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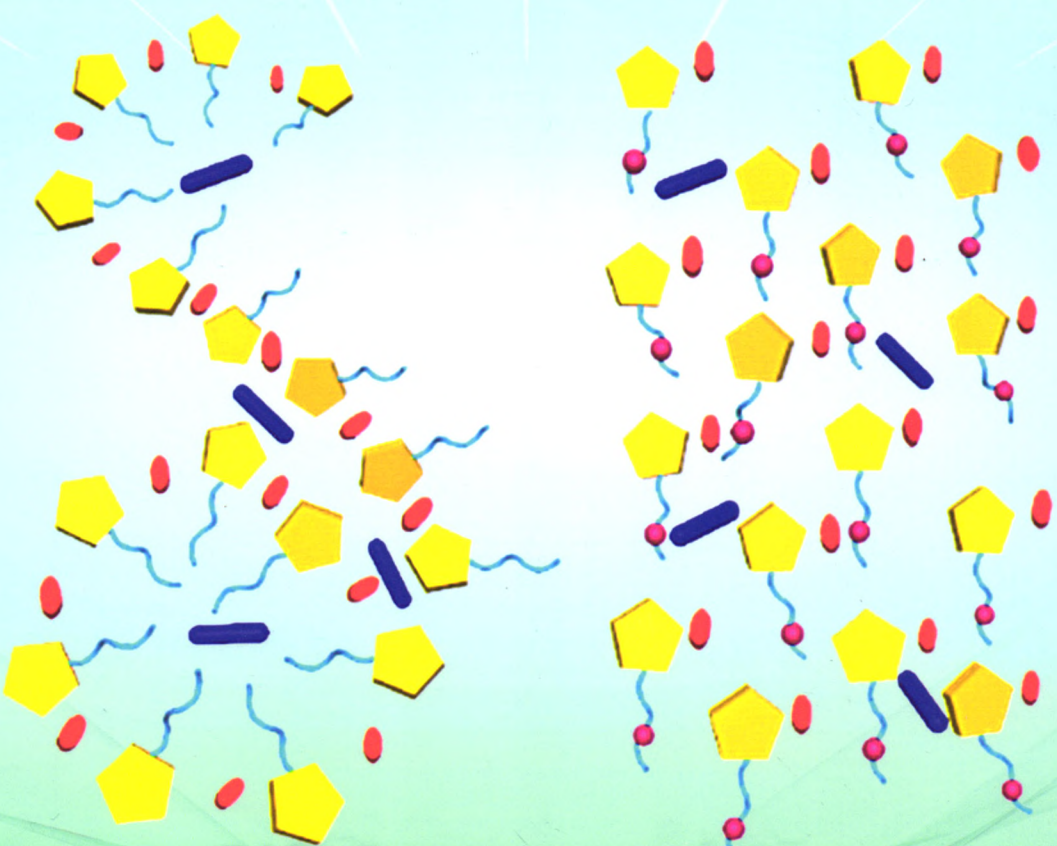
ISSN 1000-6818
CN 11-1892/O6
CODEN WHXUEU

物理化学学报

ACTA PHYSICO-CHIMICA SINICA

第31卷 第8期 Vol.31 No.8 2015



[bmim][PF_6] [moemim][PF_6]

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 31 卷第 8 期(2015 年 8 月 15 日)

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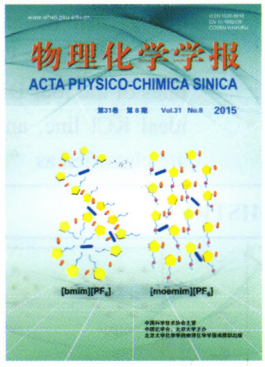
本期责任编辑: 黄　路

ACTA PHYSICO-CHIMICA SINICA
Vol.31 No.8 (August 15, 2015)

COVER



The cover image presents the different local structures of ionic liquids [bmim] [PF_6] and [moemim] [PF_6] detected by molecular probe C153. On page 1452, LI Bo-Xuan *et al.* demonstrate that the structural heterogeneity and microviscosity of [bmim] [PF_6] are lower than those of the ether-functionalized ionic liquid [moemim] [PF_6], suggesting that the good structure and property tunability of ionic liquids by molecular design can broaden their applications for different purposes.

