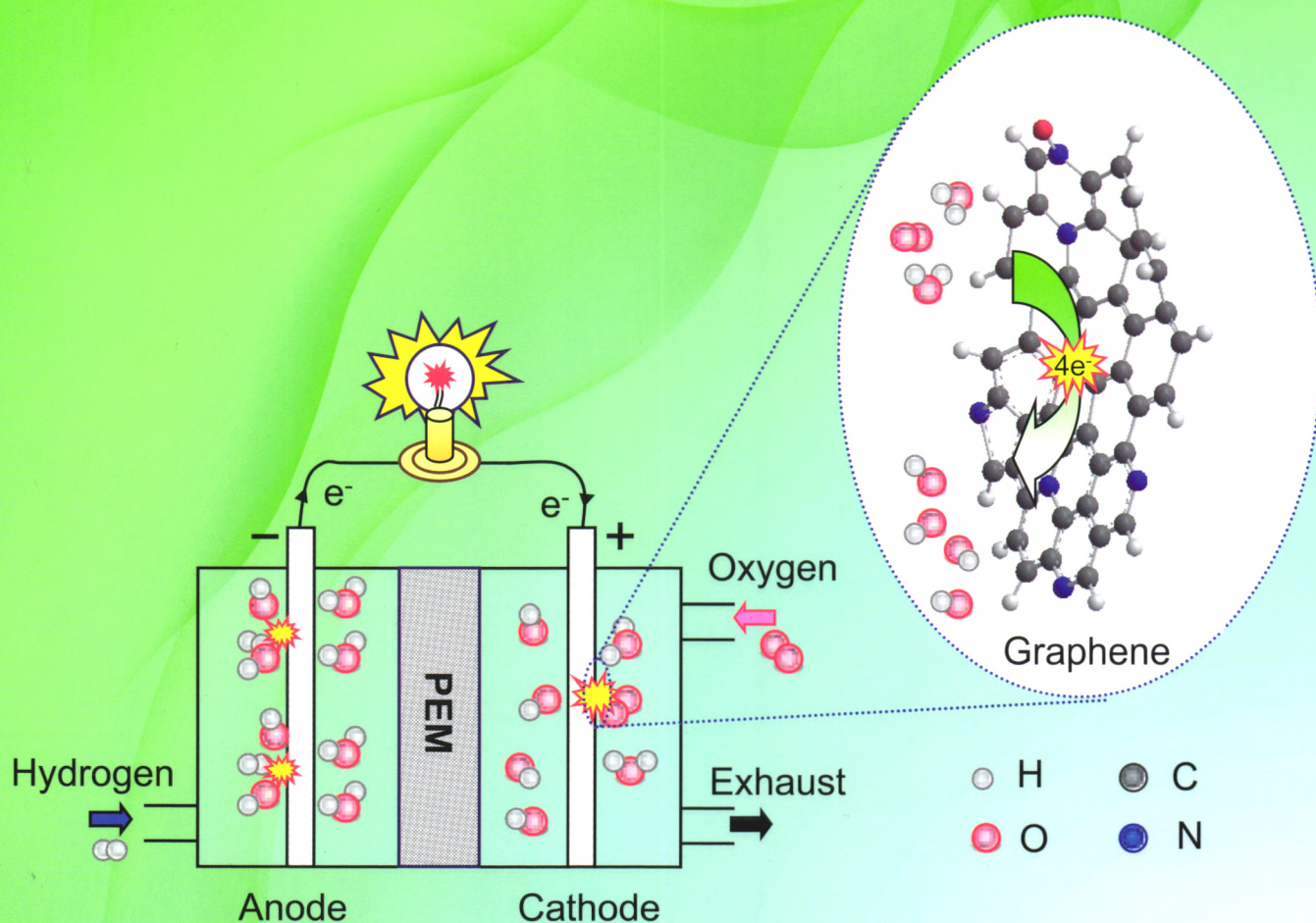


物理化学学报

ACTA PHYSICO-CHIMICA SINICA

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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

目 次

综 述

离子液体的辐射效应研究进展 王硕珏 敖银勇 周瀚洋 袁立永 彭 静 翟茂林(1597)

热力学, 动力学和结构化学

离子液体 1-乙基-3-甲基咪唑三氟甲基磺酸盐与水之间的氢键作用 宋大勇 陈 静(1605)

