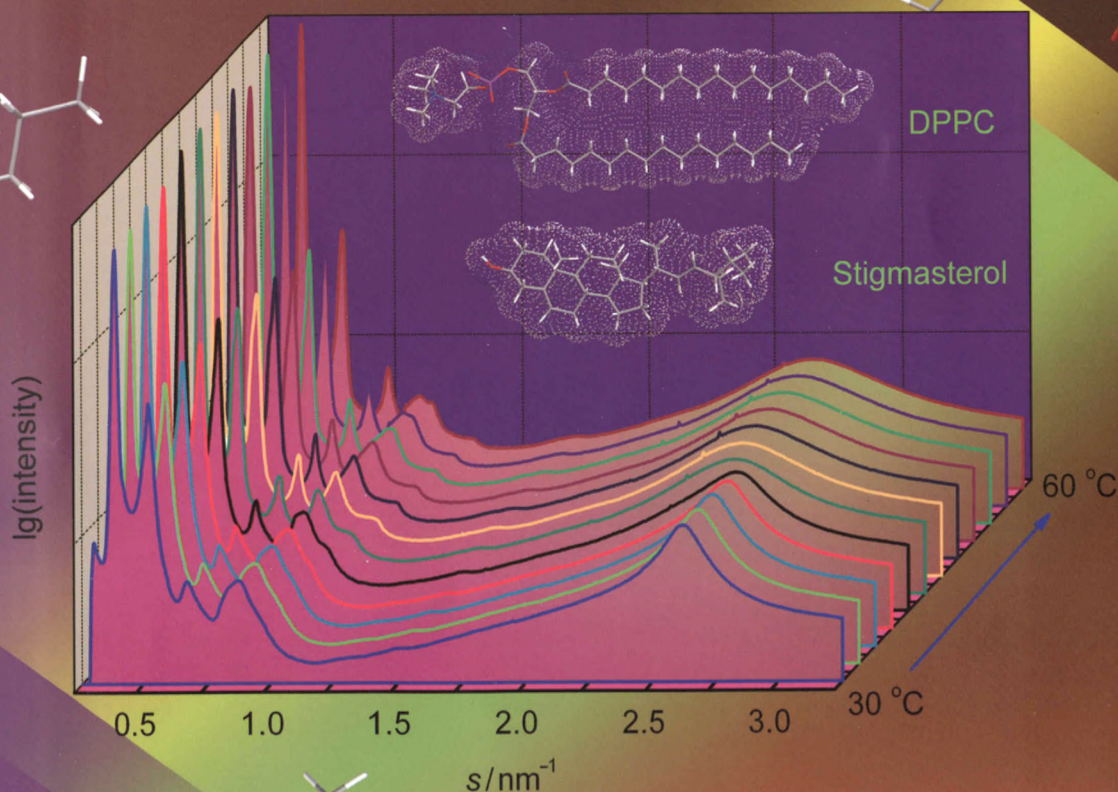


物理化学学报

ACTA PHYSICO-CHIMICA SINICA

第 28 卷 第 8 期 Vol.28 No.8 2012



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中国化学会、北京大学主办
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物理化学学报(Wuli Huaxue Xuebao)
第 28 卷第 8 期(2012 年 8 月)

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..... 郑 斌 张安峰 刘 民 丁凡舒 代成义 宋春山 郭新闻(1943)

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..... 张荣斌 梁 蕾 曾宪荣 商金艳 汪 涛 蔡建信(1951)

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..... 杨晓艳 孙 松 丁建军 张 义 张曼曼 高 琛 鲍 骏(1957)

Cu-Fe基双孔载体催化剂结构和低碳醇合成反应性能..... 刘建国 定明月 王铁军 马隆龙(1964)

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..... 李慧泉 崔玉民 吴兴才 华 林 洪文珊(1985)

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..... 申剑磊 杨新国 黄 燎 沈启立 刘振辉 张凤菊(1992)

