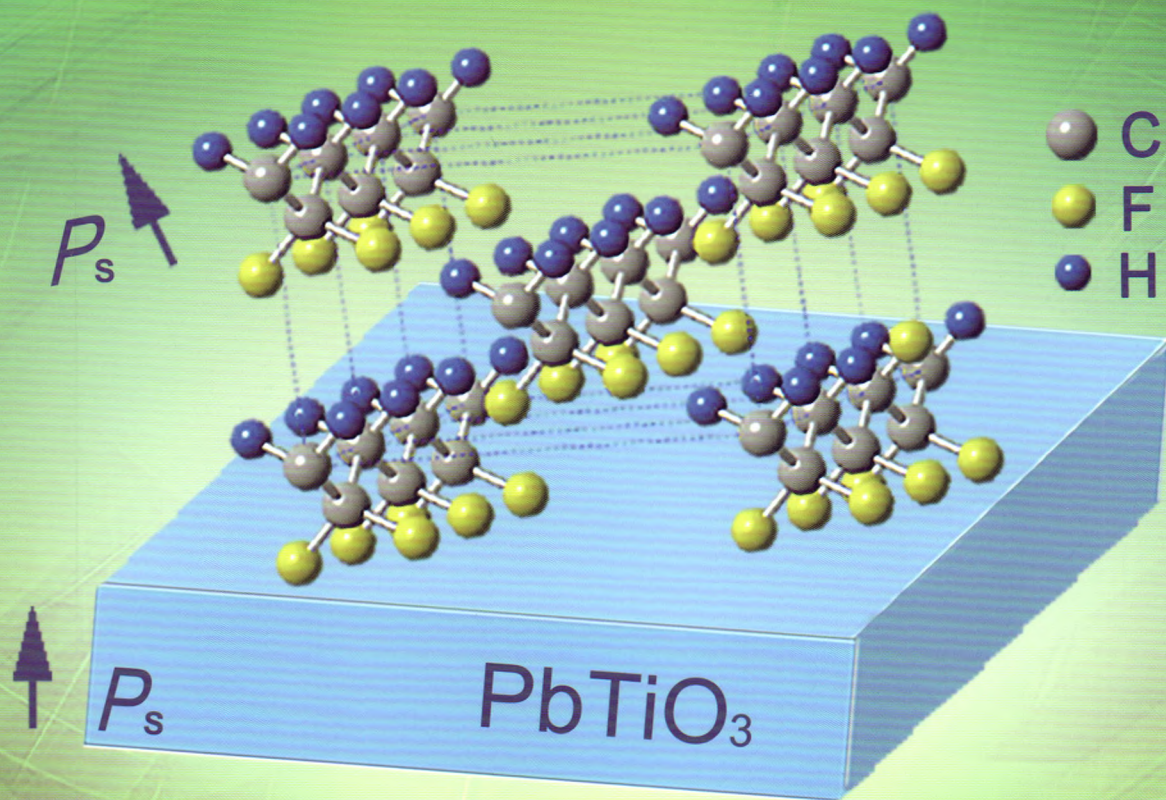


物理化学学报

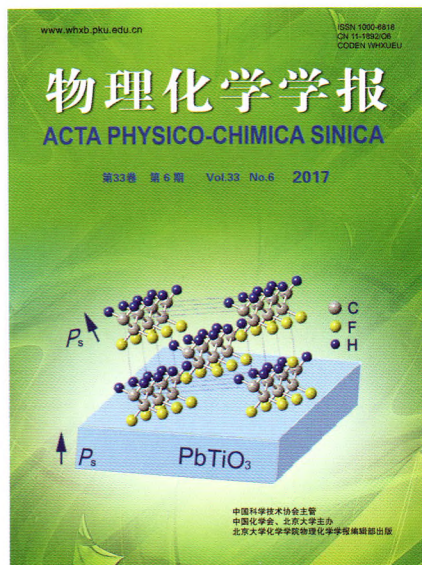
ACTA PHYSICO-CHIMICA SINICA

第33卷 第6期 Vol.33 No.6 2017



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

COVER



The cover image presents that an electric polarization interaction between semi-crystallized ferroelectric polymer P(VDF-TrFE) (denoted by PVTF) and inorganic ferroelectric PbTiO_3 is proposed to induce an oriented growth of PVTF. On page 1261, LIU *et al.* report that single-domain ferroelectric PbTiO_3 nanoplates can effectively mediate a nucleation and growth of the crystalline phase within PVTF, giving rise to an oriented film and significantly improved properties owing to an alignment of the polarization directions of the polymer and the nanoplates.

