Restricted Cytotoxic T Lymphocyte Epitopes Based on High-Dimensional Descriptor Nonlinear Screening

HAN Na YUAN Zhe-Ming
CHEN Yuan DAI Zhi-Jun
WANG Zhi-Ming

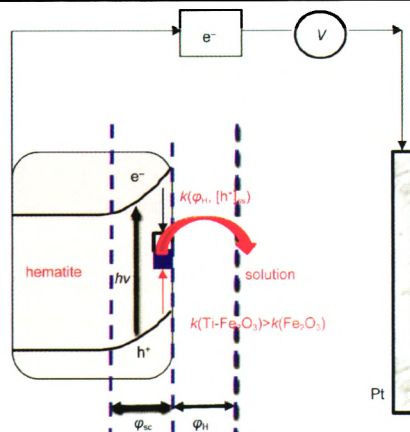


The preferred amino acid distribution at each position of HLA-A*0201 restricted cytotoxic T lymphocyte epitopes reveals the relationship between sequence and affinity activity.

Acta Phys. -Chim. Sin. **2013**, 29 (9), 1945–1953

Influence of the Potential on the Charge-Transfer Rate Constant of Photooxidation of Water over α -Fe₂O₃ and Ti-Doped α -Fe₂O₃

SHANGGUAN Peng-Peng
TONG Shao-Ping LI Hai-Li
LENG Wen-Hua

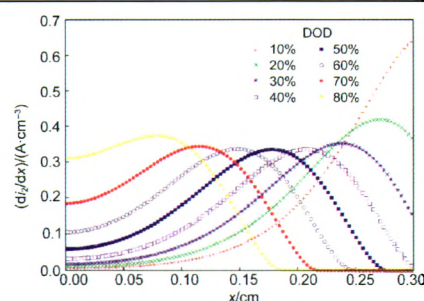


Potential can drop across the Helmholtz layer of undoped and Ti-doped α -Fe₂O₃ and influence the rate constant of water photooxidation.

Acta Phys. -Chim. Sin. **2013**, 29 (9), 1954–1960

Numerical Simulation of Discharge Process and Failure Mechanisms of Zinc Electrode

SONG Hui XU Xian-Zhi
LI Fen

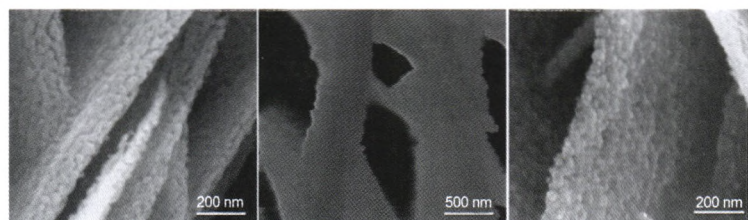


A uniform distribution of transfer current density during discharge is expected for an ideal zinc electrode.

Acta Phys. -Chim. Sin. **2013**, 29 (9), 1961–1974

Increasing Specific Surface Area of (110)-Oriented ZnO Nanosheets by Sulfuration-Oxidization Treatment for Photoelectrode Applications

WEI Yu-Long BAO Chun-Xiong
GAO Hao HUANG Huan
YU Tao ZOU Zhi-Gang

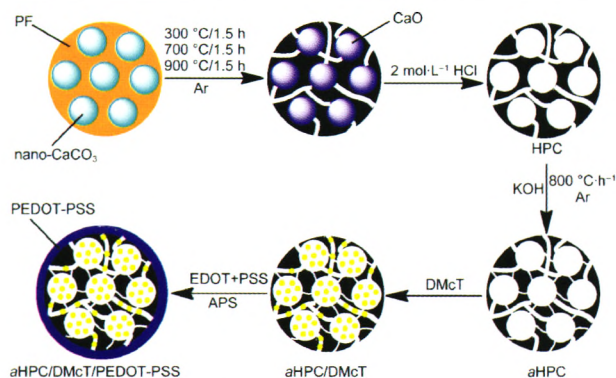


Sulfuration-oxidization treatment induces morphological change in ZnO nanosheets.

