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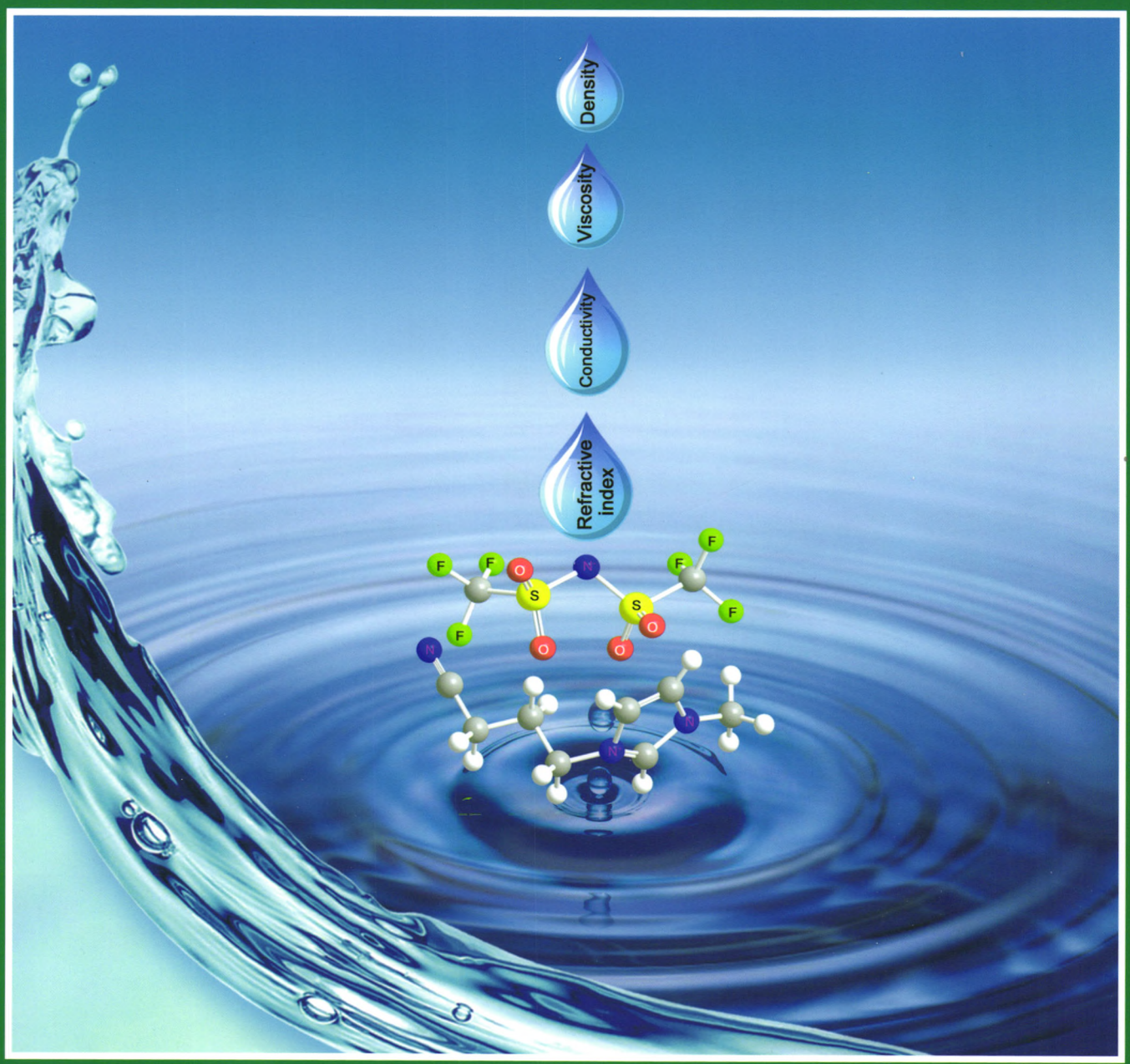
物理化学学报

ACTA PHYSICO-CHIMICA SINICA



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中国化学会、北京大学主办
北京大学化学学院物理化学学报编辑部出版
万方数据

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Vol.32 No.3

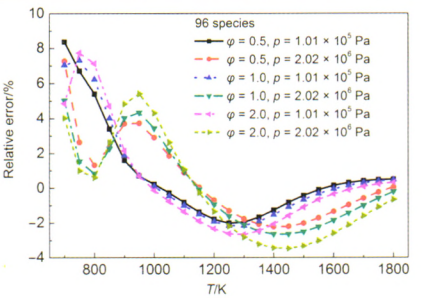
物理化学学报 (WULI HUAXUE XUEBAO) 第 32 卷第 3 期
ACTA PHYSICO-CHIMICA SINICA, Vol.32, No.3