基于三苯胺和螺(芴-9,9'-氧杂蒽)的星射形蓝光寡聚材料的合成与光电性质

..... 初增泽 王 丹 张 超 邹德春(2000)

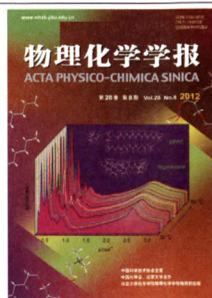
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..... 郭瑞光 陈 琳 尉志武(2008)

本期责任编辑: 黄 路

COVER



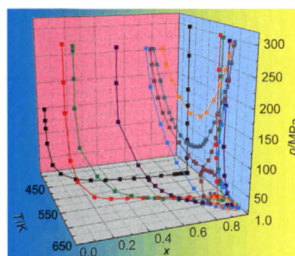
The cover image presents the temperature-dependent synchrotron small-angle and wide-angle X-ray diffraction patterns of a lipid dispersion containing 85% dipalmitoylphosphatidylcholine (DPPC) and 15% stigmasterol. The molecular structures of the two lipids are also shown. On page 2008, WU *et al.* demonstrate that the *d*-spacings of SAXS of Lo phase change slightly, while those of WAXS change markedly, with sterol concentration and temperature.

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Gas-Liquid Phase Boundary Lines and Critical Curve for the Water+Methane System

TIAN Yu-Qin TIAN Yi-Ling
ZHAO Lin ZHU Rong-Jiao
MA Chao

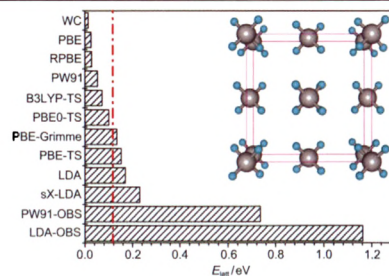


The isothermal gas-liquid phase boundary lines and critical curve were determined for the water + methane system.

Acta Phys. -Chim. Sin. **2012**, 28 (8), 1803–1808

Lattice Energies and Elastic Properties of Solid Methane: Assessment of Different Density Functionals

ZHENG Zhao-Yang ZHAO Ji-Jun

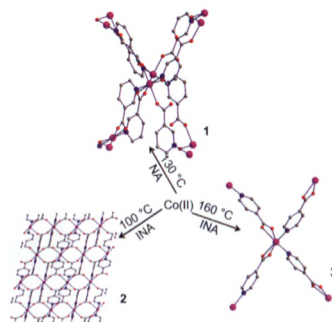


For solid methane, DFT-D methods perform better than standard and hybrid DFT functionals, but overcorrect the dispersion interaction.

Acta Phys. -Chim. Sin. **2012**, 28 (8), 1809–1814

Crystal Structures and Pore Stability of Coordination Polymers Constructed by Nicotinic Acid and Isonicotinic Acid with Co(II)

HUA Xiao-Hui LI Wei-Hong
XU Yi-Zhuang WU Jin-Guang

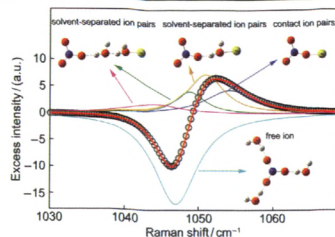


Various coordination modes of nicotinic acid and isonicotinic acid to Co(II) lead to 1D channels and variable pore stabilities.

Acta Phys. -Chim. Sin. **2012**, 28 (8), 1815–1822

Ion Pairs in Aqueous Magnesium Nitrate Solution by Excess Raman Spectroscopy

WANG Chen-Chen LIN Ke
HU Nai-Yin ZHOU Xiao-Guo
LIU Shi-Lin



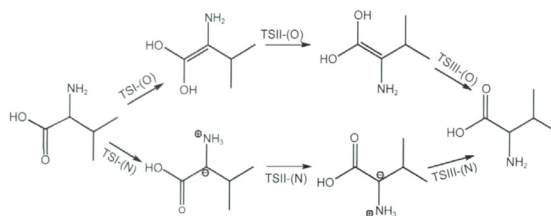
Raman spectroscopy of the ion associations in magnesium nitrate solution identifies various ion pairs. From the Raman analysis of NO_3^- symmetric $-\text{OH}$ stretching regions, contact ion pairs and solvent separated ion pairs are found to exist in varying amounts in different concentration regions.