Acta Phys. -Chim. Sin. **2013**, 29 (9), 1975–1980

Hierarchically Porous Carbon/DMcT/PEDOT-PSS Ternary Composite as a Cathode Material for Lithium-Ion Battery

CHI Ting-Yu LI Han
WANG Geng-Chao

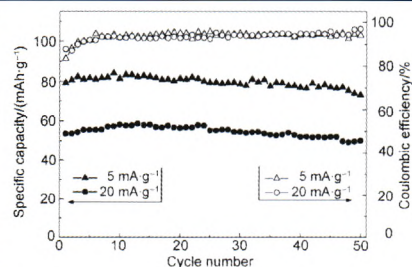
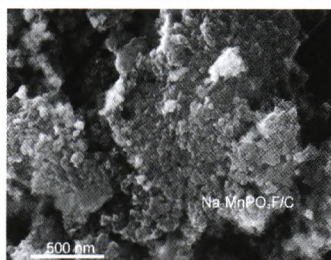


The activated hierarchically porous carbon (aHPC)/DMcT/PEDOT-PSS ternary composite was prepared through a solution immersion and *in situ* oxidative polymerization method. The specific capacity and cycling stability of the ternary composite were significantly improved by the absorption of aHPC and the surface coating of PEDOT-PSS.

Acta Phys. -Chim. Sin. **2013**, 29 (9), 1981–1988

Synthesis of $\text{Na}_2\text{MnPO}_4\text{F/C}$ with Different Carbon Sources and Their Performances as Cathode for Lithium Ion Battery

ZHONG Yan-Jun LI Jun-Tao
WU Zhen-Guo ZHONG Ben-He
GUO Xiao-Dong HUANG Ling
SUN Shi-Gang

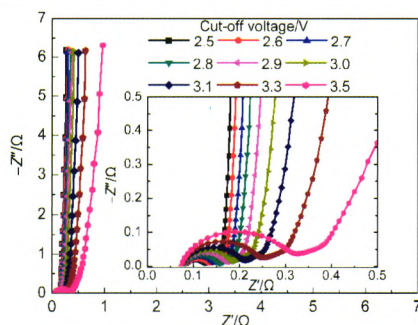


Four carbons sources, i.e., stearic acid, citric acid, poly(ethylene glycol) 6000, and β -cyclodextrin, were used to synthesize $\text{Na}_2\text{MnPO}_4\text{F/C}$ composites by wet ball milling and *in situ* pyrolytic carbon coating. A series of investigations confirmed that the sample prepared using citric acid had a micro-nano structure and the smallest primary particle size, and exhibited the best electrochemical performances.

Acta Phys. -Chim. Sin. **2013**, 29 (9), 1989–1997

Organic Electrolytes for Activated Carbon-Based Supercapacitors with Flexible Package

HUANG Bo SUN Xian-Zhong
ZHANG Xiong ZHANG Da-Cheng
MA Yan-Wei



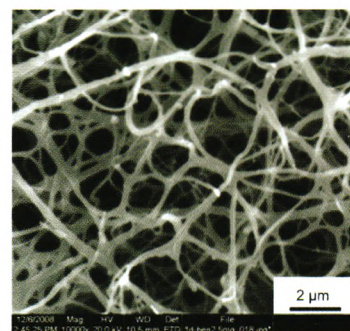
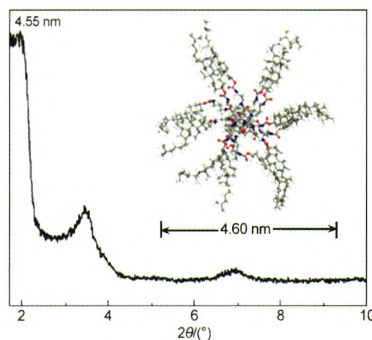
A novel organic electrolyte, triethylmethylammonium tetrafluoroborate/acetonitrile + propylene carbonate, was characterized electrochemically and its performance was compared with that of other electrolytes at 3 V.

Acta Phys. -Chim. Sin. **2013**, 29 (9), 1998–2004

SOFT MATTER

Synthesis and Gelation Properties of Cholesterol-Based New Low-Molecular-Mass Gelators

XUE Min MIAO Qing
FANG Yu

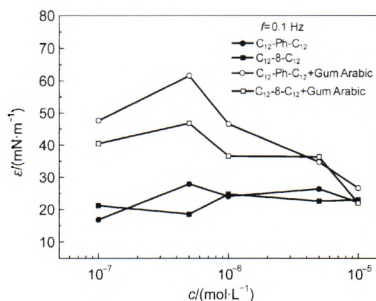


Gels with excellent properties, such as room temperature gelation, thixotropic properties, and gel film formation, were synthesized.