COVER

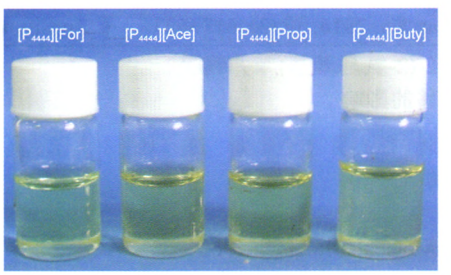
The cover image presents the structure and basic properties of functional ionic liuqid 1-(cyanopropyl)-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide. On page 617, LIU *et al.* demonstrate that the methylene introduction can lead to the decrease of density and dynamic viscosity, increase of electrical conductivity for cyano type ionic liquid, and the results are significant for design and application of the new type ionic liquids in industry and engineering.

CONTENTS

论文 ARTICLE



Directed relation graph-based methods for skeletal reduction of combustion reaction mechanisms are systematically compared.



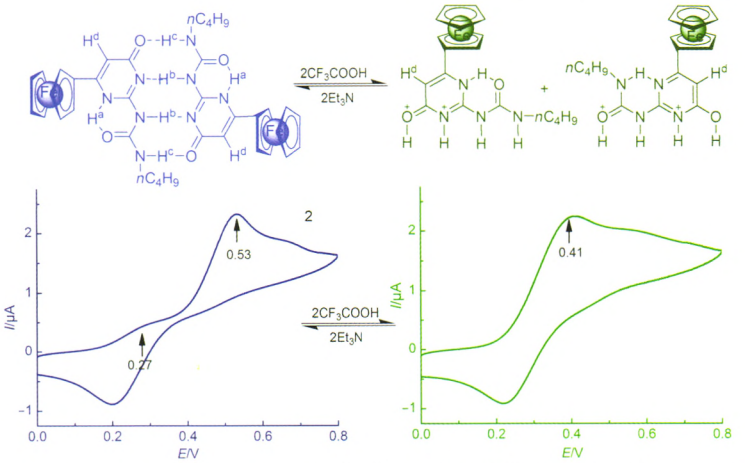
The physicochemical properties and CO_2 solubility of tetrabutylphosphonium carboxylate ionic liquids were measured.

脲基嘧啶酮四氢键二茂铁二聚体：电子相互作用的调控

王素敏　赵绒娜　王奇观　郭　浩
李金华　张文慧

Ureidopyrimidinone Quadruple Hydrogen-Bonded Ferrocene Dimer: Control of Electronic Communication

WANG Su-Min　ZHAO Rong-Na
WANG Qi-Guan　GUO Hao
LI Jin-Hua　ZHANG Wen-Hui



Electronic communication across the hydrogen-bonded bridge in a ferrocene dimer was reversibly controlled upon protonation/deprotonation of the bridging ureidopyrimidinone unit.

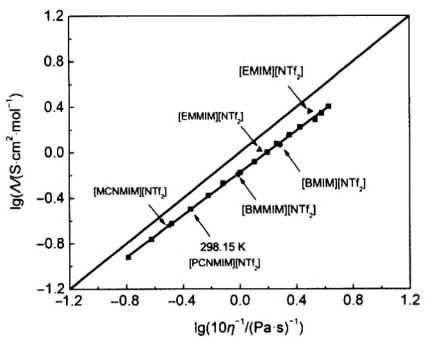
Acta Phys. -Chim. Sin. **2016,** *32* (3), 611−616

1-丁腈-3-甲基咪唑双三氟甲基磺酸亚胺的性质

刘青山　刘　惠　牟　林

Properties of 1-(Cyanopropyl)-3-methylimidazolium Bis[(trifluoromethyl)sulfonyl]imide

LIU Qing-Shan　LIU Hui
MOU Lin



lgΛ dependence on lgη^{-1} was ploted for the functional ionic liquid [PCNMIM][NTf_2] and five imidazolium ionic liquids. The curve approximates to a straight line, which indicates that the functional ionic liquid obeys the Walden rule. The position of the ideal line was established using diluted aqueous KCl solutions.