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亮点 HIGHLIGHT

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锂-氧气电池中的水添加剂的关键作用：减少副产物和降低过电位(Reducing By-Products and Overpotential in Li-O₂ Batteries by Water Addition)..... 庄 林(ZHUANG Lin)(1075)

自组装策略调控表面反应(Steering On-Surface Reactions with Self-Assembly Strategy) 刘忠范(LIU Zhong-Fan)(1077)

高效光催化分解水制氢的人工光合组装体(Artificial Photosynthetic Framework for Exceptional Solar H₂ Evolution)..... 刘忠范(LIU Zhong-Fan)(1079)

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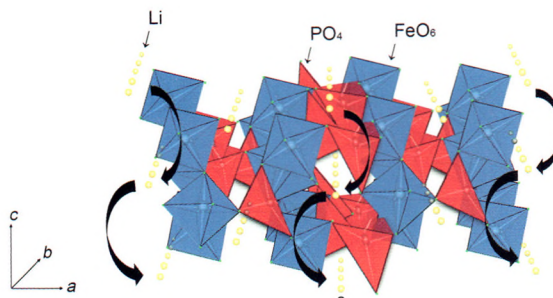
基于分子识别的外泌体纳米界面原位DNA组装(*In situ* DNA Assembly on the Surfaces of Nanosized Exosomes Based on Molecular Recognition) 符 婷 PENG Rui-Zi LIU Qiao-Ling(1083)

LiFePO₄ 电化学反应机理、制备及改性研究新进展

张英杰 朱子翼 董鹏 邱振平 梁慧新
李雪

New Research Progress of the Electrochemical Reaction Mechanism, Preparation and Modification for LiFePO₄

ZHANG Ying-Jie ZHU Zi-Yi
DONG Peng QIU Zhen-Ping
LIANG Hui-Xin LI Xue



A review of the research on the structure, electrochemical reaction mechanism, preparation technology and modification of LiFePO₄ was reviewed.

Acta Phys. -Chim. Sin. 2017, 33 (6), 1085–1107

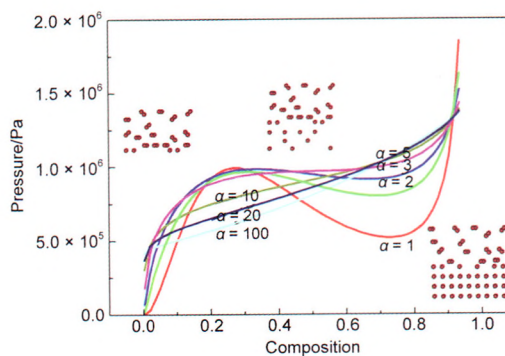
论文 ARTICLE

金属粉末的吸氢统计热力学模型

吴广新 彭望君 张捷宇

Statistic Thermodynamic Model of Hydrogen Absorption on Metal Powders

WU Guang-Xin PENG Wang-Jun
ZHANG Jie-Yu



Apparent compressibility factor α has been introduced to correct the volume change of high pressure gas. With the value of α increasing from 1 to 100, it can be seen that the shape of the curves changes from S-type to linear-type. Hence, our new model could describe the experiments more suitable.