低温合成超导体 $\text{Ba}_{1-x}\text{K}_x\text{BiO}_3$ 刘 孟 李国宝 王稼国 廖复辉 林建华(1611)

理论与计算化学

有机污染物在碳纳米管吸附的定量结构-性质关系 刘 芬 邹建卫 胡桂香 蒋勇军(1616)

分子动力学模拟研究纳米碳管中甲醇-水混合溶液的结构与输运性质
..... 高文秀 王洪磊 李慎敏(1625)

电化学和新能源

吡啶基镁卤化物/四氢呋喃可充镁电池电解液

..... 非路热·吐尔逊 祖丽皮亚·沙地克 努丽燕娜 杨 军 王久林(1634)

锂离子电池正极材料 $\text{Li}_{1.2}\text{Mn}_{0.54-x}\text{Ni}_{0.13}\text{Co}_{0.13}\text{Zr}_x\text{O}_2$ 的制备及电化学性能

..... 任祥忠 刘 涛 孙灵娜 张培新(1641)

静电自组装方法合成的具有多孔三维网络结构的 Fe_3O_4 /石墨烯复合材料作为高性能锂离子电池负极材料

..... 刘建华 刘宾虹 李洲鹏(1650)

功能化石墨烯/聚苯胺复合电极材料的制备和电化学性能 汪丽丽 邢瑞光 张邦文 侯 渊(1659)

Ag/C 包覆对 $\text{Li}[\text{Li}_{0.2}\text{Mn}_{0.54}\text{Ni}_{0.13}\text{Co}_{0.13}]\text{O}_2$ 电化学性能的影响

..... 薛庆瑞 李建玲 徐国峰 侯朋飞 晏 刚 代 宇 王新东 高 飞(1667)

在 LiCl-KCl-ZnCl_2 熔盐体系中电化学共还原提取铈

..... 薛 云 周志萍 颜永得 张密林 李 星 纪德彬 韩 伟 张 萌(1674)

单分散 PtNi 纳米粒子特殊的红外光学性能 周新文 杜娟娟 孙世刚(1681)

软物质

L-苯丙氨酸衍生物与脂肪胺构筑双组分超分子凝胶

..... 钟金莲 潘 虹 罗序中 洪三国 张 宁 黄建滨(1688)

催化和表面科学

可见光辐射下活性炭-铁酸镍杂化催化剂光催化氧化氨氮 肖 波 刘守清(1697)

Fe 掺杂 g- C_3N_4 的制备及其可见光催化性能

..... 金瑞瑞 游继光 张 倩 刘 丹 胡绍争 桂建舟(1706)

$\text{Cu}_3\text{B}_2\text{O}_6/\text{CuB}_2\text{O}_4$ 单晶的制备及其可见光催化降解亚甲基蓝

..... 陈爱民 薄盈盈 邵晨熠 汪 晶 胡 军(1713)

石墨烯氢氧化钴复合催化剂的一步合成及其对酸性橙的催化降解

..... 李洁冰 伊 玉 时鹏辉 王 倩 李登新 ASIF Hussain 杨 明(1720)

微米级 MEL 分子筛聚集体的制备 陈红丽 朱树燕 何建琴 王一萌(1727)

钾调变 Mo/SBA-15 催化剂用于乙烷选择氧化制乙醛

..... 李建梅 刘 坚 任立伟 刘清龙 赵 震 韦岳长 段爱军 姜桂元(1736)

微量Li助剂对Co/AC催化剂合成高碳醇性能的影响
..... 董文达 朱何俊 丁云杰 裴彦鹏 杜虹 王涛(1745)

光化学和辐射化学

不同掺杂浓度Tm³⁺:LiLuF₄单晶的1800 nm荧光发射
..... 李珊珊 夏海平 符立 董艳明 张加忠 谷雪梅 章践立 王冬杰 江浩川 陈宝玖(1752)

不同形貌的金字塔结构对硅片表面钝化和异质结太阳能电池的影响
..... 王利果 张晓丹 王奉友 王宁 姜元建 郝秋艳 许盛之 魏长春 赵颖(1758)

