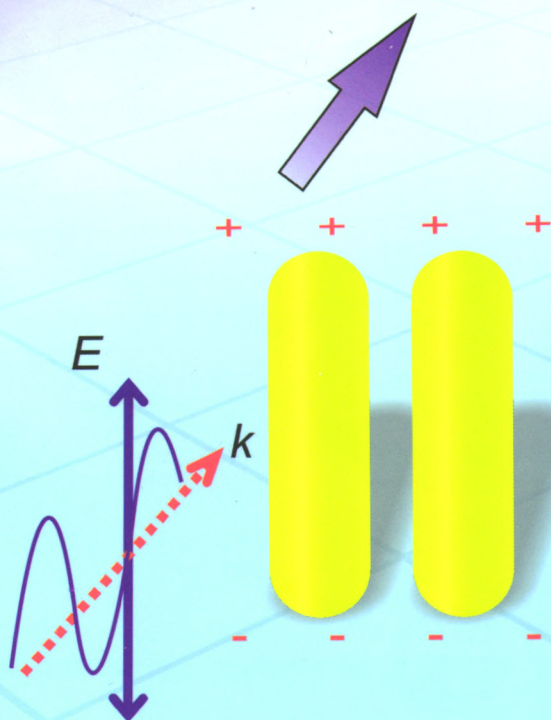
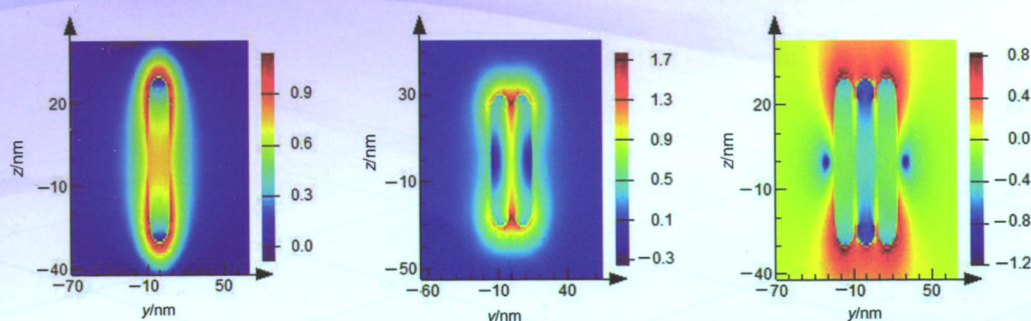


物理化学学报

ACTA PHYSICO-CHIMICA SINICA

第30卷 第10期 Vol.30 No.10 2014



中国科学技术协会主管
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 30 卷第 10 期(2014 年 10 月)

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..... 焦志锋 董莉莉 郭晓宁 靳国强 郭向云 王晓敏(1941)

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甲基多巴透过 POPC 磷脂双层膜过程的分子动力学模拟 卞富永 张继伟 王 丹 徐四川(1947)

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..... 李文章 刘 洋 李 洁 杨亚辉 陈启元(1957)

花瓣状微球 MoS₂/石墨烯复合材料的制备及其电化学性能 张传香 张晓雪 陶海军(1963)

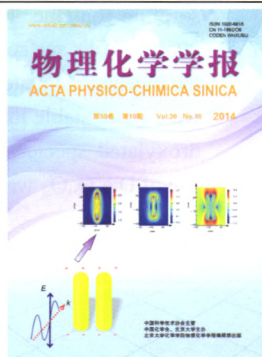
可控阵列微纳结构超疏水铜表面冰霜传质特性

..... 张友法 吴 洁 余新泉 梁彩华 吴 俊(1970)

撤稿声明(Notice of Retraction) (1946)

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COVER



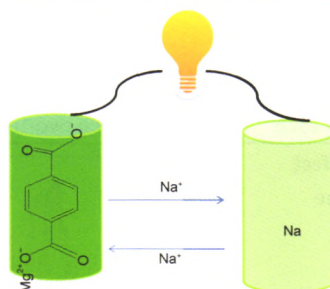
The cover image presents the electric field intensity distribution of S-S oriented gold nanorods (GNRs) with different numbers. On page 1827, LI *et al.* demonstrate that the longitudinal surface plasmon resonance for S-S oriented GNRs blue-shifts with increasing the number (or decreasing the gap spacing), the transverse surface plasmon resonance red-shifts obviously with increasing the number (or decreasing the gap spacing) when the polarized light is applied parallel to the direction of S-S oriented GNRs.