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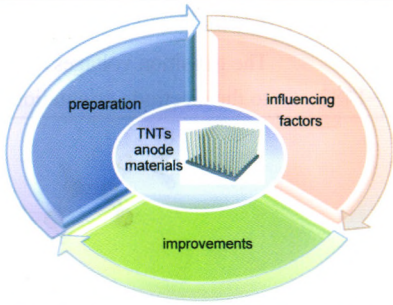
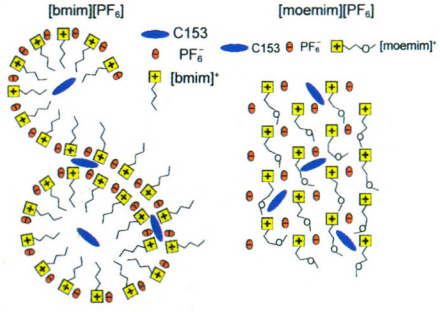
REVIEW

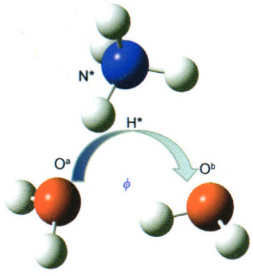


This paper reviews the preparation methods of TiO_2 nanotubes, summarizes the factors influencing their preparation, and discusses approaches improving their electrochemical performance as an anode material for lithium ion batteries.

THERMODYNAMICS, KINETICS, AND STRUCTURAL CHEMISTRY



The structural heterogeneities and microviscosities of [bmim] [PF_6] and [moemim] [PF_6] ionic liquids were investigated.

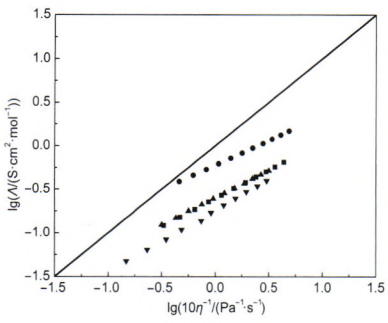


Hydrogen bond switching can trigger a fast jump rotation of ammonium ion in aqueous solutions.

Properties of Four Deep Eutectic Solvents: Density, Electrical Conductivity, Dynamic Viscosity and Refractive Index

SU Hong-Zhen YIN Jing-Mei
LIU Qing-Shan LI Chang-Ping

Acta Phys. -Chim. Sin. **2015,** *31* (8), 1468−1473



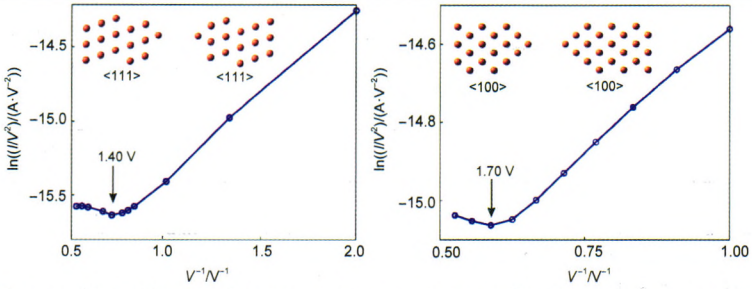
The lgΛ (molar electrical conductivity) dependence on lgη^{-1} (dynamic viscosity) was plotted for four deep eutectic solvents. The curves are approximately straight lines, which indicates that the deep eutectic solvents obey the Walden rule. The lines of the four DESs lie below the ideal KCl line, and the four DESs are classified as "subionic".

THEORETICAL AND COMPUTATIONAL CHEMISTRY

Theoretical Investigation of the Transition Voltages of Cu-Vacuum-Cu Tunneling Junctions

BAI Mei-Lin WANG Ming-Lang
HOU Shi-Min

Acta Phys. -Chim. Sin. **2015,** *31* (8), 1474−1482

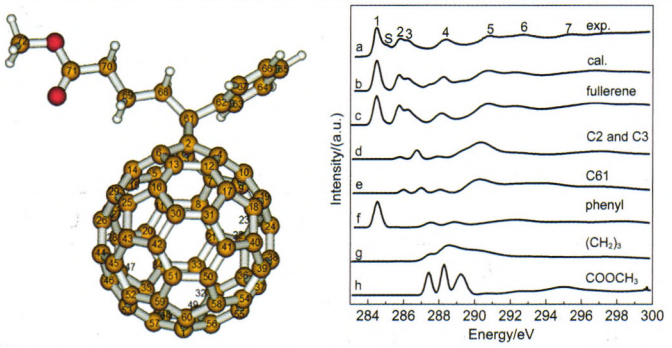


The transition voltages of copper-vacuum-copper tunneling junctions are sensitive to the electrode orientation and the atomic configurations of surface protrusions.