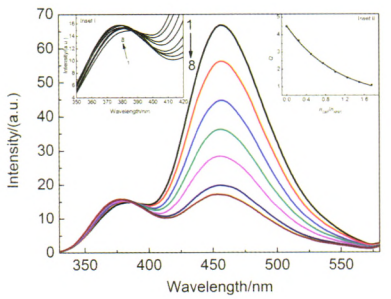
Acta Phys. -Chim. Sin. **2016,** *32* (3), 617−623

超分子作用对2-(2-氨基苯基)苯并噻唑分子内质子转移的影响

向俊峰　易平贵　任志勇　于贤勇　陈　建
刘　武　李桃梅

Effect of Supra-Molecular Interaction on the Intramolecular Proton Transfer of 2-(2-Aminophenyl)benzothiazole

XIANG Jun-Feng　YI Ping-Gui
REN Zhi-Yong　YU Xian-Yong
CHEN Jian　LIU Wu
LI Tao-Mei



The fluorescence spectra and efficiency of proton transfer of 2-(2-aminophenyl)benzothiazole depended on environment. Experimental and theoretical evidence indicated that 2-(2-aminophenyl)benzothiazole formed a 1 : 1 complex with cucurbit[7]uril.

Acta Phys. -Chim. Sin. **2016,** *32* (3), 624−630

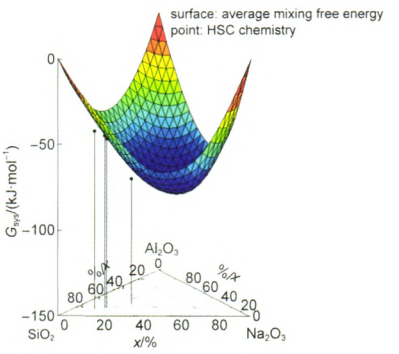
基于团簇结构模型的Na_2O-Al_2O_3-SiO_2三元体系熔体吉布斯混合摩尔自由能计算

李永康　尤静林　王　建　王　敏
马　楠　魏广超

Molar Gibbs Mixing Free Energy Calculation for a Na_2O-Al_2O_3-SiO_2 Ternary Melt Based on the Cluster Model

LI Yong-Kang　YOU Jing-Lin
WANG Jian　WANG Min
MA Nan　WEI Guang-Chao

Acta Phys. -Chim. Sin. **2016,** *32* (3), 631−637



The cluster model of molten Na_2O-Al_2O_3-SiO_2 aluminosilicates is used to show that the Gibbs mixing free energy of this ternary system is the sum of all the cluster units that exist according to the Boltzmann distribution law.

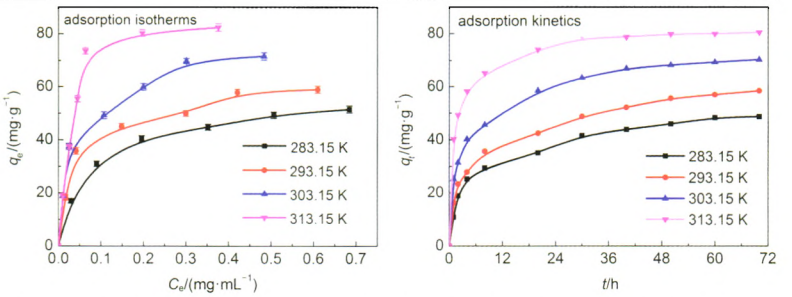
介孔TiO_2对溶菌酶吸附的动力学和热力学

洪启亮　董依慧　庄　伟　饶　超　刘　畅

Kinetics and Thermodynamics of Lysozyme Adsorption on Mesoporous Titanium Dioxide

HONG Qi-Liang　DONG Yi-Hui
ZHUANG Wei　RAO Chao
LIU Chang

Acta Phys. -Chim. Sin. **2016,** *32* (3), 638−646



The adsorption of lysozyme onto mesoporous titanium dioxide was stable, which is a spontaneous and endothermic process.

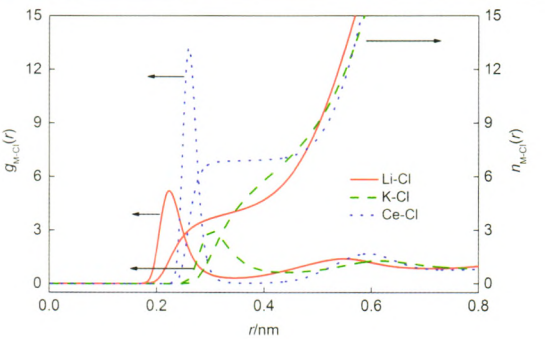
$LiCl$-KCl-$CeCl_3$熔盐结构与热力学的分子动力学模拟

姜　涛　王　宁　程长明　彭述明　严六明

Molecular Dynamics Simulation on the Structure and Thermodynamics of Molten $LiCl$-KCl-$CeCl_3$

JIANG Tao　WANG Ning
CHENG Chang-Ming　PENG Shu-Ming
YAN Liu-Ming

Acta Phys. -Chim. Sin. **2016,** *32* (3), 647−655



The behavior of $CeCl_3$ in molten $LiCl$-KCl-$CeCl_3$ mixtures was investigated by molecular dynamics simulation to predict the limitations of pyrometallurgical post-processing of spent fuel.