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COMMUNICATION

Magnesium Terephthalate as an Organic Anode Material for Sodium Ion Batteries

HUANG Zong-Ling WANG Li-Ping
MOU Cheng-Xu LI Jing-Ze



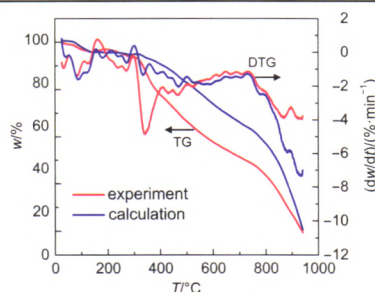
A sustainable and environmentally friendly organic material composed of magnesium terephthalate was used as an anode for sodium ion batteries.

Acta Phys. -Chim. Sin. **2014**, 30 (10), 1787–1793

THERMODYNAMICS, KINETICS, AND STRUCTURAL CHEMISTRY

Synergy Effect in Co-Gasification of Lignite and Char of Pine Sawdust

YANG Xiao-Qin LIU Xue-Jing
LIU Hai-Xiong YUE Xiao-Ming
CAO Jing-Pei ZHOU Min

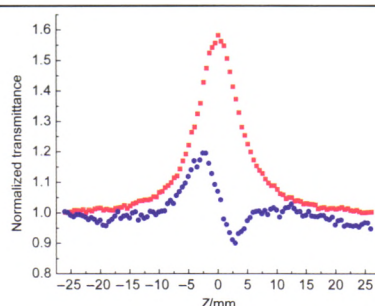


Co-gasification of pine sawdust torrefied at 400 °C with Shengli lignite had the best synergetic efficiency (as high as 13.16%) compared to pine sawdust torrefied at 200 and 300 °C.

Acta Phys. -Chim. Sin. **2014**, 30 (10), 1794–1800

Synthesis and Nonlinear Optical Properties of Porphyrin-Salen Type Homo- and Hetero-Binuclear Metal Complexes

LIU Huan ZANG Na
ZHAO Fang-Yao LIU Kun
LI Yue RUAN Wen-Juan

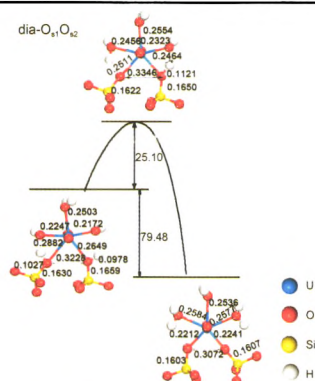


The third-order nonlinear optical properties of two new ligands, their homo- and hetero- binuclear complexes, and their mononuclear complexes were investigated by Z scan techniques.

Acta Phys. -Chim. Sin. **2014**, 30 (10), 1801–1809

Adsorption of the Uranyl Ion on the Hydroxylated α -Quartz (101) Surface

GU Jia-Fang CHEN Wen-Kai

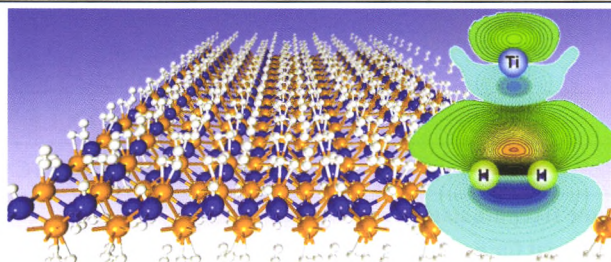


The adsorption energies and electronic structures of uranyl ion adsorption on the hydroxylated α -quartz (101) surface indicated that the bidentate hydrated uranyl species were more stable than bidentate hydroxylated species, and the bridge site of $\text{Dia-O}_{\text{Si}}\text{O}_{\text{Si}}$ was the most stable adsorption site.