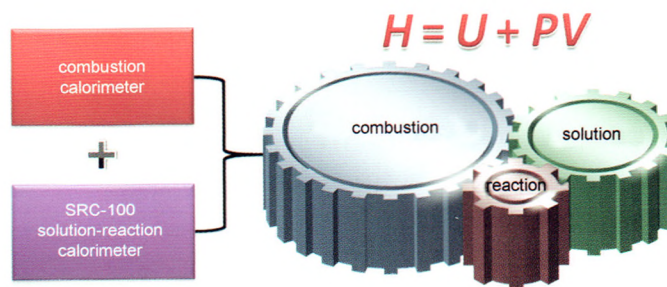
Acta Phys. -Chim. Sin. 2017, 33 (6), 1108–1113

一种精密恒温环境微量燃烧-溶解-反应多用量热计的设计及应用

李旭 李强国 蒋建宏 谷惠文 李传华
肖圣雄 李霞

Design and Application of a Precise Iso-peribol Combustion-Solution-Reaction Microcalorimeter

LI Xu LI Qiang-Guo
JIANG Jian-Hong GU Hui-Wen
LI Chuan-Hua XIAO Sheng-Xiong
LI Xia



In this work, a precise and versatile isoperibol combustion-solution-reaction microcalorimeter was developed based on the SRC-100 type solution-reaction isoperibol calorimeter.

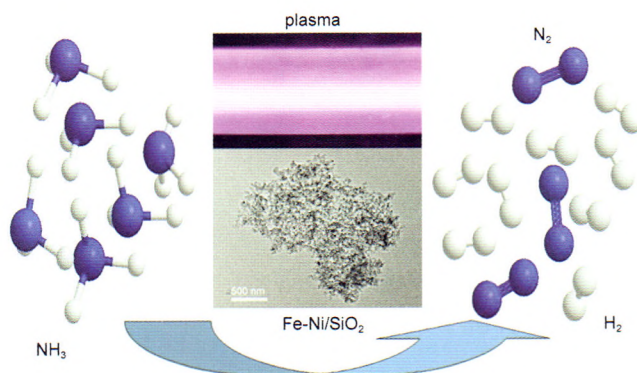
Acta Phys. -Chim. Sin. 2017, 33 (6), 1114–1122

负载型双金属催化剂的制备及其等离子体催化
氨分解制氢性能

孙帅其 易颜辉 王 丽 张家良 郭洪臣

Preparation and Performance of Supported
Bimetallic Catalysts for Hydrogen Production from
Ammonia Decomposition by Plasma Catalysis

SUN Shuai-Qi YI Yan-Hui
WANG Li ZHANG Jia-Liang
GUO Hong-Chen



The Fe-Ni bimetallic particles with spinel structure favors ammonia decompo-
sition under plasma condition.

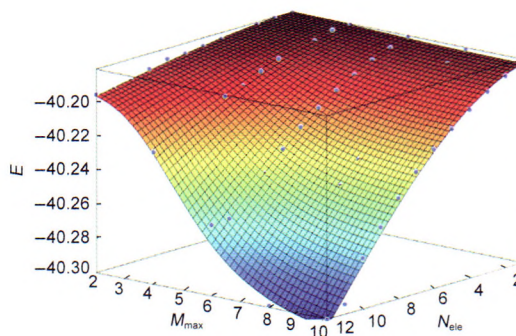
Acta Phys. -Chim. Sin. 2017, 33 (6), 1123–1129

完全活性空间组态相互作用能量的拟合和外推

曹静思 陈飞武

Fitting and Extrapolation of Configuration
Interaction Energies in Complete Active Space

CAO Jing-Si CHEN Fei-Wu



It is possible to extrapolate the full configuration interaction energy with the
maximum unoccupied active orbitals by fitting the configuration interaction en-
ergies in complete active space.

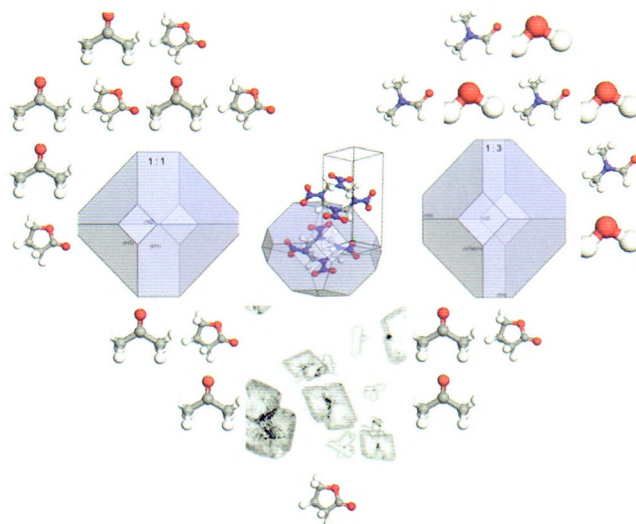
Acta Phys. -Chim. Sin. 2017, 33 (6), 1130–1139