First-Principles Study on the Near-Edge X-ray Absorption Fine Structure Spectroscopy of the Fullerene-Derivative PCBM

MA Yong WANG Guang-Wei
SUN Shao-Tao SONG Xiu-Neng

Acta Phys. -Chim. Sin. **2015,** *31* (8), 1483−1488

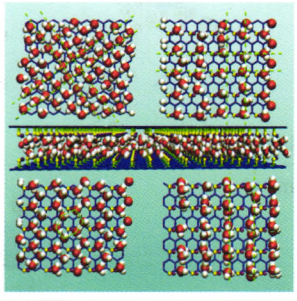


The feature peak of PCBM was assigned by component analysis of the C 1*s* near-edge X-ray absorption fine structure spectroscopy.

Molecular Dynamics Simulation of Water Molecules in Confined Slit Pores of Graphene

ZHAO Meng-Yao YANG Xue-Ping
YANG Xiao-Ning

Acta Phys. -Chim. Sin. **2015,** *31* (8), 1489−1498

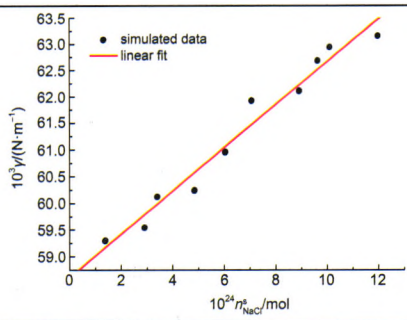


The microstructure and dynamics of water molecules confined inside graphene-based subnanometer pores have been investigated by molecular dynamics simulations.

Surface Absorption of a Solution at Equilibrium

CHEN Fei-Wu LU Tian
WU Zhao

Acta Phys. -Chim. Sin. **2015,** *31* (8), 1499−1503

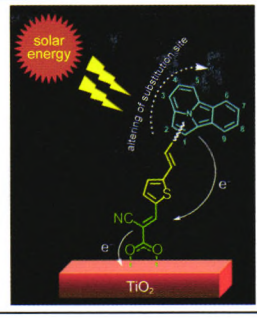


A new thermodynamic state function and a new surface adsorption equation are derived to describe surface adsorption of a solution at equilibrium.

Molecular Design of Indolizino Derivative as Sensitizers for Organic Dye-Sensitized Solar Cells

HOU Li-Mei WEN Zhi
LI Yin-Xiang HU Hua-You
KAN Yu-He SU Zhong-Min

Acta Phys. -Chim. Sin. **2015,** *31* (8), 1504−1512



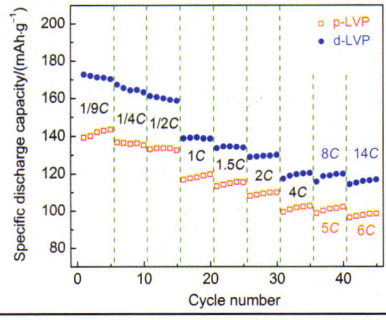
New D-π-A metal-free sensitizers with indolizino[3, 4, 5-ab]isoindole (INI) as an electronic donor were investigated and proposed as promising candidates for fabrication of high-performance dye-sensitized solar cells owing to a high maximum short-circuit current density.