Acta Phys. -Chim. Sin. **2014**, 30 (10), 1810–1820

Hydrogen Chemisorption and Physisorption on the Two-Dimensional TiC Sheet Surface

YANG Jian-Hui JI Jia-Lin
LI Lin WEI Shi-Hao

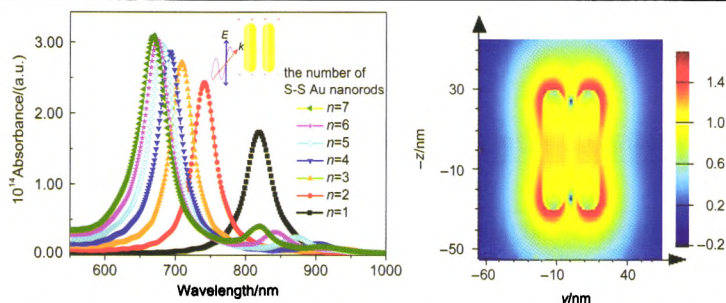


The H_2 storage capacity of the TiC monolayer sheet was calculated to be up to 7.69%, of which two-fifths was Kubas adsorption.

Acta Phys. -Chim. Sin. **2014**, 30 (10), 1821–1826

Surface Plasmon Resonance Coupling Effect of Assembled Gold Nanorods Based on the FDTD Simulation

LI Yu-Ling KAN Cai-Xia
WANG Chang-Shun LIU Jin-Sheng
XU Hai-Ying NI Yuan
XU Wei KE Jun-Hua
SHI Da-Ning

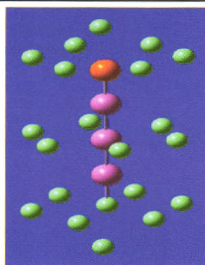


Coupling surface plasmon resonance (SPR) appears with an increase in the number of assembled Au nanorods and electric field distribution.

Acta Phys. -Chim. Sin. **2014**, 30 (10), 1827–1836

Structures and Energetics of $(p\text{-H}_2)_n\text{-HCCCN}$ Clusters

YUAN Ting SUN Xue-Li
ZHU Hua

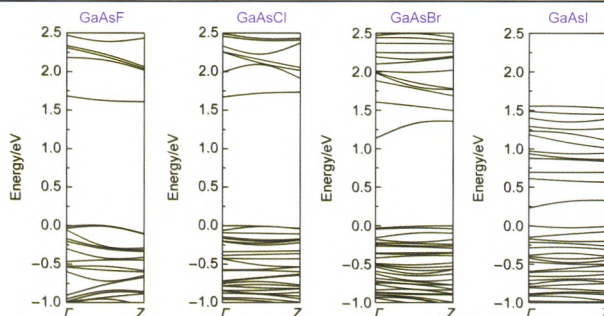


20 *para*- H_2 molecules fill the first solvation shell around HCCCN molecule.

Acta Phys. -Chim. Sin. **2014**, 30 (10), 1837–1840

Electronic Structure Modulation of GaAs Nanowires by Surface Modification

CUI Jian-Gong ZHANG Xia
YAN Xin LI Jun-Shuai
HUANG Yong-Qing REN Xiao-Min

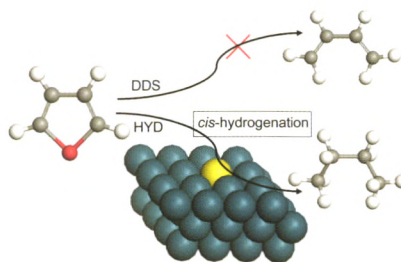


Acta Phys. -Chim. Sin. **2014**, 30 (10), 1841–1846

Surface modification can be used to tune the bandgap and the bandgap types.

Hydrodesulfurization Mechanisms of Thiophene Catalyzed by Au/Pd(111) Bimetallic Surface

ZHANG Lian-Yang SHI Wei
XIA Sheng-Jie NI Zhe-Ming



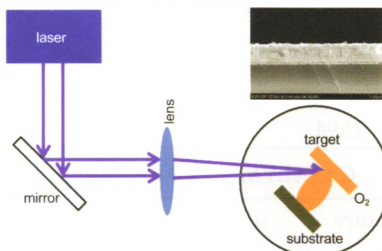
On the basis of thermodynamic and kinetic analyses of the elementary steps, a *cis*-hydrodesulfurization pathway is proposed for the hydrodesulfurization of thiophene on a Au/Pd (111) bimetallic surface.