混合溶剂对 β -HMX结晶形貌影响的分子动力学
模拟

陈 芳 刘圆圆 王建龙 苏宁宁 李丽洁
陈红春

Investigation of the Co-Solvent Effect on the Crystal
Morphology of β -HMX Using Molecular Dynamics
Simulations

CHEN Fang LIU Yuan-Yuan
WANG Jian-Long SU Ning-Ning
LI Li-Jie CHEN Hong-Chun



The crystal morphologies of β -HMX in co-solvents of acetone/ γ -butyrolactone
and dimethylformamide/H₂O were investigated.

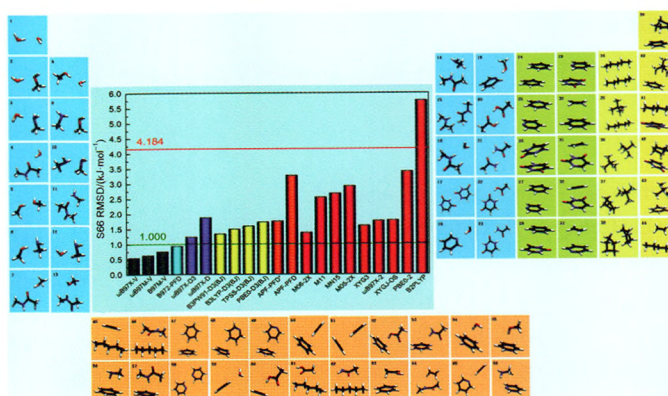
Acta Phys. -Chim. Sin. 2017, 33 (6), 1140–1148

B972-PFD: 一种高精度的色散校正密度泛函方法

何 禹 王一波

B972-PFD: A High Accuracy Density Functional Method for Dispersion Correction

HE Yu WANG Yi-Bo

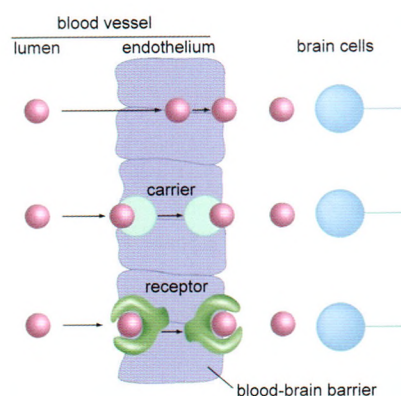


B972-PFD, a density functional method for dispersion correction, having $1 \text{ kJ} \cdot \text{L}^{-1}$ accuracy range with respect to the benchmark CCSD(T)/CBS calculations on the S66 data set.

Acta Phys. -Chim. Sin. **2017**, 33 (6), 1149–1159

Prediction of Blood-to-Brain Barrier Partitioning of Drugs and Organic Compounds Using a QSPR Approach

GOLMOHAMMADI Hassan
DASHTBOZORGI Zahra
KHOOSHECHIN Sajad



The blood-brain barrier (BBB) separates the brain from the blood stream and limits the transport of many substances from systemic circulation into brain tissue.