材料物理化学

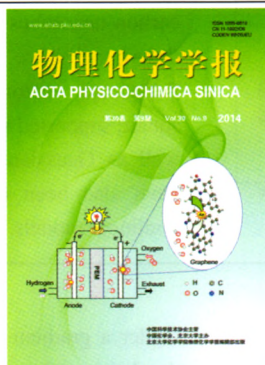
多糖凝胶的孔径和化学结构对单壁碳纳米管流动性和选择性分离的影响
..... 杨鹏 檀付瑞 张静 金赫华 李红波 刘春华 李清文(1764)

基于金银合金薄膜的波长检测型表面等离子体共振传感器 张喆 刘杰 逯丹凤 祁志美(1771)

氮掺杂石墨烯的制备及其对氧还原反应的电催化性能 彭三 郭慧林 亢晓峰(1778)

本期责任编辑: 於秀芝

COVER



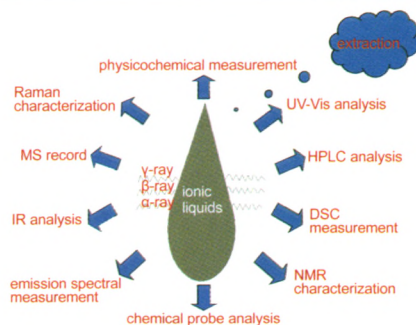
The cover image presents the schematic representation for fuel cells and the oxygen reduction reaction (ORR) on nitrogen-doped graphene. On page 1778, PENG *et al.* demonstrate that nitrogen-doped graphene can be obtained by reducing graphene oxide with dimethyl ketoxime. The results show that pyridinic-N is beneficial to direct four-electron reaction of oxygen and nitrogen-doped graphene exhibits a high selectivity for ORR with a remarkably good tolerance of methanol cross-over effects.

CONTENTS

REVIEW

Research Progress in Radiation Effects on Ionic Liquids

WANG Shuo-Jue AO Yin-Yong
ZHOU Han-Yang YUAN Li-Yong
PENG Jing ZHAI Mao-Lin



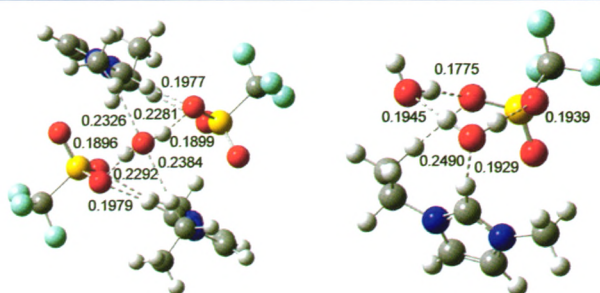
Research progress in radiation effects on ionic liquids is presented.

Acta Phys. -Chim. Sin. 2014, 30 (9), 1597–1604

THERMODYNAMICS, KINETICS, AND STRUCTURAL CHEMISTRY

Hydrogen-Bonding Interactions between Ionic Liquid 1-Ethyl-3-methylimidazolium Trifluoromethanesulfonate and Water

SONG Da-Yong CHEN Jing

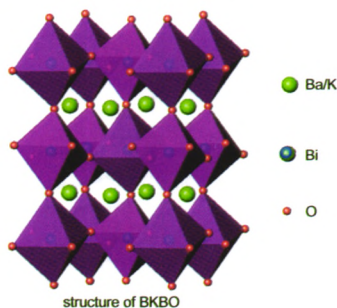


The hydrogen-bonding interaction site is the alkyl C—H at low concentrations and the aromatic C—H at high concentrations.

Acta Phys. -Chim. Sin. 2014, 30 (9), 1605–1610

Low-Temperature Synthesis of Superconductor $Ba_{1-x}K_xBiO_3$

LIU Meng LI Guo-Bao
WANG Jia-Guo LIAO Fu-Hui
LIN Jian-Hua



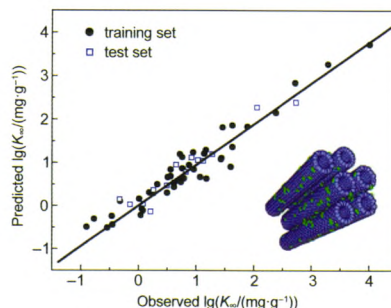
$Ba_{1-x}K_xBiO_3$ (BKBO) and the parent compound $BaBiO_3$, both have cubic perovskite structures; BKBO can be synthesized from $BaBiO_3$, using a topotactic reaction.