Acta Phys. -Chim. Sin. **2014**, 30 (10), 1847–1854

ELECTROCHEMISTRY AND NEW ENERGY

Fabrication and Electrochemical Behavior of a Pure-Phase Li_2MnO_3 Thin Film for Cathode Material of Li-Ion Batteries

ZHENG Jie-Yun WANG Rui
LI Hong

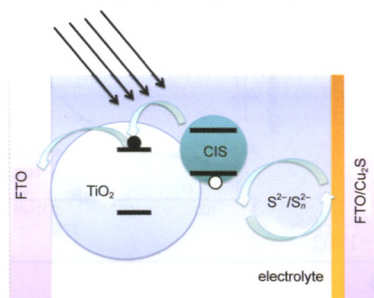


Pure phase thin film cathode materials can be fabricated by pulsed laser deposition.

Acta Phys. -Chim. Sin. **2014**, 30 (10), 1855–1860

Size-Dependent Electron Injection and Photoelectronic Properties of CuInS_2 Quantum Dot Sensitized Solar Cells

ZHU De-Hua ZHONG Rong
CAO Yu PENG Zhi-Hui
FENG Ai-Xin XIANG Wei-Dong
ZHAO Jia-Long

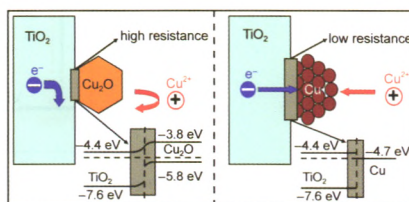


The performance of CuInS_2 quantum dot sensitized solar cells was optimized by varying the size of the quantum dots.

Acta Phys. -Chim. Sin. **2014**, 30 (10), 1861–1866

Bias-Determined Cu_2O and Cu Growth on TiO_2 Surface and Their Photoelectrochemical Properties

JIANG Chun-Xiang HU Yu-Xiang
DONG Wen ZHENG Fen-Gang
SU Xiao-Dong FANG Liang
SHEN Ming-Rong

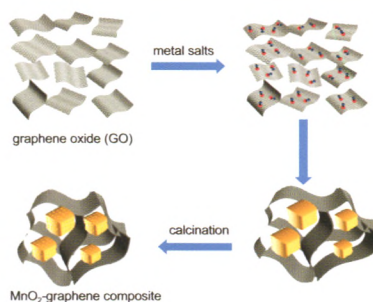


$\text{Cu}_2\text{O}/\text{TiO}_2$ and Cu/TiO_2 films were fabricated by electrodeposition and they were found to have different growth modes and enhanced photoelectrochemical properties.

Acta Phys. -Chim. Sin. **2014**, 30 (10), 1867–1875

Synthesis of a Mesoporous Manganese Dioxide-Graphene Composite by a Simple Template-Free Strategy for High-Performance Supercapacitors

TANG Jia-Yong CAO Pei-Qi
FU Yan-Bao LI Peng-Hui
MA Xiao-Hua

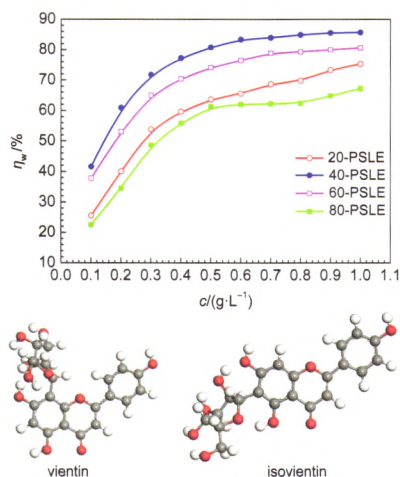


Graphene sheets, as a conductive bridge, can improve the specific capacity and structural stability of MnO_2 particles.

Acta Phys. -Chim. Sin. **2014**, 30 (10), 1876–1882

Inhibition Effect of Bamboo Leaf Extract on the Corrosion of Aluminum in HCl Solution

LI Xiang-Hong DENG Shu-Duan
XIE Xiao-Guang DU Guan-Ben



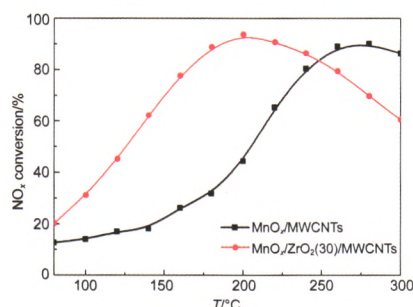
Bamboo leaf extract from A bamboo leaf inhibitor (designated PSLE) effectively retards aluminum corrosion in HCl solution. The inhibition efficiency decreases as follows: 40-PSLE>60-PSLE>20-PSLE>80-PSLE.