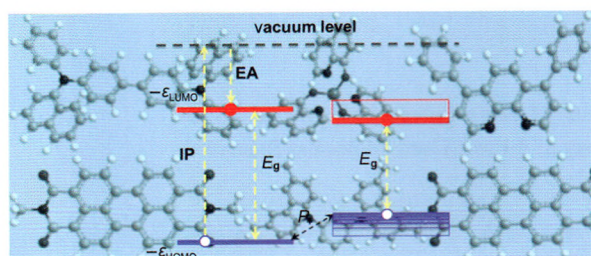
Acta Phys. -Chim. Sin. **2017**, 33 (6), 1160–1170

有机半导体的电子电离能、亲和势和极化能的密度泛函理论研究

郭姿含 胡竹斌 孙真荣 孙海涛

Density Functional Theory Studies on Ionization Energies, Electron Affinities, and Polarization Energies of Organic Semiconductors

GUO Zi-Han HU Zhu-Bin
SUN Zhen-Rong SUN Hai-Tao



A combination of the polarizable continuum model and the optimally tuned range-separated functional method was proposed and proved an easily applicable and computationally efficient theoretical tool for studying the energy levels of organic solid materials.

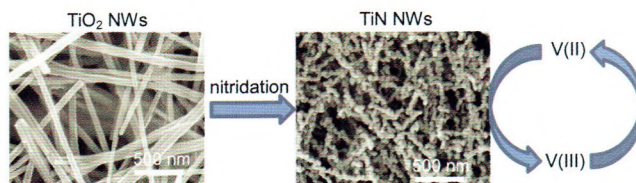
Acta Phys. -Chim. Sin. **2017**, 33 (6), 1171–1180

氮化钛纳米线的结构特征及其对 V(II)/V(III) 的电极过程

赵峰鸣 闻刚 孔丽瑶 褚有群 马淳安

Structure Characteristic of Titanium Nitride Nanowires and Its Electrode Processes for V(II)/V(III) Redox Couple

ZHAO Feng-Ming WEN Gang
KONG Li-Yao CHU You-Qun
MA Chun-An



TiN NWs, which were directly prepared on a Ti foil by a hydrothermal method followed by nitridation in ammonia atmosphere, exhibit excellent electrochemical activity towards the V(II)/V(III) redox couple.

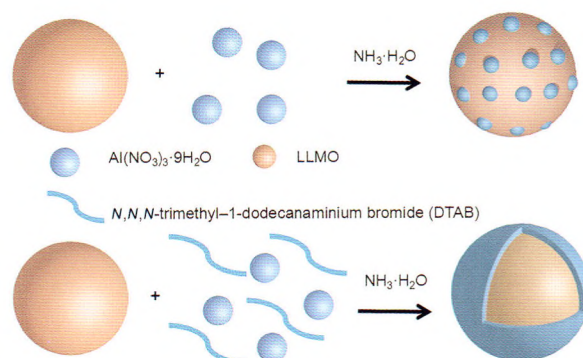
Acta Phys.-Chim. Sin. **2017**, 33 (6), 1181–1188

表面活性剂对氧化铝修饰富锂锰基正极材料的影响

甘永平 林沛沛 黄辉 夏阳 梁初
张俊 王奕顺 韩健峰 周彩红 张文魁

Effects of Surfactants on Al₂O₃-Modified Li-Rich Layered Metal Oxide Cathode Materials for Advanced Li-Ion Batteries

GAN Yong-Ping LIN Pei-Pei
HUANG Hui XIA Yang
LIANG Chu ZHANG Jun
WANG Yi-Shun HAN Jian-Feng
ZHOU Cai-Hong ZHANG Wen-Kui



DTAB as surfactant could guarantee uniform dispersion of Al₂O₃ nanoparticles on the LLMO surface, such that the composites exhibited superior electrochemical performance.

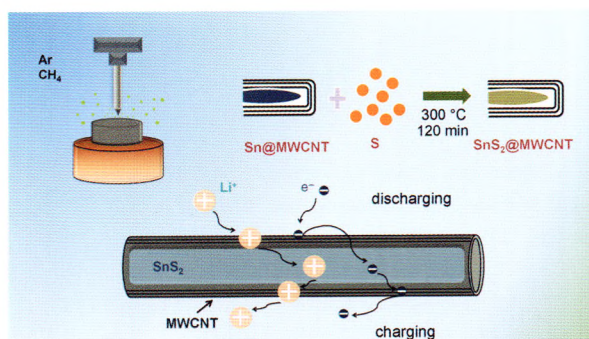
Acta Phys.-Chim. Sin. **2017**, 33 (6), 1189–1196