Acta Phys. -Chim. Sin. **2013**, 29 (9), 2005–2012

Impact of the Addition of Gum Arabic on the Interface Dilational Properties of Gemini Surfactants

XIONG Ke-Jie SHU Zhan-Xia
NIE Hai-Yu DU Feng-Pei

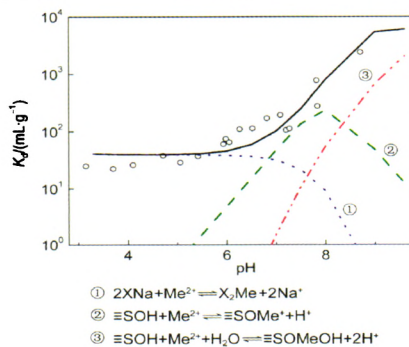


The addition of 1%(w) Gum Arabic in Gemini surfactant solutions caused the interfacial tension and the interfacial dilational modulus to show different trends. This was explained as an electrostatic interaction between the Gum Arabic and surfactant molecules.

Acta Phys. -Chim. Sin. **2013**, 29 (9), 2013–2018

Adsorption of Co(II) and Ni(II) on Beishan Granite: Surface Complexation Model and Linear Free Energy Relationship

CHEN Zong-Yuan ZHANG Rui
YANG Xing-Long WU Wang-Suo
GUO Zhi-Jun LIU Chun-Li

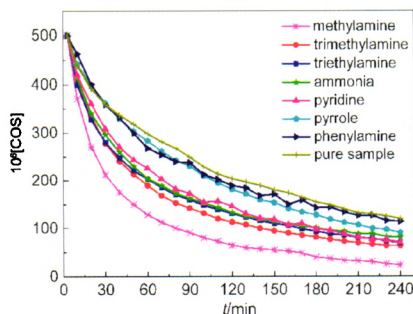


The adsorption of Co(II) and Ni(II) on granite was quantitatively interpreted by a model with one cation exchange reaction and two inner-sphere surface complexation reactions.

Acta Phys. -Chim. Sin. **2013**, 29 (9), 2019–2026

Effects of Ammonia and Amines on Heterogeneous Oxidation of Carbonyl Sulfide on Hematite

ZHANG Shuan-Qin KONG Ling-Dong
ZHAO Xi Roeland JANSEN
CHEN Jian-Min

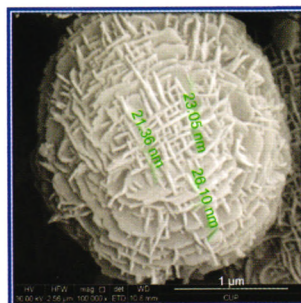


Ammonia and amines pre-adsorbed on hematite enhanced the reactivity of carbonyl sulfide and different amines affected the reactivity differently.

Acta Phys. -Chim. Sin. **2013**, 29 (9), 2027–2034

Synthesis and Characterization of Nanosheet ZSM-5 Zeolites with Different SiO₂/Al₂O₃ Molar Ratios

WANG Wu-Gang ZHANG Shao-Long
ZHANG Lan-Lan WANG Yan
LIU Xiao-Ling GONG Yan-Jun
DOU Tao

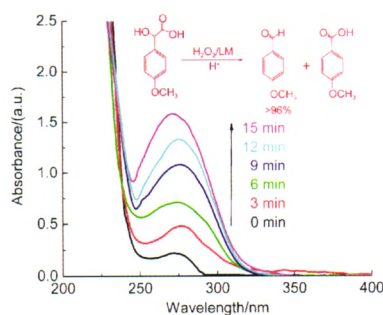


Syntheses of nanosheet ZSM-5 zeolites with different SiO₂/Al₂O₃ molar ratios were investigated in detail and a three-phase region for synthesis of the nanosheet ZSM-5 zeolite was provided.