Acta Phys. -Chim. Sin. **2014**, *30* (10), 1883–1894

CATALYSIS AND SURFACE SCIENCE

Structural Properties and Low-Temperature SCR Activity of Zirconium-Modified MnO_x/MWCNTs Catalysts

YANG Chao LIU Xiao-Qing
HUANG Bi-Chun WU You-Ming

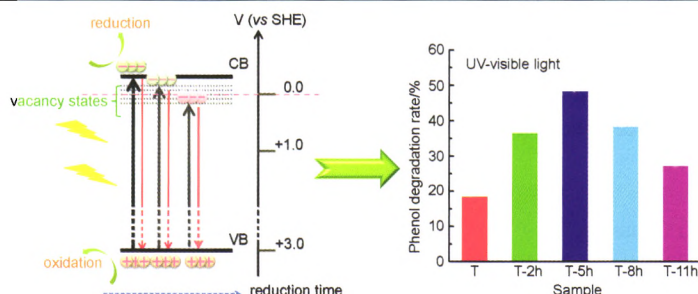


The significant promotion effects of zirconium on MnO_x/MWCNTs catalysts come from the improvement of surface properties: the valence state of Mn, the dispersion of active components, and surface acidity.

Acta Phys. -Chim. Sin. **2014**, *30* (10), 1895–1902

Hydrogenated Rutile TiO₂ Nanorods and Their Photocatalytic Activity

CUI Hai-Qin JING Li-Qiang
XIE Ming-Zheng LI Zhi-Jun

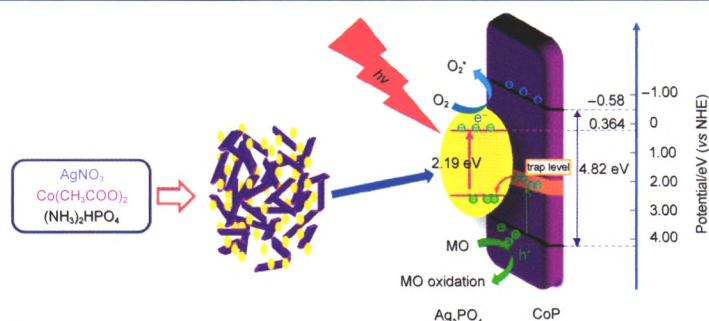


A specific amount of defects and/or vacancies can induce new and appropriate surface states below the conduction band (CB) of TiO₂, which improves photocatalytic reactions.

Acta Phys. -Chim. Sin. **2014**, *30* (10), 1903–1908

Preparation and Characterization of Co₃(PO₄)₂/Ag₃PO₄ Nanocomposites for Visible- Light Photocatalysis

GU Yong-Qin WANG Bo
GU Xiu-Quan ZHAO Yu-Long
QIANG Ying-Huai ZHANG Shuang
ZHU Lei

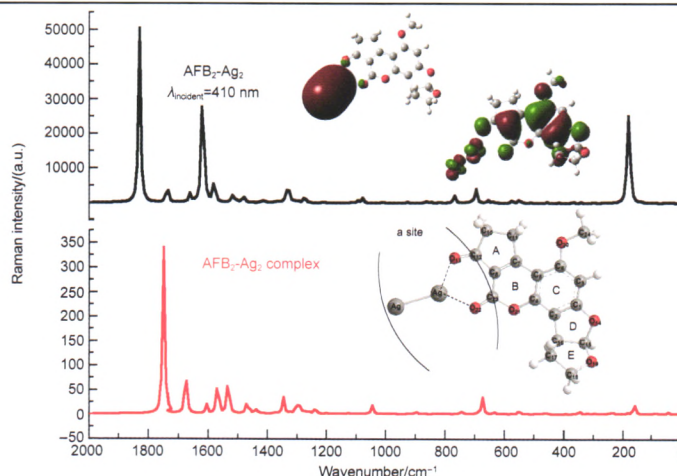


We succeeded in synthesizing Co₃(PO₄)₂(CoP)/Ag₃PO₄ hybrids with higher photocatalytic activity and recyclability during the degradation of methyl orange (MO) than single-phase Ag₃PO₄ NPs because of their suitable band offset at interfaces.