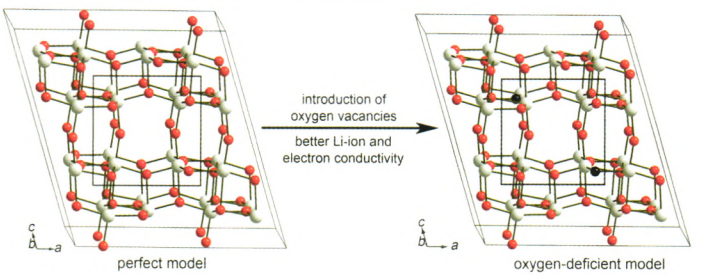
氧缺陷TiO_2-B作为可充电锂离子电池负极材料的第一性原理研究

孔令明　祝宝林　庞先勇　王贵昌

First-Principles Study on TiO_2-B with Oxygen Vacancies as a Negative Material of Rechargeable Lithium-Ion Batteries

KONG Ling-Ming　ZHU Bao-Lin
PANG Xian-Yong　WANG Gui-Chang

Acta Phys. -Chim. Sin. **2016,** *32* (3), 656−664



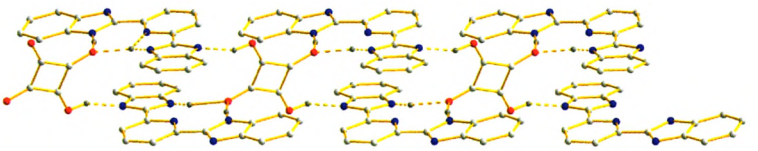
Oxygen-deficient TiO_2-B has higher Li-ion and electron conductivities than defect-free TiO_2-B and is a promising material for use in advanced rechargeable Li-ion batteries.

方酸与2,6-二苯并咪唑的超分子自组装及氢键实验与理论研究

胡爱彬　潘志权　程清蓉　周　红

Experimental and Theoretical Evidence for Supramolecular Self-Assembly and Hydrogen Bonding between Squaric Acid and 2,6-Bis(2-benzimidazolyl)pyridine

HU Ai-Bin　PAN Zhi-Quan
CHENG Qing-Rong　ZHOU Hong



Self-assembly of a supramolecular polymer driven by squaric acid was investigated by X-ray diffraction and theoretical analyses.

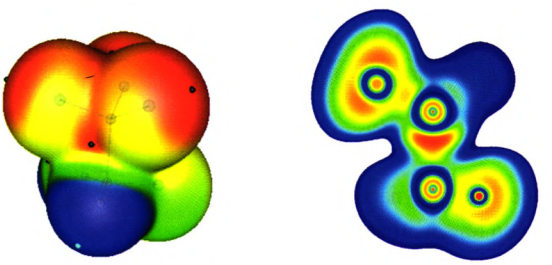
Acta Phys. -Chim. Sin. **2016,** *32* (3), 665−670

$PO_2X\cdots PX_3/PH_2X$ (X = F, Cl, Br, CH_3, NH_2)复合物中π-hole磷键作用的电子密度拓扑分析

王月红　李晓艳　曾艳丽　孟令鹏　张雪英

Topological Analyses of Electron Density on π-hole Pnicogen Bonds in $PO_2X\cdots PX_3/PH_2X$ (X = F, Cl, Br, CH_3, NH_2) Complexes

WANG Yue-Hong　LI Xiao-Yan
ZENG Yan-Li　MENG Ling-Peng
ZHANG Xue-Ying



A theoretical study shows that substituent groups greatly influence the properties of π-hole pnicogen bond interactions.

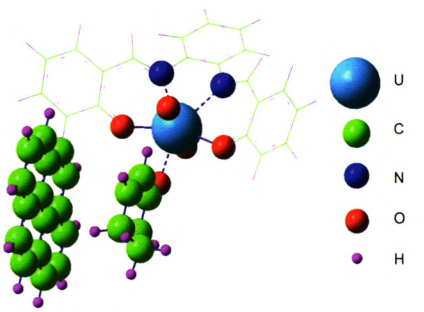
Acta Phys. -Chim. Sin. **2016,** *32* (3), 671−682

铀酰-Salophen受体对α,β-不饱和羰基化合物及手性客体的分子识别

高　莎　兰文波　林英武　廖力夫　聂长明

Molecular Recognition of α,β-Unsaturated Carbonyl Compounds and Chiral Guests by Uranyl-Salophen Receptors

GAO Sha　LAN Wen-Bo
LIN Ying-Wu　LIAO Li-Fu
NIE Chang-Ming



Theoretical calculations reveal that uranyl-salophens have the ability to selectively recognize some specific molecules.