Acta Phys.-Chim. Sin. **2012**, 28 (8), 1823–1829

THEORETICAL AND COMPUTATIONAL CHEMISTRY

Two Possible Photoreaction Pathways of L-Valine Optical Isomerization

MA Chi-Cheng PU Min
WEI Min LI Jun-Nan
LI Zhi-Hong

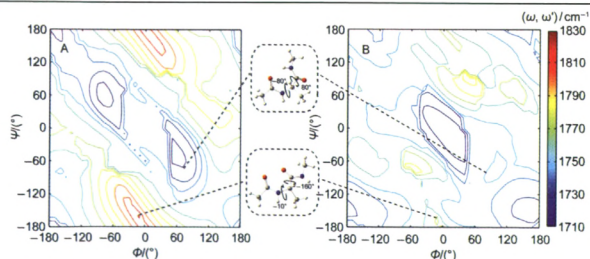


Two photoreaction pathways are proposed in which the intrinsic variation is the hydrogen transfer of carbonyl O or amino N atom in the excited state.

Acta Phys.-Chim. Sin. **2012**, 28 (8), 1830–1836

Secondary Structure and Vibrational Spectral Feature of Alanine Dipeptide

CAI Kai-Cong LIU Shan-Hong
LIU Di-Wen LIN Shen

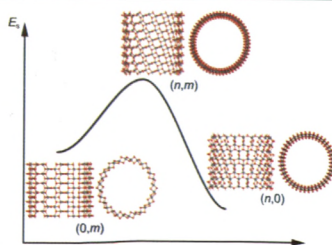


The amide-I modes of alanine dipeptide were used as vibrational probe to reveal the structural features of polypeptides.

Acta Phys.-Chim. Sin. **2012**, 28 (8), 1837–1842

A Tight-Binding Density Functional Theory Study on Single-Walled Nanotubes from Anatase TiO_2 (101) Sheets

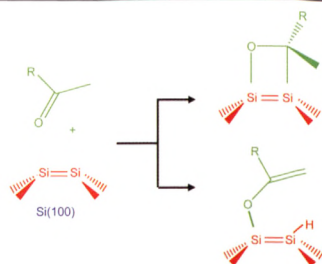
LIU Hao LIN Meng-Hai
TAN Kai



The strain energy (E_s) of TiO_2 nanotubes is dependent on the chirality of nanotube at a given diameter.

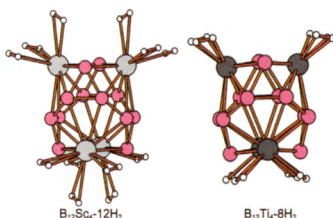
Acta Phys.-Chim. Sin. **2012**, 28 (8), 1843–1848

ZHANG Ji-Chao CHENG Xue-Li
CHENG Yu-Qiao MENG Xiang-Hua
LIU Yong-Jun LIU Cheng-Bu



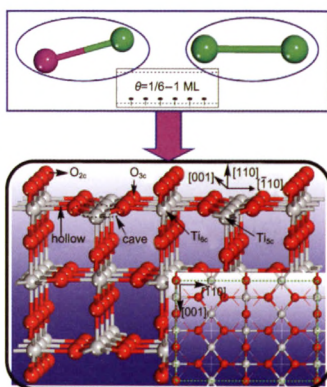
Acta Phys. -Chim. Sin. 2012, 28 (8), 1849–1853