ELECTROCHEMISTRY AND NEW ENERGY

Triple-Cation-Doped $Li_3V_2(PO_4)_3$ Cathode Material for Lithium Ion Batteries

SUN Xiao-Fei XU You-Long
ZHENG Xiao-Yu MENG Xiang-Fei
DING Peng REN Hang
LI Long

Acta Phys. -Chim. Sin. **2015,** *31* (8), 1513−1520

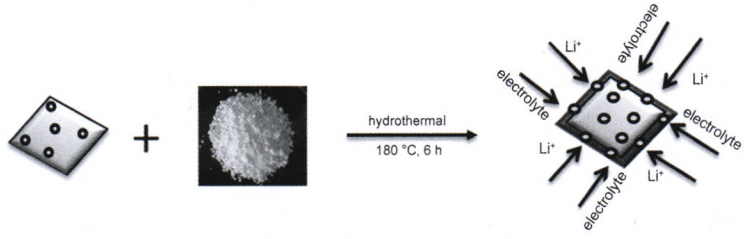


The capacity, rate, and cycling performances of $Li_3V_2(PO_4)_3$ are significantly improved by Na-Al-F co-doping along with carbon coating.

Preparation and Electrochemical Properties of Carbon-Coated $CoCO_3$ as an Anode Material for Lithium Ion Batteries

SUN Xue-Mei GAO Li-Jun

Acta Phys. -Chim. Sin. **2015,** *31* (8), 1521−1526

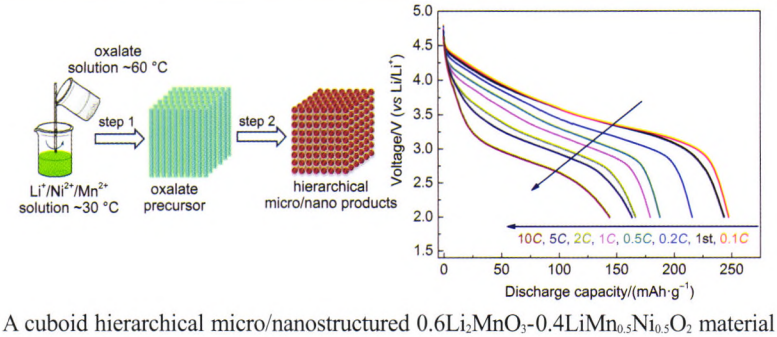


The electrical conductivity and specific capacity of $CoCO_3$ are improved after its surface is coated with carbon. The structural stability of $CoCO_3$/C during charge and discharge cycles is enhanced by carbon coating.

Facile Synthesis of $0.6Li_2MnO_3$-$0.4LiNi_{0.5}Mn_{0.5}O_2$ with Hierarchical Micro/Nanostructure and High Rate Capability as Cathode Material for Li-Ion Battery

SHI Xia-Xing LIAO Shi-Xuan
YUAN Bing ZHONG Yan-Jun
ZHONG Ben-He LIU Heng
GUO Xiao-Dong

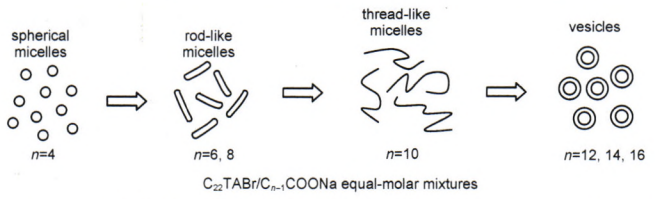
Acta Phys. -Chim. Sin. **2015,** *31* (8), 1527−1534



A cuboid hierarchical micro/nanostructured $0.6Li_2MnO_3$-$0.4LiMn_{0.5}Ni_{0.5}O_2$ material composed of small nanoparticles was synthesized by a quick and facile co-precipitation method which masterly utilizes the properties of the oxalate. The as-prepared composite delivers excellent electrochemical performance.

Self-Assembly of Cationic/Anionic Surfactants with Highly Dissymmetric Lengths of Alkyl Tails

DONG Wen-Jing ZHAO Jian-Xi



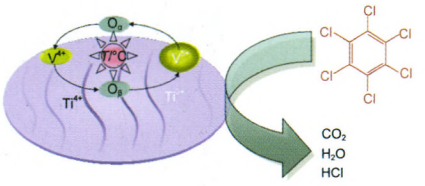
Acta Phys. -Chim. Sin. **2015,** *31* (8), 1535−1540

The dissymmetry of alkyl tail lengths strongly affected the aggregate structures in equimolar mixtures of cationic/anionic surfactants.