Acta Phys. -Chim. Sin. **2014**, *30* (10), 1909–1915

**Surface-Enhanced Raman Scattering
Mechanism of Aflatoxin B₂ Molecule
Adsorbed on Silver Cluster**

GAO Si-Min WANG Hong-Yan
LIN Yue-Xia WU Ying-Xi
HU Jun

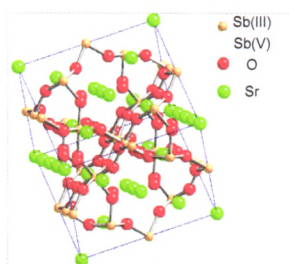


Surface-enhanced Raman scattering (SERS) at the charge transfer resonance incident wavelength is more conducive to the trace detection of the strong carcinogen Aflatoxin B₂ (AFB₂).

Acta Phys. -Chim. Sin. **2014**, 30 (10), 1916–1922

**Preparation, Characterization and Sr(II)
Adsorption Performance of Self-Doped
Antimony Oxide**

ZHANG Lan WEI Ji-Ying
ZHAO Xuan LI Fu-Zhi
JIANG Feng

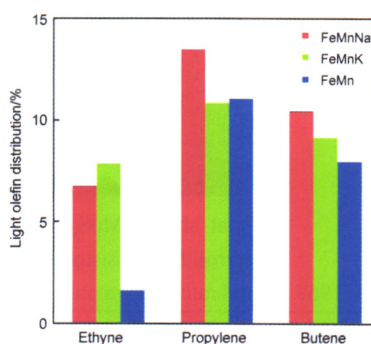


By substituting some Sb(III) atoms for Sb(V) atoms in the framework of Sb₂O₃, the Sr(II) adsorption capacity was remarkably enhanced.

Acta Phys. -Chim. Sin. **2014**, 30 (10), 1923–1931

**Comparison of FeMn, FeMnNa and FeMnK
Catalysts for the Preparation of Light Olefins
from Syngas**

LI Jiang-Bing MA Hong-Fang
ZHANG Hai-Tao SUN Qi-Wen
YING Wei-Yong FANG Ding-Ye

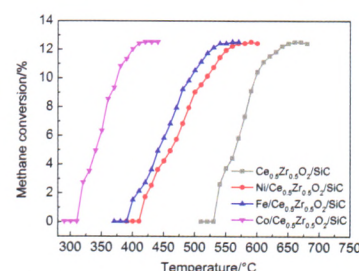
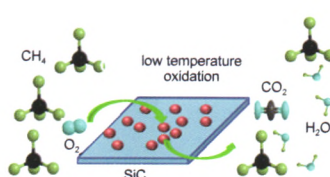


An Na-promoted FeMn catalyst was found to have better performance for light olefin synthesis from syngas compared with unpromoted and K-promoted FeMn catalysts.

Acta Phys. -Chim. Sin. **2014**, 30 (10), 1932–1940

**Methane Catalytic Combustion over Ni/SiC,
Fe/SiC and Co/SiC Modified by
Zr_{0.5}Ce_{0.5}O₂ Solid Solution**

JIAO Zhi-Feng DONG Li-Li
GUO Xiao-Ning JIN Guo-Qiang
GUO Xiang-Yun WANG Xiao-Min



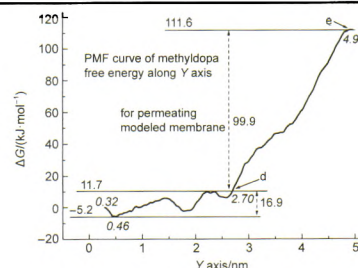
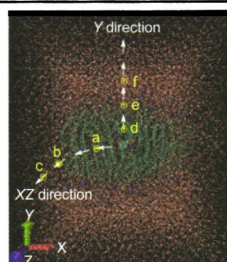
Ce_{0.5}Zr_{0.5}O₂ solid solution modified Ni/SiC, Fe/SiC, and Co/SiC catalysts showed remarkable activity and stability for deoxidation of coal-bed gas.