MA Li-Juan WANG Jian-Feng
JIA Jian-Feng WU Hai-Shun



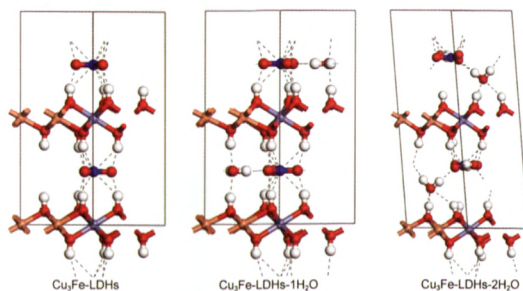
Acta Phys. -Chim. Sin. 2012, 28 (8), 1854–1860

ZHAO Wei-Na LIN Hua-Xiang
LI Yi ZHANG Yong-Fan
HUANG Xin CHEN Wen-Kai



Acta Phys. -Chim. Sin. 2012, 28 (8), 1861–1868

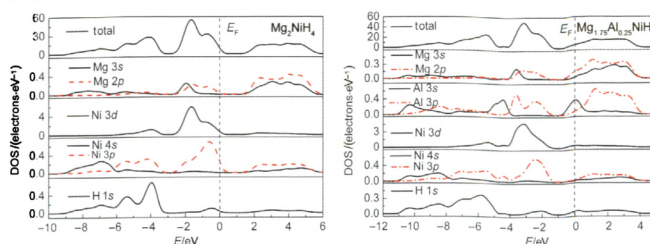
SHI Wei HU Jun
NI Zhe-Ming LI Yuan
LIU Jiao



Acta Phys. -Chim. Sin. 2012, 28 (8), 1869–1876

Effect of Doping with Aluminium on the Electronic Structure and Hydrogen Storage Properties of Mg₂Ni Alloy

LAN Zhi-Qiang XIAO Xiao
SU Xin CHEN Jie-Shi
GUO Jin

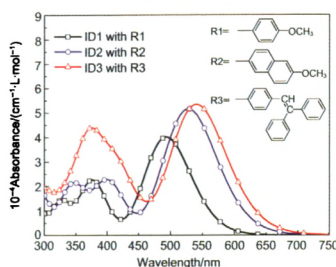


Hydrogen desorption kinetics for a Mg₂Ni hydride can be improved with the partial substitution of Al for Mg.

Acta Phys.-Chim. Sin. **2012**, 28 (8), 1877–1884

Effect of Donor Moieties on the Electronic Structures and Absorption Spectra of Indoline Dyes

LIANG Gui-Jie ZHONG Zhi-Cheng
CHEN Mei-Hua XU Jie
XU Wei-Lin HE Ping
HOU Qiu-Fei LI Zai-Fang

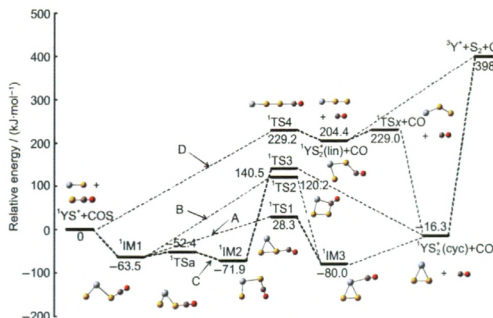


Increasing the number of phenyl groups in the donor in ID1–ID3 improves the light harvesting efficiency.

Acta Phys.-Chim. Sin. **2012**, 28 (8), 1885–1891

Theoretical Study on Gas-Phase Reaction of YS⁺ (¹Σ⁺, ³Φ) with COS of YS⁺+COS→YS₂+CO

YANG Shu YANG Xiao-Mei
XIE Xiao-Guang



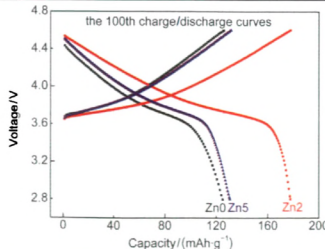
Mechanism of gas-phase S-transfer reaction (YS⁺+COS→YS₂+CO) was studied theoretically.