CATALYSIS AND SURFACE SCIENCE

Influence of Calcination Temperature on Dechlorination Performance of V_2O_5/CNTs-TiO_2 Catalysts

LI Yan ZHANG Ting-Ting
LI Yue JIA Bing
TAN Hua-Hua YU Jiang

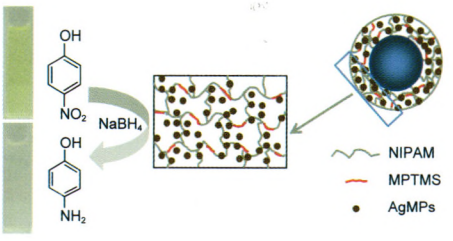


Optimization of the active components of V_2O_5/CNT-TiO_2 by calcination temperature was performed to improve the catalyst activity for the degradation of HCB.

Acta Phys. -Chim. Sin. **2015,** *31* (8), 1541−1548

Synthesis of Silver Nanoparticles Loaded onto a Structural Support and Their Catalytic Activity

ZHAO Jia LIU Li-Feng
ZHANG Ying

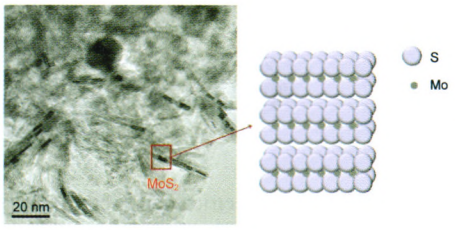


Ag nanoparticles were prepared on the surface of inorganic-organic hybrid network microgels with thermosensitivity. Poly(*N*-isopropylacrylamide) segments separated by the inorganic networks formed by 3-methacryloxypropyltrimethoxysilane are favorable for the mass transfer of reactants.

Acta Phys. -Chim. Sin. **2015,** *31* (8), 1549−1558

Effect of the Fluorine Addition Method on the Hydrodesulfurization Performance of NiMo Catalysts over Slurry Bed

SHI Lin HUANG Wei
SONG Shu-Zheng LI Zhi-Bo
LIU Shuang-Qiang

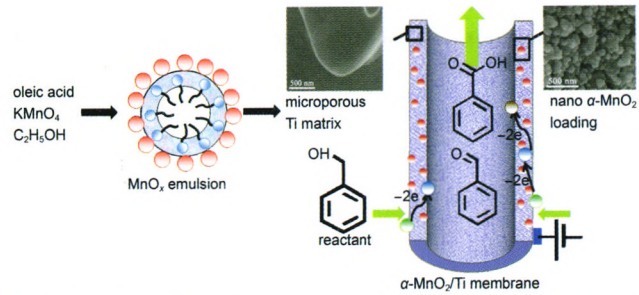


In the absence of nitric acid, adding fluoride into a NiMo-based slurry catalyst before the active component can effectively weaken the interaction between the metal and the support, and promote the generation of more MoS_2 slabs with proper stacking number (3−4 layers), which show the characteristic of highly active NiMoS(II) phases.

Acta Phys. -Chim. Sin. **2015,** *31* (8), 1559−1566

Preparation of Nano-Manganite Loaded Titanium Electrocatalytic Membrane for the Catalytic Oxidation of Benzyl Alcohol

TIAN Wen-Jie WANG Hong
YIN Zhen YANG Ying
LI Jian-Xin



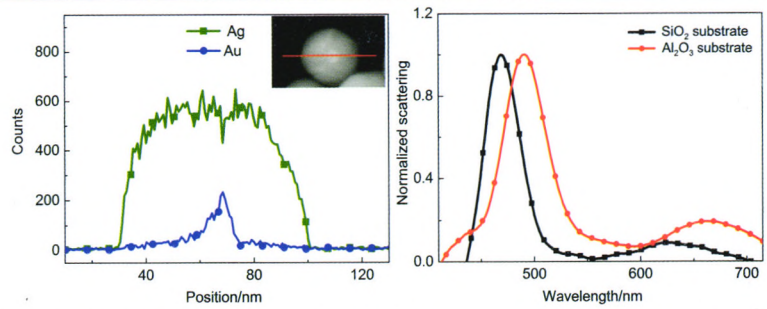
Because of the binding effects between unsaturated coordination atoms of Mn and oxygen vacancies with the Ti substrate, the α-MnO_2/Ti membrane obtained at a calcination temperature 450 °C had superior electrochemical properties and catalytic performance for selective oxidation of benzyl alcohol.

