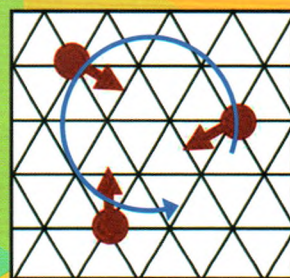
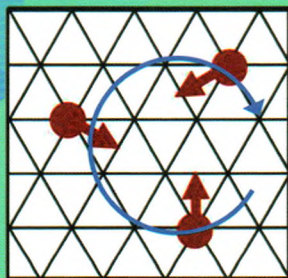
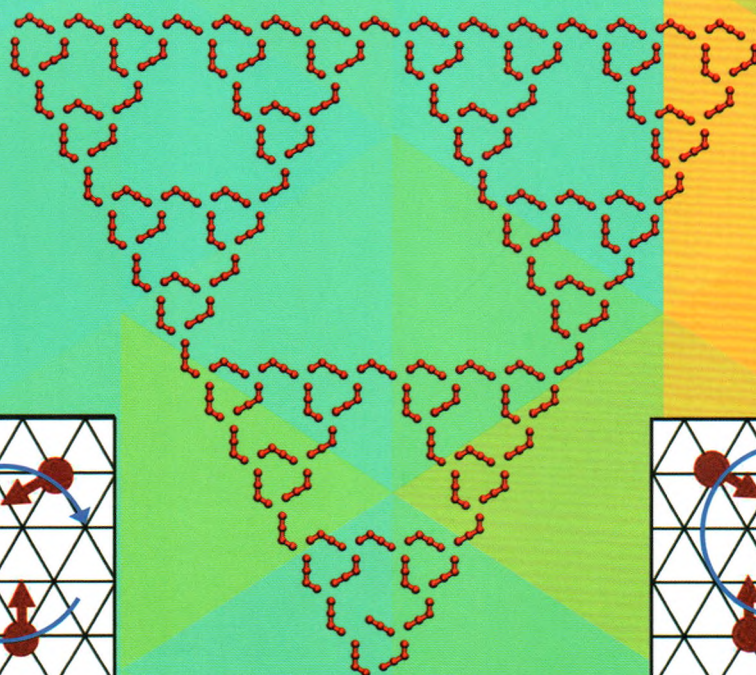
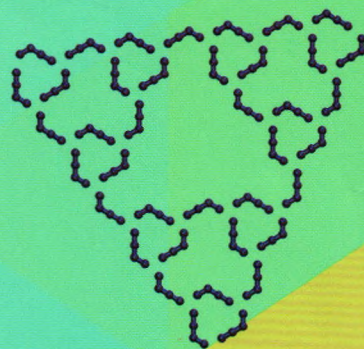


物理化学学报

ACTA PHYSICO-CHIMICA SINICA

第33卷 第3期 Vol.33 No.3 2017

Triangular
Halogen
Bond



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 the self-assembly of Sierpiński triangle fractals using Monte Carlo simulations. On page 539, ZHANG *et al.* demonstrate that the assembly pathway and outcome could be controlled by molecular design.

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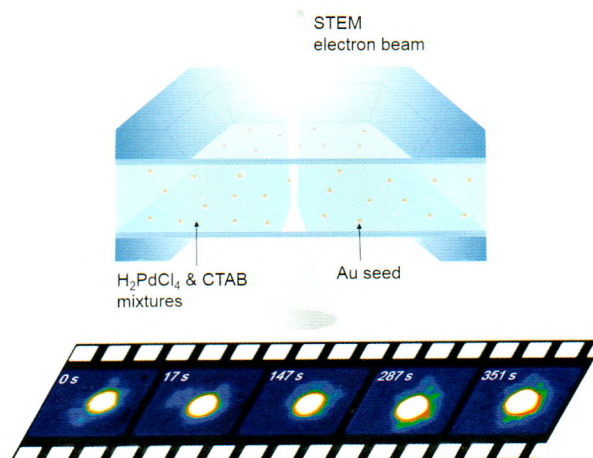
- 具有超高活性位密度的低温 fcc Ru 费托合成催化剂设计新策略(Strategy for the Design of Ru Catalyst with Ultra-High Density of Active Sites for Low Temperature FTS) 刘忠范(LIU Zhong-Fan)(441)
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- 引入液晶小分子实现高效厚膜三元有机太阳能电池(Realizing High-Performance Ternary Organic Solar Cell with Thick Active Layer by Incorporating a Liquid Crystalline Small Molecule Third Component) 李永舫(LI Yong-Fang)(447)
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- 原子尺度原位揭示纳米粒子相变微观机制(*In situ* Atomically Revealing the Microscopic Mechanism of Phase Transition in Single Nanoparticles) 赵进才(ZHAO Jin-Cai)(454)
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周晓琴 张 辉 张 泽 陈 新 金传洪