多壁纳米碳管约束二硫化锡作为锂离子电池负极的电化学行为

谷泽宇 高嵩 黄昊 靳晓哲 吴爱民
曹国忠

Electrochemical Behavior of MWCNT-Constraint SnS₂ Nanostructure as the Anode for Lithium-Ion Batteries

GU Ze-Yu GAO Song
HUANG Hao JIN Xiao-Zhe
WU Ai-Min CAO Guo-Zhong

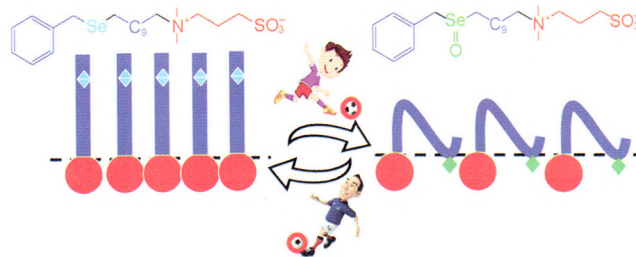


Carbon-constant SnS₂ nanoparticles were synthesized by a facile 2-step method and gave excellent electrochemical performance as the anode of Li-ion batteries.

Acta Phys.-Chim. Sin. **2017**, 33 (6), 1197–1204

含硒磺基甜菜碱表面活性剂界面性能的氧化-还原响应行为

孔伟伟 郭爽 张永民 刘雪峰



Redox-Responsive Interfacial Properties of Se-Containing Sulfobetaine Surfactant

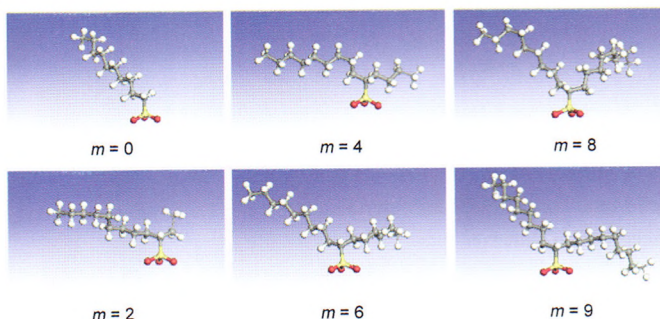
KONG Wei-Wei GUO Shuang
ZHANG Yong-Min LIU Xue-Feng

Acta Phys.-Chim. Sin. **2017**, *33* (6), 1205–1213

Both macroscopic and microscopic interfacial properties of Se-containing surfactant solution can be smart-controlled by a simple redox reaction.

双链阴离子表面活性剂 1-烷基-癸基磺酸钠在气/液界面聚集行为：分子动力学模拟研究

陈贻建 周洪涛 葛际江 徐桂英



Aggregation Behavior of Double-Chained Anionic Surfactant 1-C_m-C₉-SO₃Na at Air/Liquid Interface: Molecular Dynamics Simulation

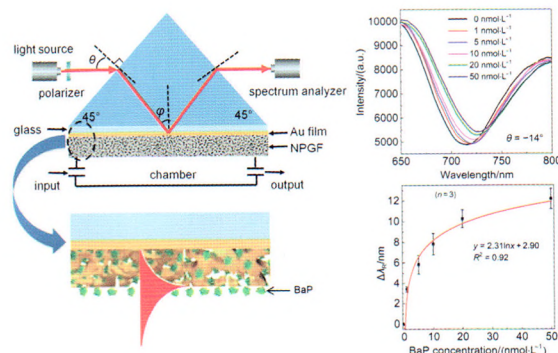
CHEN Yi-Jian ZHOU Hong-Tao
GE Ji-Jiang XU Gui-Ying

Acta Phys.-Chim. Sin. **2017**, *33* (6), 1214–1222

The m value of branched carbon chain greatly influences the properties of 1-C_m-C₉-SO₃Na. The performance of 1-C_m-C₉-SO₃Na first increases, and then decreases with the increase of m (0, 2, 4, 6, 8 and 9), the surfactant with $m = 4$ giving the best interfacial performance.