Acta Phys. -Chim. Sin. 2014, 30 (9), 1611–1615

THEORETICAL AND COMPUTATIONAL CHEMISTRY

Quantitative Structure–Property Relationship Studies on the Adsorption of Aromatic Contaminants by Carbon Nanotubes

LIU Fen ZOU Jian-Wei
HU Gui-Xiang JIANG Yong-Jun

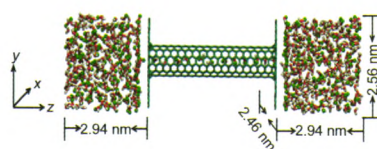


Excellent linear relationships between the adsorption equilibrium constants of organic contaminants by carbon nanotubes and the structural descriptors have been established. Supported vector machine, least-square supported vector machine, as well as Gaussian process methods have also been used to construct nonlinear models.

Acta Phys. -Chim. Sin. **2014**, 30 (9), 1616–1624

Molecular Dynamics Simulation Study of Structural and Transport Properties of Methanol-Water Mixture in Carbon Nanotubes

GAO Wen-Xiu WANG Hong-Lei
LI Shen-Min



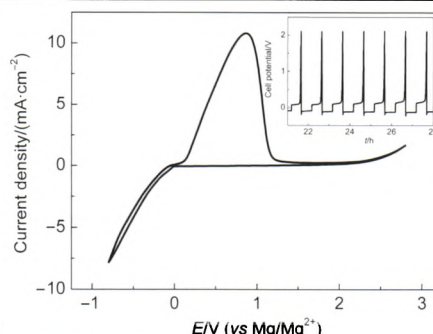
Under a gradient electric field, hydrophobic carbon nanotube becomes hydrophilic, resulting in the phenomenon of methanol-water separation disappearing.

Acta Phys. -Chim. Sin. **2014**, 30 (9), 1625–1633

ELECTROCHEMISTRY AND NEW ENERGY

Pyrazolyl Magnesium Halide/Tetrahydrofuran Solutions for Rechargeable Magnesium Battery Electrolytes

FEILURE Tuerxun ZULIPIYA Shadike
NULI Yan-Na YANG Jun
WANG Jiu-Lin

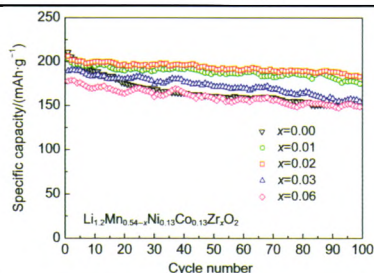


An electrolyte consisting of 1 mol·L⁻¹ 1-methylpyrazole-PhMgCl (1:1 molar ratio)/THF has an anodic oxidation decomposition potential of 2.4 V (vs Mg/Mg²⁺) on stainless steel, a low overpotential for magnesium deposition-dissolution, and high cycling reversibility.

Acta Phys. -Chim. Sin. **2014**, 30 (9), 1634–1640

Preparation and Electrochemical Performances of Li_{1.2}Mn_{0.54-x}Ni_{0.13}Co_{0.13}Zr_xO₂ Cathode Materials for Lithium-Ion Batteries

REN Xiang-Zhong LIU Tao
SUN Ling-Na ZHANG Pei-Xin

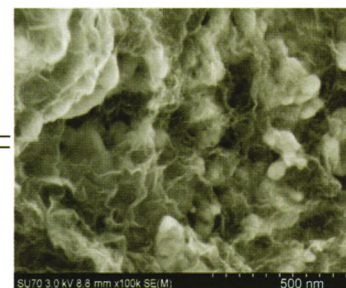
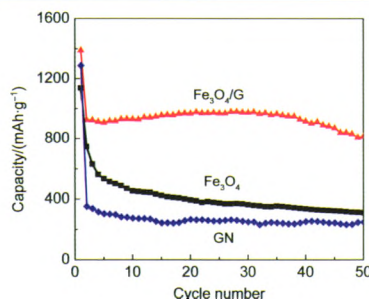


Zirconium substitution is a convenient and effective method for improving the electrochemical performance of the lithium-rich layered Li_{1.2}Mn_{0.54}Ni_{0.13}Co_{0.13}O₂ cathode material.