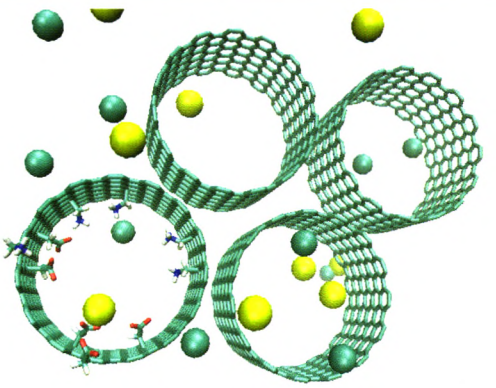
Acta Phys. -Chim. Sin. **2016,** *32* (3), 683−690

直径大于2 nm的(15,15)碳纳米管的仿生生物改性及其脱盐行为的分子模拟

李　清　杨登峰　王建花　武　琪　刘清芝

Biomimetic Modification and Desalination Behavior of (15,15) Carbon Nanotubes with a Diameter Larger than 2 nm

LI Qing　YANG Deng-Feng
WANG Jian-Hua　WU Qi
LIU Qing-Zhi



Carbon nanotubes modified with oppositely charged groups in their interior and at their entrance could improve salt desalination and maintain high water flux.

Acta Phys. -Chim. Sin. **2016,** *32* (3), 691−700

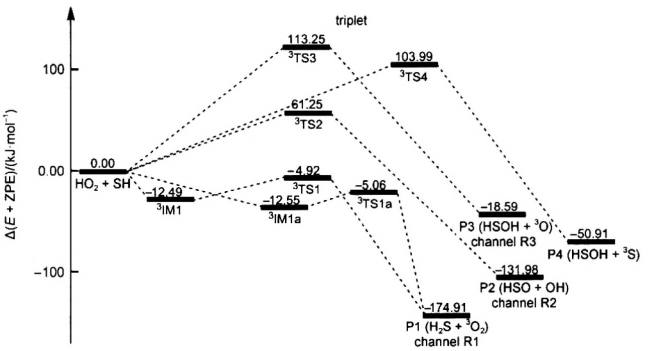
HS + HO_2气相反应机理及主通道速率常数的理论研究

张田雷　杨　晨　凤旭凯　王竹青　王　睿
刘秋丽　张　鹏　王文亮

Theoretical Study on the Atmospheric Reaction of HS with HO_2: Mechanism and Rate Constants of the Major Channel

ZHANG Tian-Lei　YANG Chen
FENG Xu-Kai　WANG Zhu-Qing
WANG Rui　LIU Qiu-Li
ZHANG Peng　WANG Wen-Liang

Acta Phys. -Chim. Sin. **2016,** *32* (3), 701−710



Theoretical investigations indicate that the favorable channel of the HO_2 + HS reaction, namely, the product channel of H_2S and $^3O_2$, occurs on the triplet potential energy surfaces with apparent activation energies ranging from − 5.06 to −4.92 kJ·mol^{-1}.

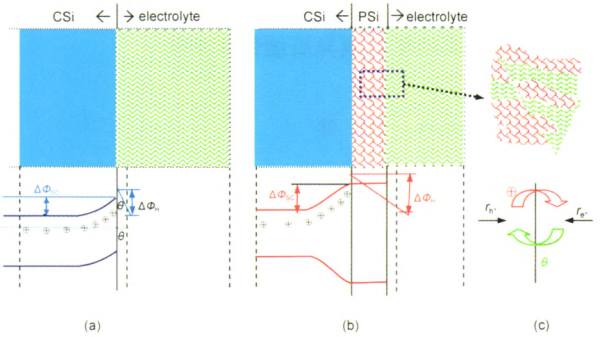
多孔与平面硅电极界面的电化学行为

吕京美　程　璇

Electrochemical Behavior of Porous and Flat Silicon Electrode Interfaces

LÜ Jing-Mei　CHENG Xuan

Acta Phys. -Chim. Sin. **2016,** *32* (3), 711−716



Changes of electrochemical parameters suggested that the porous silicon layer formation on single-crystal silicon electrodes increased the thickness of the Helmholtz layer and influenced the potential distribution.