Acta Phys. -Chim. Sin. **2014**, 30 (10), 1941–1946

BIOPHYSICAL CHEMISTRY

Molecular Dynamics Simulation of the Permeation of Methylidopa through POPC Phospholipid Bilayer Membrane

BIAN Fu-Yong ZHANG Ji-Wei
WANG Dan XU Si-Chuan



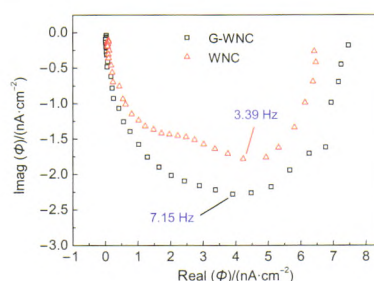
Molecular dynamics of the process of methylidopa diffusion within and permeation through the 1-palmitoyl-2-oleoyl-glycero-3-phosphate dylcholine (POPC) phospholipid bilayer membrane were studied.

Acta Phys. -Chim. Sin. **2014**, *30* (10), 1947–1956

PHYSICAL CHEMISTRY OF MATERIALS

Synthesis and Interfacial Electron Transfer of a Composite Film of Graphene and Tungsten Oxide

LI Wen-Zhang LIU Yang
LI Jie YANG Ya-Hui
CHEN Qi-Yuan

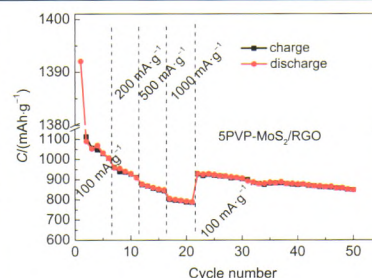
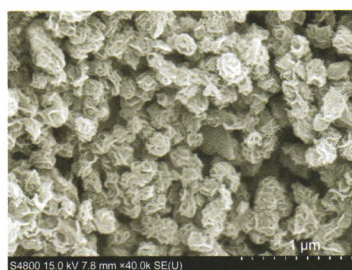


The electron-hole lifetime increased for tungsten oxide films after the incorporation of graphene, and the efficiency of photoelectric conversion improved significantly.

Acta Phys. -Chim. Sin. **2014**, *30* (10), 1957–1962

Synthesis and Electrochemical Properties of MoS₂/Graphene Composites with Petal-Shaped Microspheres

ZHANG Chuan-Xiang ZHANG Xiao-Xue
TAO Hai-Jun

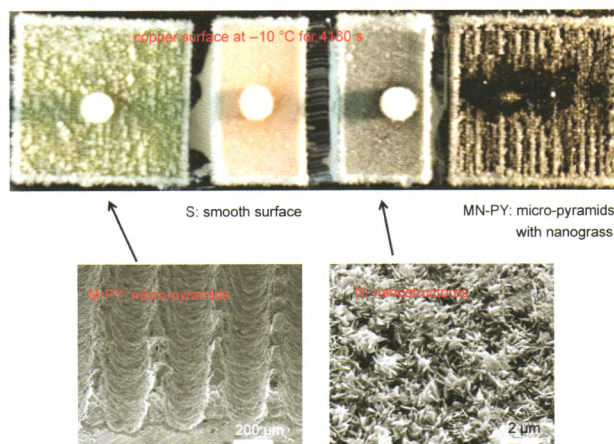


Petal-shaped MoS₂/RGO composite electrode materials prepared by polyvinylpyrrolidone-assisted synthesis showed good dispersion, capacity, cycle stability, and rate performance as lithium ion battery anode materials.

Acta Phys. -Chim. Sin. **2014**, *30* (10), 1963–1969

Frost and Ice Transport on Superhydrophobic Copper Surfaces with Patterned Micro- and Nano-Structures

ZHANG You-Fa WU Jie
YU Xin-Quan LIANG Cai-Hua
WU Jun



Two-tier roughness on copper effectively improves superhydrophobicity, and retards the formation and growth of frost and ice.

Acta Phys. -Chim. Sin. **2014**, *30* (10), 1970–1978

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