Acta Phys.-Chim. Sin. **2012**, 28 (8), 1892–1898

ELECTROCHEMISTRY AND NEW ENERGY

Improved Electrochemical Stability of Zn-Doped LiNi_{1/3}Co_{1/3}Mn_{1/3}O₂ Cathode Materials

LI Jie-Bin XU You-Long
DU Xian-Feng SUN Xiao-Fei
XIONG Li-Long

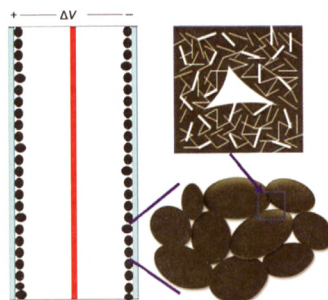


The improved electrochemical stability of Zn-doped LiNi_{1/3}Co_{1/3}Mn_{1/3}O₂ is attributed to reduced electrode polarization and impedance values, and an increased Li-ion diffusion coefficient.

Acta Phys.-Chim. Sin. **2012**, 28 (8), 1899–1905

Preparation and Electrochemical Performance of Microporous Carbon Microspheres Obtained from Potato Starch

FU Xiao-Ting JIA Fan
LI Wen-Bin CHEN Ming-Ming
WANG Cheng-Yang

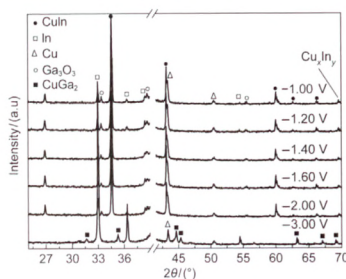


Owing to the microporous structure and spherical shape, the starch based activated microspheres showed superior capacitive performance.

Acta Phys.-Chim. Sin. **2012**, 28 (8), 1906–1912

Electrodeposited Gallium on Gallium and Copper/Indium Substrates

ZHANG Chao AO Jian-Ping
WANG Li JIANG Tao
SUN Guo-Zhong HE Qing
ZHOU Zhi-Qiang SUN Yun

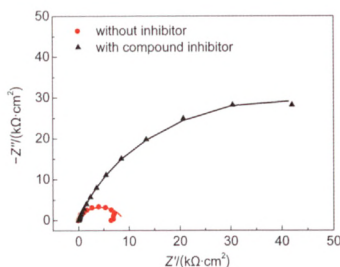


Ga electrodeposition on Cu/In films from acidic aqueous solutions produces CuGa_2 at the Cu/In interface. Subsequent annealing of the films in an Se atmosphere produces high quality $\text{Cu}(\text{In}_{1-x}\text{Ga}_x)\text{Se}_2$ (CIGS) thin films and the efficiency of the solar cell prepared using these films is 9.42%.

Acta Phys.-Chim. Sin. **2012**, 28 (8), 1913–1922

Effect of Sodium D-Gluconate-Based Inhibitor in Preventing Corrosion of Reinforcing Steel in Simulated Concrete Pore Solutions

YANG Rong-Jie GUO Ya
TANG Fang-Miao WANG Xiao-Ping
DU Rong-Gui LIN Chang-Jian

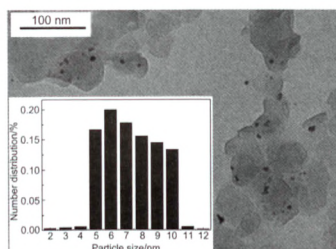


The compound inhibitor with sodium D-gluconate, Na_2MoO_4 , and thiourea had a significant corrosion inhibition effect on the reinforcing steel in the simulated concrete pore solution with NaCl. The radii of capacitive semicircles for the steel decreased in the solution with the inhibitor.