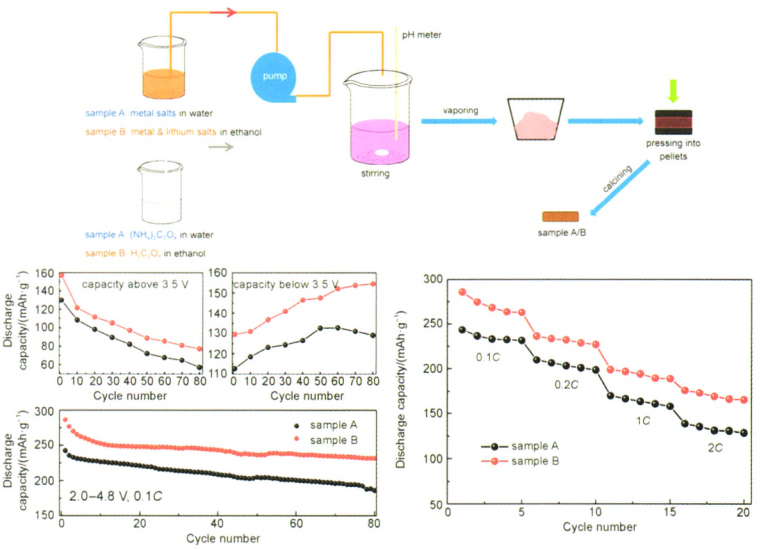
采用基于乙醇体系的一步草酸共沉淀法制备层状富锂锰基正极材料

寇建文　王　昭　包丽颖　苏岳锋
胡　宇　陈　来　徐少禹　陈　芬
陈人杰　孙逢春　吴　锋

Layered Lithium-Rich Cathode Materials Synthesized by an Ethanol-Based One-Step Oxalate Coprecipitation Method

KOU Jian-Wen　WANG Zhao
BAO Li-Ying　SU Yue-Feng
HU Yu　CHEN Lai
XU Shao-Yu　CHEN Fen
CHEN Ren-Jie　SUN Feng-Chun
WU Feng

Acta Phys. -Chim. Sin. **2016,** *32* (3), 717−722



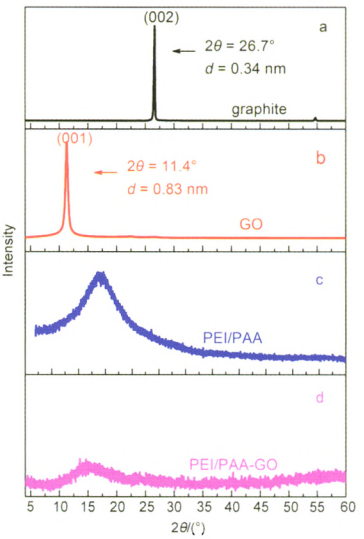
Layered lithium-rich cathode materials with enhanced electrochemical performance were synthesized by a novel ethanol-based one-step oxalate coprecipitation method.

氧化石墨烯/聚电解质层层自组装制备单价离子选择性膜

赵胜君　张　伟　邓会宁　刘　伟

Layer-by-Layer Assembly of Graphene Oxide and Polyelectrolyte Composite Membranes for Monovalent Cation Separation

ZHAO Sheng-Jun　ZHANG Wei
DENG Hui-Ning　LIU Wei



Acta Phys. -Chim. Sin. **2016,** *32* (3), 723−727

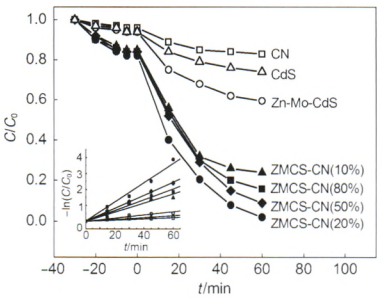
The addition of GO effectively enhances the antifouling and selectivity for monovalent ions of PEI/PAA multilayer membranes.