纳米多孔金膜表面等离子体共振效应的理论分析和传感应用

王丽 逯丹凤 高然 程进 张喆
祁志美



Theoretical Analyses and Chemical Sensing Application of Surface Plasmon Resonance Effect of Nanoporous Gold Films

WANG Li LU Dan-Feng
GAO Ran CHENG Jin
ZHANG Zhe QI Zhi-Mei

Acta Phys.-Chim. Sin. **2017**, *33* (6), 1223–1229

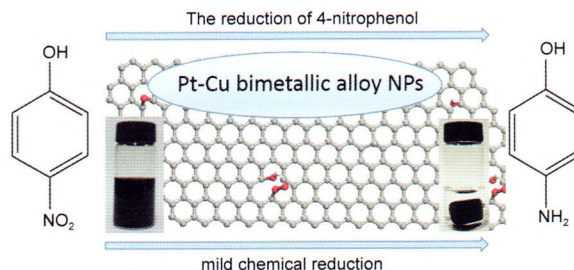
The surface plasmon resonance effect of nanoporous gold films was theoretically analyzed and used to detect small molecules, like bisphenol A and benzo[a]pyrene.

高活性、可循环的Pt-Cu@3D石墨烯复合催化剂的制备和催化性能

王美淞 邹培培 黄艳丽 王媛媛 戴立益

Three-Dimensional Graphene-Based Pt-Cu Nanoparticles-Containing Composite as Highly Active and Recyclable Catalyst

WANG Mei-Song ZOU Pei-Pei
HUANG Yan-Li WANG Yuan-Yuan
DAI Li-Yi



Acta Phys. -Chim. Sin. **2017**, 33 (6), 1230–1235

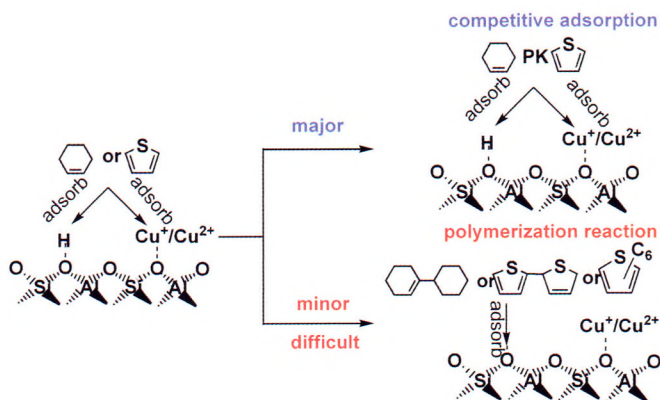
Pt-Cu@3DG composite hydrogel, prepared by mild chemical reduction, was used as an efficient, inexpensive, recyclable, and stable catalyst.

环己烯对噻吩在CuY分子筛上吸附的影响机制

莫周胜 秦玉才 张晓彤 段林海 宋丽娟

Influencing Mechanism of Cyclohexene on Thiophene Adsorption over CuY Zeolites

MO Zhou-Sheng QIN Yu-Cai
ZHANG Xiao-Tong DUAN Lin-Hai
SONG Li-Juan



Acta Phys. -Chim. Sin. **2017**, 33 (6), 1236–1241

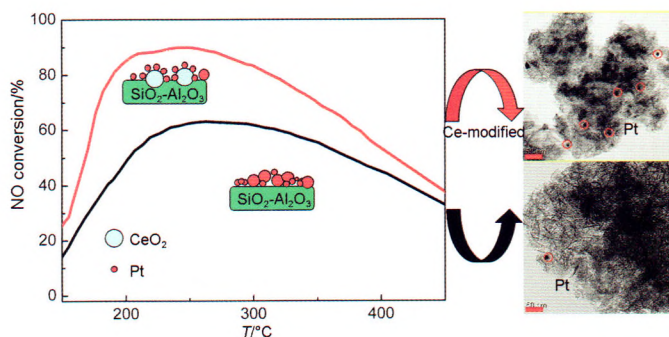
Cyclohexene affects thiophene adsorption over CuY zeolites via competitive adsorption rather than polymerization.