Acta Phys.-Chim. Sin. **2012**, 28 (8), 1923–1928

Layered Double Hydroxide Supported Palladium Nanoparticles for Electrocatalytic Oxidation of Hydrazine

JIN Rong-Rong LI Li-Fang
XU Xue-Feng LIAN Ying-Hui
ZHAO Fan

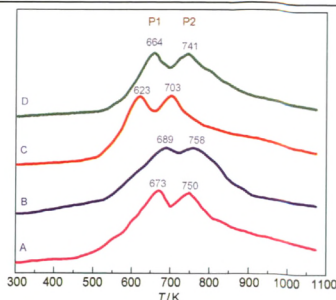


Layered double hydroxide supported palladium nanomaterials exhibit excellent electrocatalytic activity with regard to the oxidation of hydrazine.

Acta Phys.-Chim. Sin. **2012**, 28 (8), 1929–1935

Effect of Doping M (M=Mn, Y) into $\text{Ce}_{0.50}\text{Zr}_{0.50}\text{O}_2$ on the Properties of $\text{MnO}_x/\text{Ce}_{0.50-0.7}\text{Zr}_{0.50-0.3}\text{M}_2\text{O}_7/\text{Al}_2\text{O}_3$ for Catalytic Combustion of Ethyl Acetate

CAO Hong-Yan WANG Jian-Li
YAN Sheng-Hui LIU Zhi-Min
GONG Mao-Chu CHEN Yao-Qiang

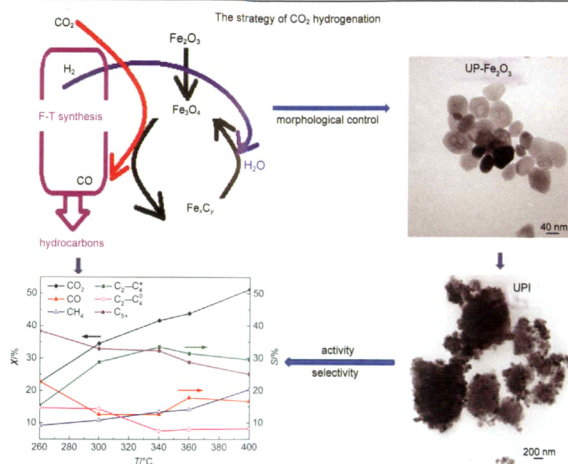


The incorporation of Y results in lower reduction temperature. The incorporation of Mn results in larger reduction peak area.

Acta Phys.-Chim. Sin. **2012**, 28 (8), 1936–1942

Properties of the Nano-Particle Fe-Based Catalyst for the Hydrogenation of Carbon Dioxide to Hydrocarbons

ZHENG Bin ZHANG An-Feng
LIU Min DING Fan-Shu
DAI Cheng-Yi SONG Chun-Shan
GUO Xin-Wen

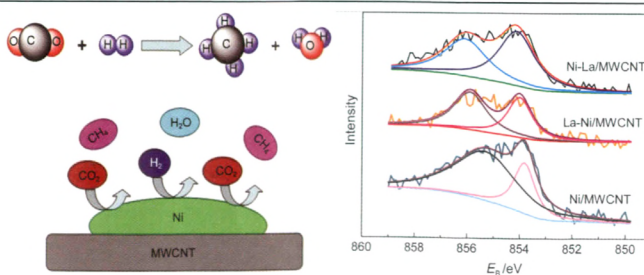


The nano-UPI catalyst is highly active towards the hydrogenation of CO_2 , prompting a thorough study on the effect of particle size.

Acta Phys.-Chim. Sin. **2012**, 28 (8), 1943–1950

Catalytic Properties of Ni/MWCNT and La-Promoted Ni/MWCNT for Methanation Reaction of Carbon Dioxide

ZHANG Rong-Bin LIANG Lei
ZENG Xian-Rong SHANG Jin-Yan
WANG Tao CAI Jian-Xin

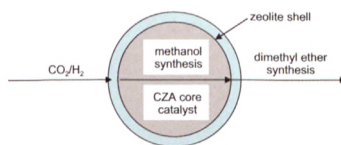


The addition of rare earth La to Ni/MWCNT catalyst improves its catalytic performance in the methanation reaction of CO_2 .