Acta Phys. -Chim. Sin. **2014**, 30 (9), 1641–1649

Fe₃O₄/Graphene Composites with a Porous 3D Network Structure Synthesized through Self-Assembly under Electrostatic Interactions as Anode Materials of High-Performance Li-Ion Batteries

LIU Jian-Hua LIU Bin-Hong
LI Zhou-Peng

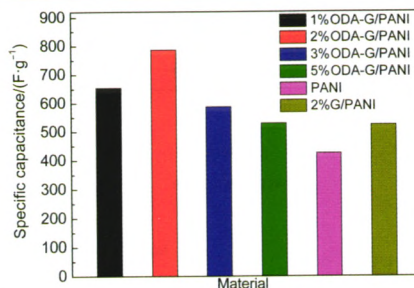


Fe₃O₄/graphene composites with a porous 3D graphene network exhibited good electrochemical performance as the anode material for Li-ion batteries.

Acta Phys. -Chim. Sin. **2014**, 30 (9), 1650–1658

Preparation and Electrochemical Properties of Functionalized Graphene/Polyaniline Composite Electrode Materials

WANG Li-Li XING Rui-Guang
ZHANG Bang-Wen HOU Yuan

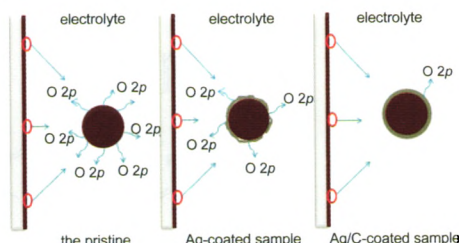


Octadecylamine functionalized graphene (ODA-G) and polyaniline (PANI) composites were prepared using a facile solvent-blending procedure. The composite material can greatly improve the stability and high specific capacitance of polyaniline.

Acta Phys. -Chim. Sin. **2014**, *30* (9), 1659–1666

Effects of Surface Modification with Ag/C on Electrochemical Properties of $\text{Li}[\text{Li}_{0.2}\text{Mn}_{0.54}\text{Ni}_{0.13}\text{Co}_{0.13}]\text{O}_2$

XUE Qing-Rui LI Jian-Ling
XU Guo-Feng HOU Peng-Fei
YAN Gang DAI Yu
WANG Xin-Dong GAO Fei

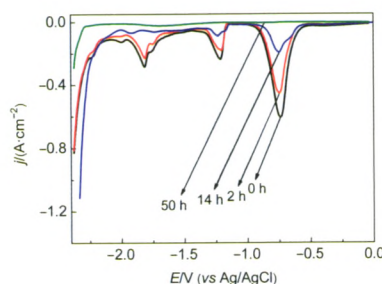


An Ag/C coating layer improved the electrochemical performance of $\text{Li}[\text{Li}_{0.2}\text{Mn}_{0.54}\text{Ni}_{0.13}\text{Co}_{0.13}]\text{O}_2$ by suppressing oxygen release and stabilizing the interface between particle surfaces and the electrolyte.

Acta Phys. -Chim. Sin. **2014**, *30* (9), 1667–1673

Electrochemical Co-Reduction Extraction of Neodymium in LiCl-KCl-ZnCl_2 Molten Salt System

XUE Yun ZHOU Zhi-Ping
YAN Yong-De ZHANG Mi-Lin
LI Xing JI De-Bin
HAN Wei ZHANG Meng

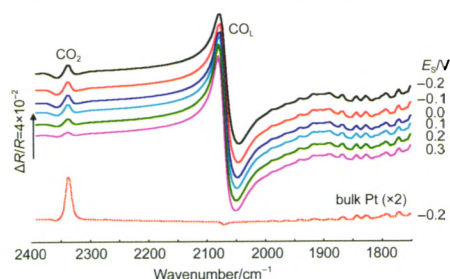


Based on the electrochemical results, square-wave voltammetry was used to determine the concentration variations of Nd during potentiostatic electrolysis.