三元金属硫化物-石墨相氮化碳异质结催化剂的制备及光催化性能

王彦娟　孙佳瑶　封瑞江　张　健

Preparation of Ternary Metal Sulfide/g-C_3N_4 Heterojunction Catalysts and Their Photocatalytic Activity under visible Light

WANG Yan-Juan　SUN Jia-Yao
FENG Rui-Jiang　ZHANG Jian



Acta Phys. -Chim. Sin. **2016,** *32* (3), 728−736

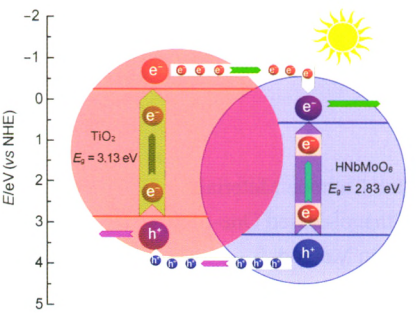
At an optimal g-C_3N_4 mass fraction of 20%, the as-prepared Zn-Mo-CdS/g-C_3N_4 heterojunction photocatalyst displayed the highest rate constant for RhB degradation under visible light, which was 30 and 10 times higher than those of single g-C_3N_4 and Zn-Mo-CdS, respectively.

TiO_2-$HNbMoO_6$复合材料的结构特征及其光催化性能

胡丽芳　何　杰　刘　媛　赵芸蕾　陈　凯

Structural Features and Photocatalytic Performance of TiO_2-$HNbMoO_6$ Composite

HU Li-Fang　HE Jie
LIU Yuan　ZHAO Yun-Lei
CHEN Kai



Acta Phys. -Chim. Sin. **2016,** *32* (3), 737−744

The TiO_2 nanoparticle was highly dispersed on the surface of $HNbMoO_6$ and was combined with Nb−O bond to constitute the heterojunctions. The narrower band gap and the higher activity of TiO_2-$HNbMoO_6$ may be attributed to a synergistic effect of $HNbMoO_6$ and TiO_2.

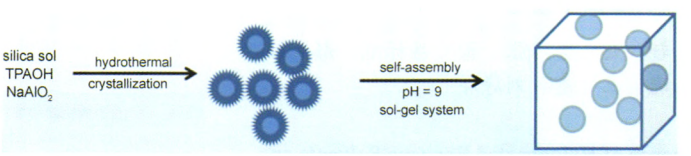
核壳MFI/CHA分子筛的合成及催化性能

张　玲　王海彦　蒋忠祥　王钰佳

Synthesis and Catalytic Activity of Core-Shell MFI/CHA Zeolites

ZHANG Ling　WANG Hai-Yan
JIANG Zhong-Xiang　WANG Yu-Jia

Acta Phys. -Chim. Sin. **2016,** *32* (3), 745−752



Core-shell MFI/CHA zeolites were synthesized by a two-step hydrothermal synthesis strategy (epitaxial growth).

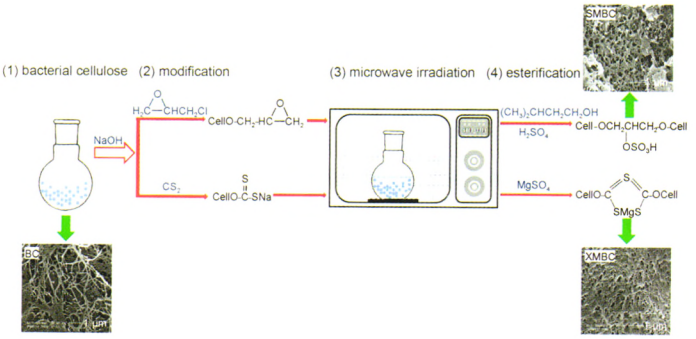
微波辅助细菌纤维素酯的制备及对Pb(II)的高效去除

王　吟　孙凤玲　张晓东　陶　红　杨一琼

Microwave-Assisted Synthesis of Esterified Bacterial Celluloses to Effectively Remove Pb(II)

WANG Yin　SUN Feng-Ling
ZHANG Xiao-Dong　TAO Hong
YANG Yi-Qiong

Acta Phys. -Chim. Sin. **2016,** *32* (3), 753−762



Esterification using microwave synthesis promoted the incorporation of thiol groups onto bacterial cellulose, which increased its adsorption capacity for Pb(II).

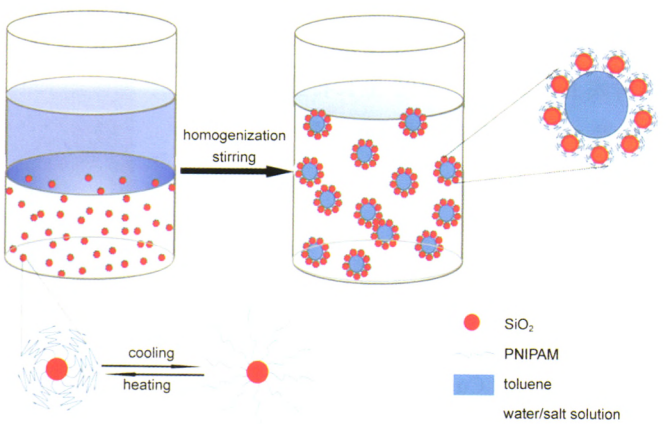
阴离子对SiO_2-PNIPAM构筑温敏Pickering乳液稳定性的影响

陈　芳　陈助国　孙会昭　孟繁想　马晓燕

Anion Effect on the Tunable Stability of a Thermoresponsive Pickering Emulsion Based on SiO_2-PNIPAM