Acta Phys.-Chim. Sin. **2012**, 28 (8), 1951–1956

Preparation, Structure and Performance of [CuO-ZnO-Al₂O₃]/[HZSM-5] Core-Shell Bifunctional Catalysts for One-Step Synthesis of Dimethyl Ether from CO₂+H₂

YANG Xiao-Yan SUN Song
DING Jian-Jun ZHANG Yi
ZHANG Man-Man GAO Chen
BAO Jun

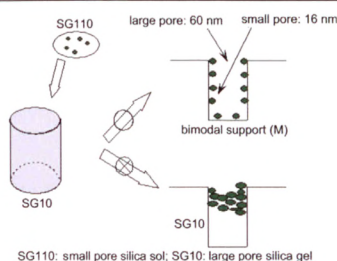


A novel bifunctional catalyst with core-shell structure shows high selectivity for one-step synthesis of dimethyl ether from CO₂ hydrogenation.

Acta Phys. -Chim. Sin. **2012**, 28 (8), 1957–1963

Structure and Performance of Cu-Fe Bimodal Support for Higher Alcohol Syntheses

LIU Jian-Guo DING Ming-Yue
WANG Tie-Jun MA Long-Long

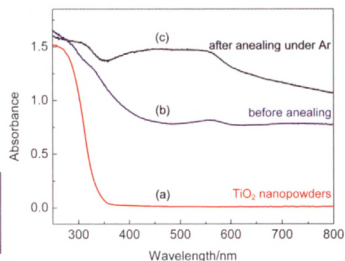
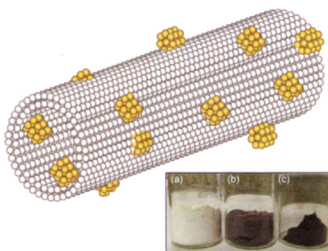


We investigated Fe/Cu molar ratio of Cu-Fe bimodal support for higher alcohol syntheses, and found that the Cu₃₀Fe₃₀KM catalyst showed optimal catalytic activity and space-time yield of mixed alcohols.

Acta Phys. -Chim. Sin. **2012**, 28 (8), 1964–1970

One-Step Hydrothermal Synthesis and Visible-Light Photocatalytic Activity of Ultrafine Cu-Nanodot-Modified TiO₂ Nanotubes

ZHAO Peng-Jun WU Rong
HOU Juan CHANG Ai-Min
GUAN Fang ZHANG Bo

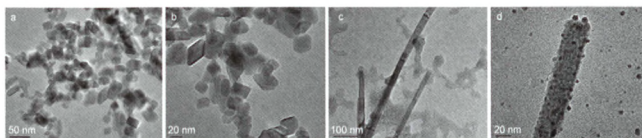


Titanate nanotubes modified by copper nanospheres, with high photocatalytic activity, have been synthesized through a one-step hydrothermal process.

Acta Phys. -Chim. Sin. **2012**, 28 (8), 1971–1977

Visible Light Photocatalytic Properties of Bi_{1.25}La_{0.75}Ti₃O₁₂ Nanowires

LIN Xue LÜ Peng
GUAN Qing-Feng LI Hai-Bo
LI Hong-Ji CAI Jie
ZOU Yang

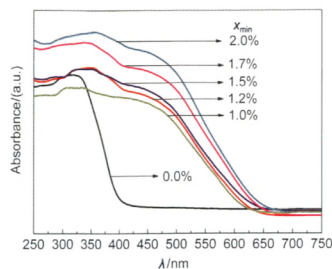


Bi_{1.25}La_{0.75}Ti₃O₁₂ nanowires, synthesized hydrothermally, exhibit higher photocatalytic activities in the degradation of methyl orange (MO) under visible light irradiation compared with commercial P25 TiO₂, traditional N-doped TiO₂ (N-TiO₂), and pure bismuth titanate (Bi₄Ti₃O₁₂, BIT).