Acta Phys. -Chim. Sin. **2014**, *30* (9), 1674–1680

Anomalous IR Optical Properties of Monodispersed PtNi Nanoparticles

ZHOU Xin-Wen DU Juan-Juan
SUN Shi-Gang



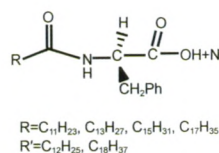
It was demonstrated that CO molecules adsorbed on PtNi nanoparticles exhibited characteristics of a bipolar IR feature with a strong enhancement.

Acta Phys. -Chim. Sin. **2014**, *30* (9), 1681–1687

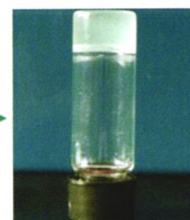
SOFT MATTER

Two-Component Supramolecular Organogels Formed from *L*-Phenylalanine Derivatives and Aliphatic Amines

ZHONG Jin-Lian PAN Hong
LUO Xu-Zhong HONG San-Guo
ZHANG Ning HUANG Jian-Bin



organic solvent
cooling after melt



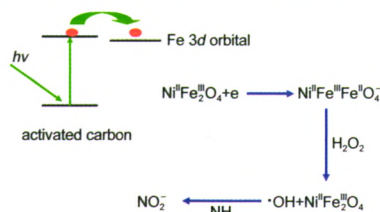
L-Phenylalanine derivatives mixed with aliphatic amines gelled various organic liquids.

Acta Phys. -Chim. Sin. **2014**, *30* (9), 1688–1696

Photocatalytic Oxidation of Ammonia via an Activated Carbon-Nickel Ferrite Hybrid Catalyst under Visible Light Irradiation

XIAO Bo LIU Shou-Qing

Acta Phys. -Chim. Sin. **2014**, *30* (9), 1697–1705

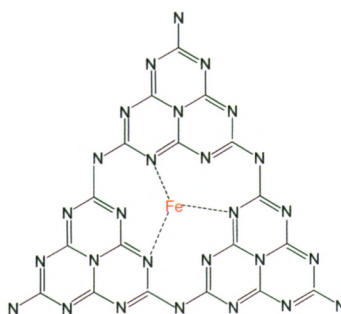


Graphene sheets in activated carbon elevate electrons to the Fe 3d orbital under visible light irradiation, triggering the photo-Fenton oxidation of ammonia.

Preparation of Fe-Doped Graphitic Carbon Nitride with Enhanced Visible-Light Photocatalytic Activity

JIN Rui-Rui YOU Ji-Guang
ZHANG Qian LIU Dan
HU Shao-Zheng GUI Jian-Zhou

Acta Phys. -Chim. Sin. **2014**, *30* (9), 1706–1712

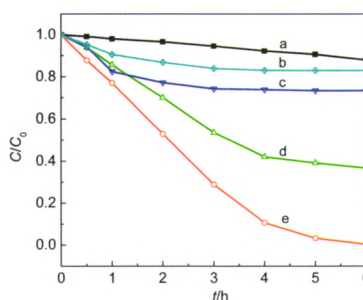


Fe^{3+} embedded in the structural units of $\text{g-C}_3\text{N}_4$ by coordination with N atoms changed the optical properties, affected the energy band structure, and increased the electron/hole separation rate.

Synthesis of Single-Crystalline $\text{Cu}_3\text{B}_2\text{O}_6/\text{CuB}_2\text{O}_4$ and Their Photocatalytic Degradation of Methylene Blue under Visible-Light Irradiation

CHEN Ai-Min BO Ying-Ying
SHAO Chen-Yi WANG Jing
HU Jun

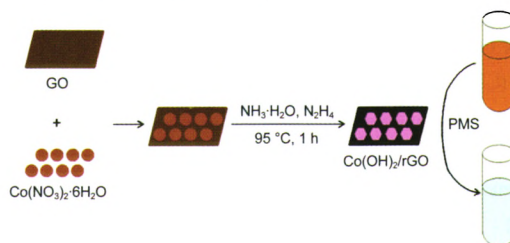
Acta Phys. -Chim. Sin. **2014**, *30* (9), 1713–1719



Single-crystalline $\text{Cu}_3\text{B}_2\text{O}_6/\text{CuB}_2\text{O}_4$ was successfully prepared using a sol-gel method. $\text{Cu}_3\text{B}_2\text{O}_6$ and CuB_2O_4 both displayed good photocatalytic activity in the photodegradation of methylene blue solution. The photocatalytic activity of $\text{Cu}_3\text{B}_2\text{O}_6$ reached 99.52%.