Acta Phys. -Chim. Sin. **2015,** *31* (8), 1567−1574

PHOTOCHEMISTRY AND RADIATION CHEMISTRY

Spherical Au@Ag Nanoparticles for Localized Surface Plasmon Resonance Scanning Probes: Synthesis and Dielectric Sensitivity

HE Xi TANG Tong-Dan
YI Jun LIU Bi-Ju
WANG Fang-Fang REN Bin
ZHOU Jian-Zhang



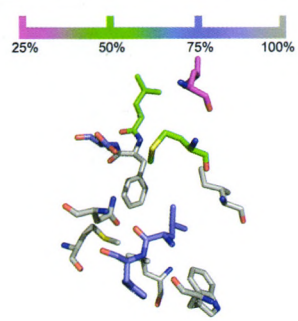
Spherical Au@Ag nanoparticles with good size uniformity and a thick Ag shell were synthesized for use as localized surface plasmon resonance microscopic probes.

Acta Phys. -Chim. Sin. **2015,** *31* (8), 1575−1583

BIOPHYSICAL CHEMISTRY

Comparison of the Selectivity of Human Adenosine Receptor Antagonists Based on Structure and Pharmacophore Features

ZENG Ling-Xiao LI Xin-Ran
JIN Hong-Wei LIU Zhen-Ming
ZHANG Liang-Ren



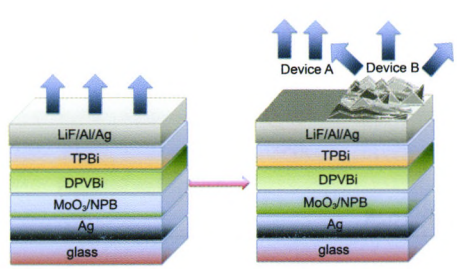
Ligand-based and receptor-based methods were implemented to investigate the selectivity of human adenosine receptor antagonists.

Acta Phys. -Chim. Sin. **2015,** *31* (8), 1584−1596

PHYSICAL CHEMISTRY OF MATERIALS

Mesoscopic Optical Structure to Enhance the Out-Coupling Efficiency of Blue Top OLED

CHUNG Yaohsien BIAN Mengying
ZHANG Mingxiao CHU Saisai
CHEN Zhijian GONG Qihuang
XIAO Lixin

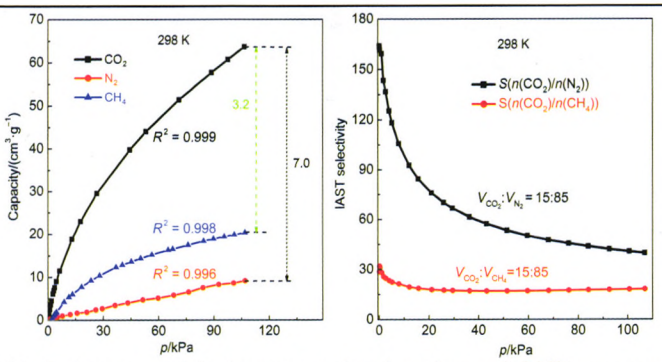


Mesoscopic optical structured 2,9-dimethyl-4,7-diphenyl-1,10-phenyl-1,10-phenanthrolin (bathocuproine, BCP) film was formed to enhance the out-coupling efficiency of blue top-emitting organic light-emitting devices (OLEDs).

Acta Phys. -Chim. Sin. **2015,** *31* (8), 1597−1601

Nitrogen-Enriched Hierarchical Porous Carbon for Carbon Dioxide Adsorption and Separation

JIN Zhen-Yu LI Tong
LU An-Hui

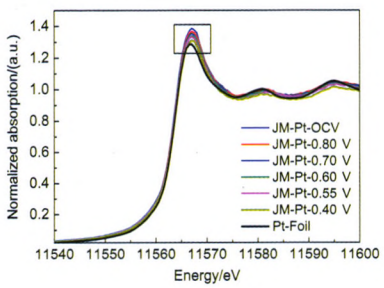


Hierarchical nitrogen-enriched porous carbon based on a Schiff base precursor shows a CO_2 capacity of 97 cm^3·g^{-1} at ambient pressure and 273 K. The CO_2/N_2 and CO_2/CH_4 separation ratios are 7.0 and 3.2, respectively. The predicted ideal adsorbed solution theory (IAST) selectivities of the two-component mixed stream are 40 (CO_2/N_2) and 18 (CO_2/CH_4) by Toth mode simulation.