CeO₂的添加对柴油车氧化催化剂Pt/SiO₂-Al₂O₃的NO氧化性能提高的影响

黄子芬 张海龙 杨铮铮 赵明 黄木兰
梁艳丽 王健礼 陈耀强

Effects of CeO₂ Addition on Improved NO Oxidation Activities of Pt/SiO₂-Al₂O₃ Diesel Oxidation Catalysts

HUANG Yu-Fen ZHANG Hai-Long
YANG Zheng-Zheng ZHAO Ming
HUANG Mu-Lan LIANG Yan-Li
WANG Jian-Li CHEN Yao-Qiang



Acta Phys. -Chim. Sin. **2017**, 33 (6), 1242–1252

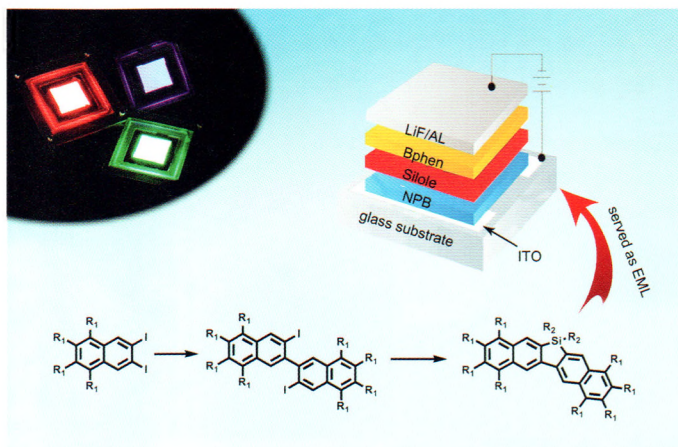
15% Ce-modified catalyst has better Pt dispersion, leading to improved reducibility and higher NO oxidation activity under diesel exhaust conditions.

二萘并噻咯的合成及性能

曲红梅 种泽鹏 陈旭 门奕灿 申海蛟

Synthesis and Properties of a Series of Dinaphthosiloles

QU Hong-Mei CHONG Ze-Peng
CHEN Xu MEN Yi-Can
SHEN Hai-Jiao



Acta Phys. -Chim. Sin. **2017**, 33 (6), 1253–1260

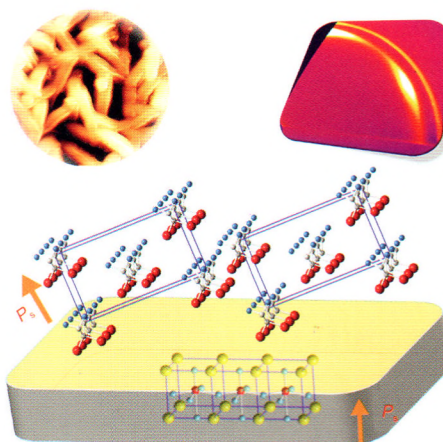
Synthesis of a series of dinaphthosiloles and investigation of their properties indicate that they can be used as light-emitting materials.

钙钛矿铁电纳米片诱导的P(VDF-TrFE)取向生长

刘金 麦江泉 李诗 任召辉 李铭
武梦娇 吴勇军 路新慧 李翔 田鹤
王宗荣 韩高荣

Perovskite Ferroelectric Nanoplates Induced a Highly Oriented Growth of P(VDF-TrFE) Films

LIU Jin MAI Jiang-Quan
LI Shi REN Zhao-Hui
LI Ming WU Meng-Jiao
WU Yong-Jun LU Xin-Hui
LI Xiang TIAN He
WANG Zong-Rong HAN Gao-Rong



Acta Phys. -Chim. Sin. **2017**, 33 (6), 1261–1266

PbTiO₃ were employed to effectively mediate the nucleation and growth of P(VDF-TrFE), resulting in an orientation and enhancement of property.

The journal has been indexed in SCIE, CA, SCOPUS, AJ, JICST, and CSTPCD. The average publication time is 66 days for the web version and 152 days for the printed version in 2016.

The journal accepts papers in English or Chinese.

物理化学学报

ACTA PHYSICO-CHIMICA SINICA



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