Acta Phys. -Chim. Sin. **2013**, 29 (9), 2035–2040

Selective Oxidation of 4-Methoxymandelic Acid Catalyzed by Mononucleonic and Binucleonic Metal Complexes

YU Wei-Feng MENG Xiang-Guang
LIU Ying LI Xiao-Hong

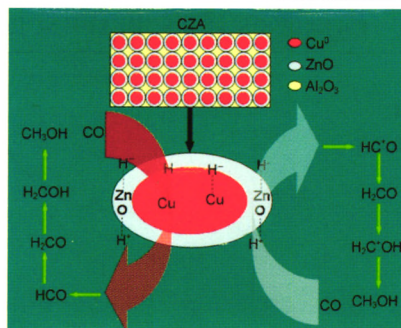


The copper complex displayed excellent catalytic ability for the selective oxidation of 4-methoxymandelic acid by H₂O₂ in a tartaric acid buffer solution.

Acta Phys. -Chim. Sin. **2013**, 29 (9), 2041–2046

Effect of Surface Promoters-Modifying on Catalytic Performance of Cu/ZnO/Al₂O₃ Methanol Synthesis Catalyst

HAO Ai-Xiang YU Yang
CHEN Hai-Bo MAO Chun-Peng
WEI Shi-Xin YIN Yu-Sheng



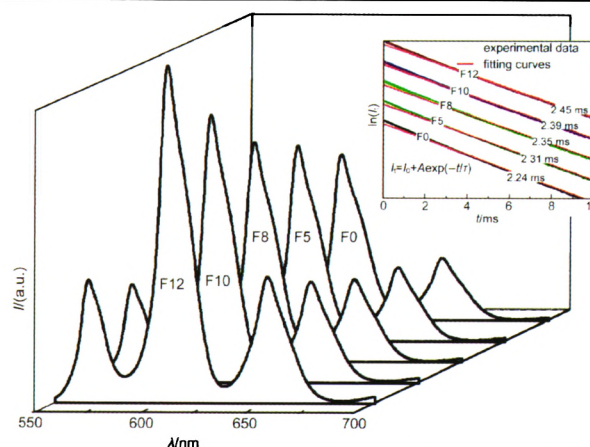
ZrO₂, as a surface promoter, can improve significantly the catalytic performance and thermal stability of a Cu/ZnO/Al₂O₃ methanol synthesis catalyst.

Acta Phys. -Chim. Sin. **2013**, 29 (9), 2047–2055

PHOTOCHEMISTRY AND RADIATION CHEMISTRY

Enhanced Photoluminescence Properties of CaF₂ in CaO-CaF₂-B₂O₃-SiO₂ Glass Doped with Sm₂O₃

QIAO Yin-Po YIN Hai-Rong
ZHANG Yan-Bin PAN Yun-Juan
QIAO Lu LIU Ting



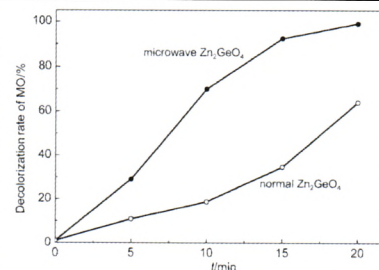
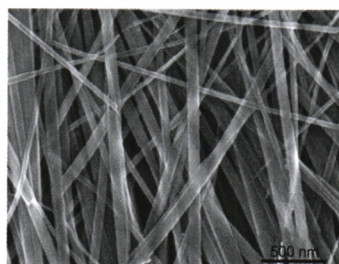
The emission intensity and fluorescent lifetime of CaO-CaF₂-B₂O₃-SiO₂ glass doped with samarium oxide can be enhanced and tuned by the CaF₂ content in the glass matrix.

Acta Phys. -Chim. Sin. **2013**, 29 (9), 2056–2061

PHYSICAL CHEMISTRY OF MATERIALS

Microwave-Hydrothermal Synthesis and Photocatalytic Activity of Zn₂GeO₄ Nanoribbons

DU Shu-Qing YUAN Yu-Feng
TU Wei-Xia



Mono-dispersed Zn₂GeO₄ nanoribbons were synthesized *via* a microwave hydrothermal method, and were found to show high photocatalytic activity with high surface area and less native defects.

Acta Phys. -Chim. Sin. **2013**, 29 (9), 2062–2068