Acta Phys. -Chim. Sin. **2015,** *31* (8), 1602−1608

***In Situ* XAFS Method for Characterizing Catalyst Structure in Proton Exchange Membrane Fuel Cells**

SHANG Ming-Feng DUAN Pei-Quan
ZHAO Tian-Tian TANG Wen-Chao
LIN Rui HUANG Yu-Ying
WANG Jian-Qiang

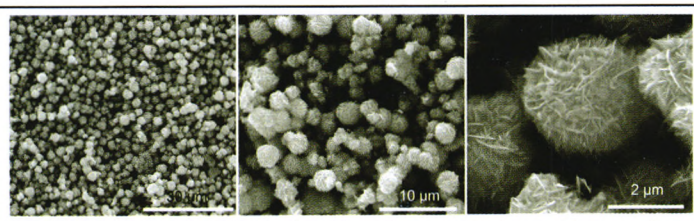


In situ XANES data were collected under the operating state of a fuel cell with Pt/C and Pd/C cathode and anode catalysts, respectively, while the cell $C-V$ and power density curves were monitored. Changes in the oxidation states of the Pt/C catalyst were observed at different potentials. Strong Pt−O bonds were induced on the surfaces of the Pt at high potential, which may hinder the performance of Pt and reduce its ORR activity.

Acta Phys. -Chim. Sin. **2015,** *31* (8), 1609−1614

Preparation of Micro/Nano ZnO Pompons and Their Catalytic Activity for the Solar Degradation of Organic Dyes

TONG La-Ga LIU Jin-Yan
WANG Cen-Chen RONG Hua
LI Wei

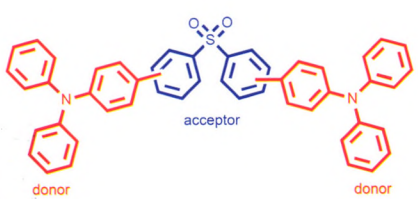


Micro/nano ZnO pompons displaying high photocatalytic reactivity and photostability under sunlight were synthesized using glutamic acid fluoborate ionic liquid.

Acta Phys. -Chim. Sin. **2015,** *31* (8), 1615−1620

Thermally Activated Delayed Fluorescence Materials Based on Triphenylamine/ Diphenyl Sulfone

HUANG Bin DAI Yu
BAN Xin-Xin JIANG Wei
ZHANG Zhao-Hang SUN Kai-Yong
LIN Bao-Ping SUN Yue-Ming



A series of thermally activated delayed fluorescence (TADF) materials based on triphenylamine and diphenyl sulfone were synthesized. These materials have small energy gaps between the singlet and triplet of 0.46, 0.39, and 0.29 eV.

Acta Phys. -Chim. Sin. **2015,** *31* (8), 1621−1628

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The Editorial Committee of Acta Physico-Chimica Sinica

物理化学学报 (WULI HUAXUE XUEBAO) 第 31 卷第 8 期 (2015.08.15)
ACTA PHYSICO-CHIMICA SINICA, Vol.31, No.8 (August 15, 2015)

月刊(1985年创刊)
Monthly (First volume appeared in 1985)

编辑出版者	北京大学化学与分子工程学院《物理化学学报》编辑部	Editor and Publisher:	Editorial Office of Acta Physico-Chimica Sinica (Wuli Huaxue Xuebao)
地　　址	北京大学化学楼(邮政编码 100871)	Address:	Chemistry Building Peking University Beijing 100871, P. R. China
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主　　编	刘忠范	Editor-in-Chief:	LIU Zhong-Fan
主管单位	中国科学技术协会	Printer:	Beijing Kexin Printing CO., LTD
印 刷 者	北京科信印刷有限公司	Distributor:	China International Book Trading Corporation (Code No 1443-MO)
国内总发行	北京报刊发行局		
国内订购	全国各邮局		
国外发行	中国国际图书贸易总公司 Code No 1443-MO		
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ISSN 1000-6818

定价：**50.00**元　　**2015** 年 **8** 月 **15** 日出版　　国内邮发代号：**82-163**