Acta Phys. -Chim. Sin. **2012**, 28 (8), 1978–1984

Structure and Properties of BiOI/TiO₂ (A) Photocatalysts with Different Bi/Ti Molar Ratios

LI Hui-Quan CUI Yu-Min
WU Xing-Cai HUA Lin
HONG Wen-Shan



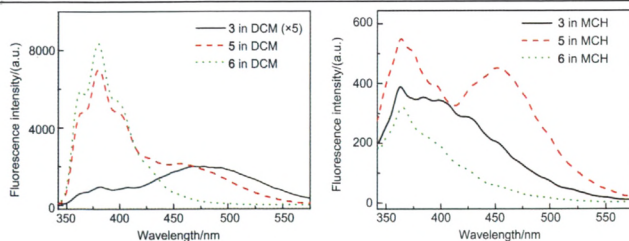
BiOI-sensitized nano-anatase increased its photoactivities. The absorption increases in the 370–630 nm and the absorption band edge redshifts.

Acta Phys. -Chim. Sin. **2012**, 28 (8), 1985–1991

PHOTOCHEMISTRY AND RADIATION CHEMISTRY

Synthesis and Photophysical Behavior of Two Novel Bis(1,8-naphthalimides) Containing Triazine Spacers

SHEN Jian-Lei YANG Xin-Guo
HUANG Liao SHEN Qi-Li
LIU Zhen-Hui ZHANG Feng-Ju

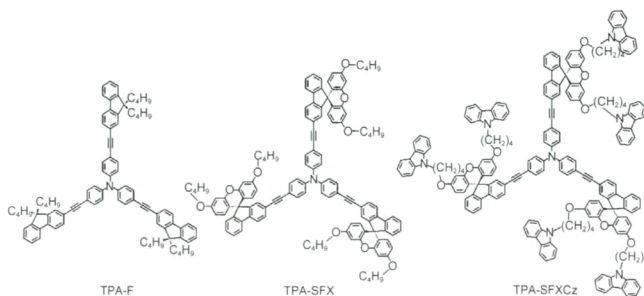


Two novel bis(1,8-naphthalimides) (**3** and **5**) containing a triazine spacer display intramolecular excimer emission in dichloromethane (DCM), chloroform or methanol, and intermolecular excimer emission in methyl cyclohexane (MCH).

Acta Phys. -Chim. Sin. **2012**, 28 (8), 1992–1999

Synthesis and Optoelectronic Properties of Blue-Emitting Star-Burst Oligomers Based on Triphenylamine and Spiro(fluorene-9,9'-xanthene)

CHU Zeng-Ze WANG Dan
ZHANG Chao ZOU De-Chun



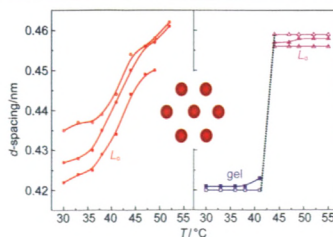
The star-burst molecular structure comprised of the non-planar triphenylamine (TPA) and spiro (fluorene-9,9'-xanthene) (SFX) moieties can effectively restrict the formation of aggregates or excimers.

Acta Phys. -Chim. Sin. **2012**, 28 (8), 2000–2007

BIOPHYSICAL CHEMISTRY

Structural Properties of the Liquid Ordered Phase of Phosphatidylcholine/Stigmasterol Liposomes: A Synchrotron X-Ray Diffraction Study

WU Rui-Guang CHEN Lin
YU Zhi-Wu



The repeat spacings of hexagonally or quasi-hexagonally arranged lipid acyl chains/sterol molecules at liquid-ordered, gel, and liquid-crystal phases.

Acta Phys. -Chim. Sin. **2012**, 28 (8), 2008–2014