Facile Synthesis of Graphene-Cobalt Hydroxide Nanocomposite and Application in Degradation of Acid Orange 7

LI Jie-Bing YI Yu
SHI Peng-Hui WANG Qian
LI Deng-Xin ASIF Hussain
YANG Ming



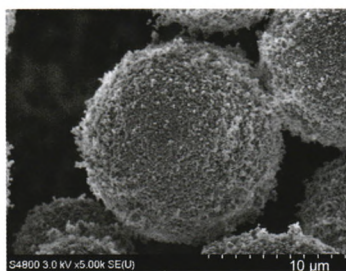
A catalyst ($\text{Co(OH)}_2/\text{rGO}$) prepared by one-step self-assembly degraded acid orange 7 in less than 12 min in aqueous solution.

Acta Phys. -Chim. Sin. **2014**, *30* (9), 1720–1726

Synthesis of Micro-Sized MEL-Type Zeolite Aggregates

CHEN Hong-Li ZHU Shu-Yan
HE Jian-Qin WANG Yi-Meng

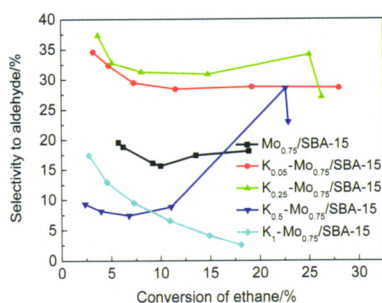
Acta Phys. -Chim. Sin. **2014**, *30* (9), 1727–1735



Micro-sized MEL aggregates were synthesized; they showed comparable catalytic activities to that of nano-sized TS-1, but were easily separated.

Selective Oxidation of Ethane to Aldehydes over Potassium-Promoted SBA-15-Supported Molybdenum Oxide Catalysts

LI Jian-Mei LIU Jian
REN Li-Wei LIU Qing-Long
ZHAO Zhen WEI Yue-Chang
DUAN Ai-Jun JIANG Gui-Yuan

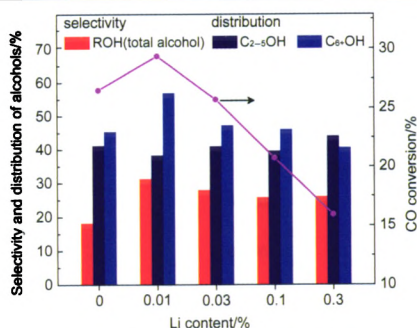


The addition of potassium to $\text{Mo}_{0.75}/\text{SBA-15}$ effectively enhances the activity of catalysts and the selectivity to the total aldehydes (formaldehyde, acetaldehyde, and acrolein), for selective oxidation of ethane.

Acta Phys.-Chim. Sin. **2014**, 30 (9), 1736–1744

Effect of Trace Amounts of Li Doping on Performance of Co/AC Catalysts for Syntheses of Mixed Linear α -Alcohols

DONG Wen-Da ZHU He-Jun
DING Yun-Jie PEI Yan-Peng
DU Hong WANG Tao



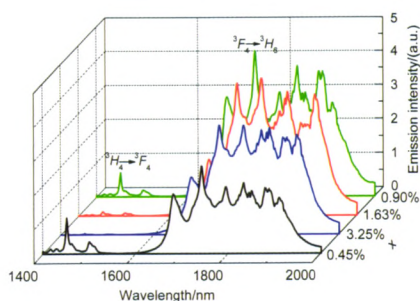
Trace amounts of Li doping in 15Co/AC catalyst led to significant improvement in catalytic performance for syntheses of alcohols. The interaction of doped Li with Co decreased the size of the Co^0 particles and promoted the formation of Co_2C species.