CHEN Fang　CHEN Zhu-Guo
SUN Hui-Zhao　MENG Fan-Xiang
MA Xiao-Yan

Acta Phys. -Chim. Sin. **2016,** *32* (3), 763−770



A thermoresponsive pickering emulsion is prepared using SiO_2-PNIPAM as particles. The stabilization difference of the pickering emulsion can be tuned by changing temperature and anion.

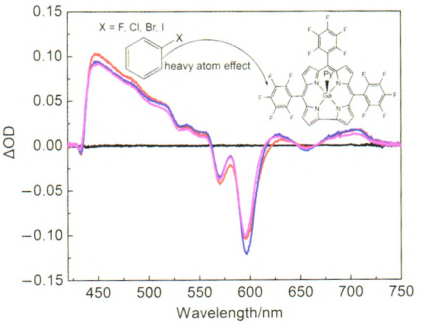
卤代苯溶剂对镓咔咯配合物光物理性质的影响：外重原子效应

占 轩 赵 芳 张 蕾 吕标彪 彭素红
应 晓 王 惠 刘海洋

Influence of Halogenated Benzene Solvents on the Photophysical Properties of Gallium Corroles: the External Heavy Atom Effect

ZHAN Xuan ZHAO Fang
ZHANG Lei LÜ Biao-Biao
PENG Su-Hong YING Xiao
WANG Hui LIU Hai-Yang

Acta Phys. -Chim. Sin. **2016,** *32* (3), 771−779



The effect of heavy atoms of halogenated benzene solvents on the photophysical properties of gallium corroles was investigated.

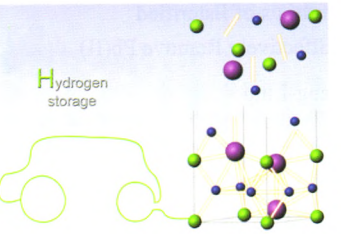
影响 $TiMn_x$ 非计量比合金储氢容量的结构因素

徐申东 方 亮 丁晓丽

Effect of Structural Factors on the Hydrogen Storage Capacity of Nonstoichiometric $TiMn_x$ Alloys

XU Shen-Dong FANG Liang
DING Xiao-Li

Acta Phys. -Chim. Sin. **2016,** *32* (3), 780−786



The Mn(2*a*)−Mn(2*a*) bonds play a dominant role in changing the tetrahedron interstitials for enhancing hydrogen storage in $TiMn_x$ alloys.

蓝宝石衬底上化学气相沉积法生长石墨烯

刘庆彬 蔚 翠 何泽召 王晶晶 李 佳
芦伟立 冯志红

Epitaxial Graphene on Sapphire Substrate by Chemical Vapor Deposition

LIU Qing-Bin YU Cui
HE Ze-Zhao WANG Jing-Jing
LI Jia LU Wei-Li
FENG Zhi-Hong

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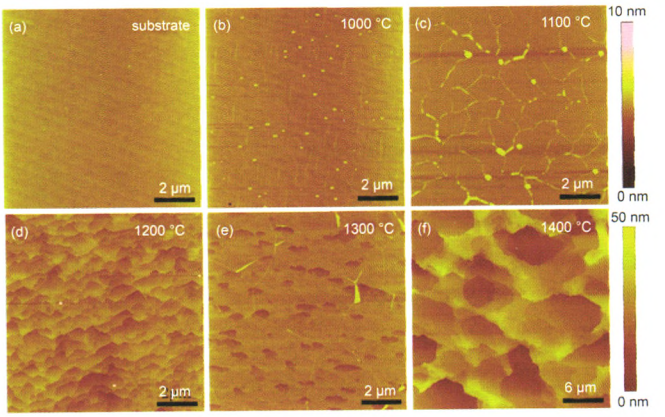

In this work, epitaxial grapheme was prepared on a sapphire substrate. A very low carbon concentration of 0.01% was used in the growth process, which results in a flat surface morphology and good crystal quality with a carrier mobility above 1000 $cm^2 \cdot V^{-1} \cdot s^{-1}$ at room temperature.

亮点 HIGHLIGHT

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