Acta Phys.-Chim. Sin. **2014**, 30 (9), 1745–1751

PHOTOCHEMISTRY AND RADIATION CHEMISTRY

Fluorescent Emissions (1800 nm) of LiLuF_4 Single Crystals Doped with Various Tm^{3+} Concentrations

LI Shan-Shan XIA Hai-Ping
FU Li DONG Yan-Ming
ZHANG Jia-Zhong GU Xue-Mei
ZHANG Jian-Li WANG Dong-Jie
JIANG Hao-Chuan CHEN Bao-Jiu

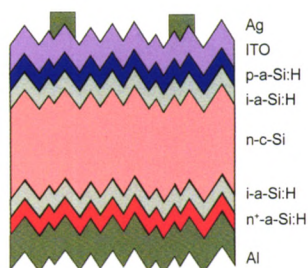


We obtained the optimum fluorescent emission (1800 nm) of LiLuF_4 single crystals singly doped with different Tm^{3+} concentrations.

Acta Phys.-Chim. Sin. **2014**, 30 (9), 1752–1757

Influence of Different Pyramidal Structural Morphologies of Crystalline Silicon Wafers for Surface Passivation and Heterojunction Solar Cells

WANG Li-Guo ZHANG Xiao-Dan
WANG Feng-You WANG Ning
JIANG Yuan-Jian HAO Qiu-Yan
XU Sheng-Zhi WEI Chang-Chun
ZHAO Ying

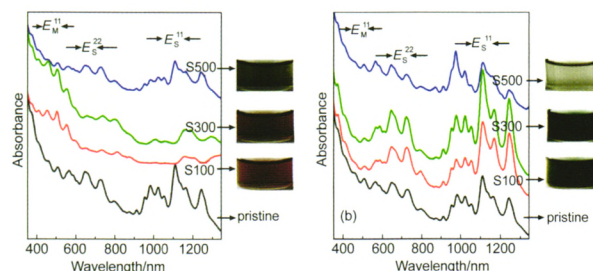


Heterojunction solar cells were fabricated on silicon wafers with nested pyramidal structures, hill rock pyramidal structures, and standard four-sided pyramidal structures.

Acta Phys.-Chim. Sin. **2014**, 30 (9), 1758–1763

Effects of Pore-Size Range and Composition of Polysaccharide Gels on Flow Behaviors and Selective Sorting of Single-Walled Carbon Nanotubes

YANG Peng TAN Fu-Rui
ZHANG Jing JIN He-Hua
LI Hong-Bo LIU Chun-Hua
LI Qing-Wen

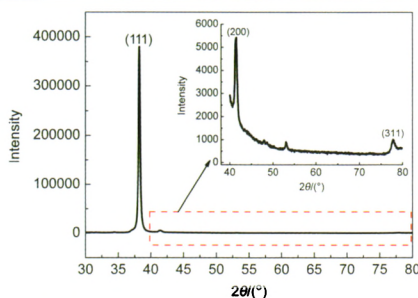


The effects of pore size and chemical composition of polysaccharide gels on the flow behavior and metal/semiconductor separation of single-walled carbon nanotubes by gel column chromatography are described.

Acta Phys. -Chim. Sin. **2014**, 30 (9), 1764–1770

Wavelength-Interrogated Surface Plasmon Resonance Sensor Based on Au-Ag Alloy Film

ZHANG Zhe LIU Jie
LU Dan-Feng QI Zhi-Mei

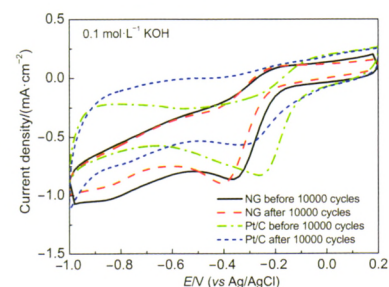
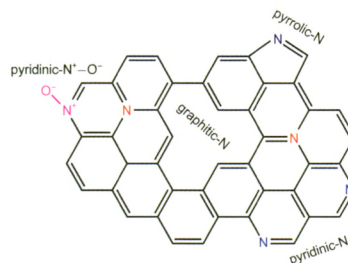


Au-Ag alloy films prepared by sputtering show greatly enhanced sensitivity in SPR sensors.

Acta Phys. -Chim. Sin. **2014**, 30 (9), 1771–1777

Preparation of Nitrogen-Doped Graphene and Its Electrocatalytic Activity for Oxygen Reduction Reaction

PENG San GUO Hui-Lin
KANG Xiao-Feng



Graphitic-N and pyridinic-N in graphene mainly determined the limiting current density and onset potential, respectively, in the oxygen reduction reaction.

Acta Phys. -Chim. Sin. **2014**, 30 (9), 1778–1786

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