Characterization of Heterostructural Palladium Deposition on Spherical Gold Nanoparticles by *In situ* Liquid Cell Transmission Electron Microscopy

ZHOU Xiao-Qin ZHANG Hui
ZHANG Ze CHEN Xin
JIN Chuan-Hong



The formation mechanisms of gold/palladium heterogeneous nanostructures were investigated *in situ via* liquid cell transmission electron microscopy.

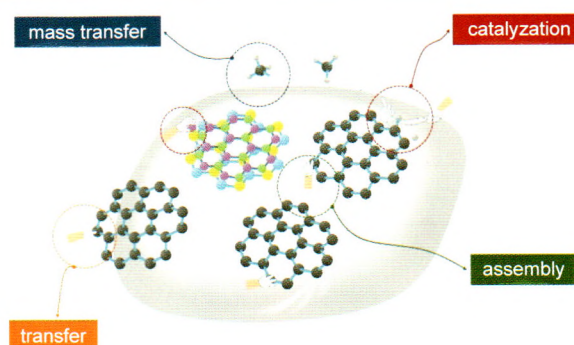
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液态金属催化剂：二维材料的点金石

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Liquid Metal Catalyst: Philosopher's Stone of Two-Dimensional Materials

ZENG Meng-Qi ZHANG Tao
TAN Li-Fang FU Lei



The unique growth, transfer, and assembly behaviors of 2D materials on liquid metal catalysts are demonstrated.

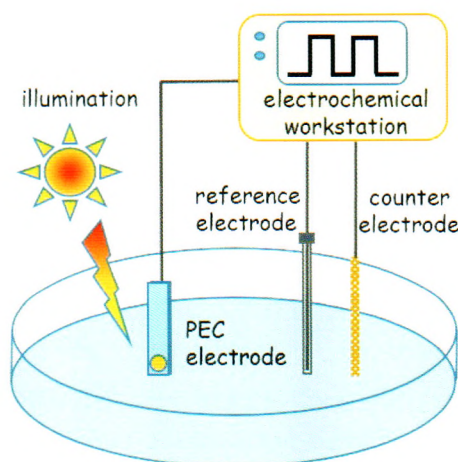
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光电化学生物分析研究进展

阮弋帆 张 楠 朱圆城 赵伟伟 徐静娟
陈洪渊

New Developments in Photoelectrochemical Bioanalysis

RUAN Yi-Fan ZHANG Nan
ZHU Yuan-Cheng ZHAO Wei-Wei
XU Jing-Juan CHEN Hong-Yuan



New developments in photoelectrochemical (PEC) bioanalysis are highlighted with recent illustrative examples in this review.

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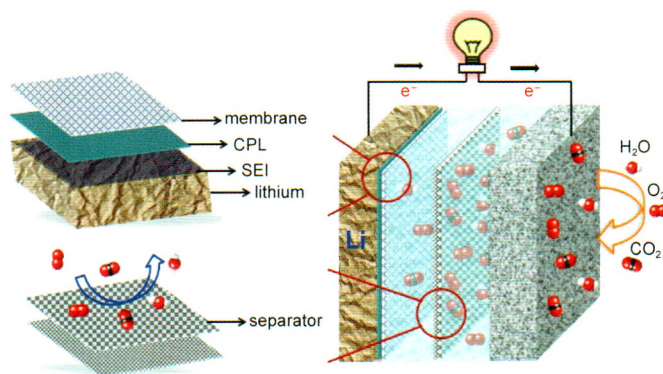
张彦涛 刘圳杰 王佳伟 王 亮 彭章泉

Recent Advances in Li Anode for Aprotic Li-O₂ Batteries

ZHANG Yan-Tao LIU Zhen-Jie

WANG Jia-Wei WANG Liang

PENG Zhang-Quan



Acta Phys. -Chim. Sin. **2017**, 33 (3), 486–499

Advanced strategies to protect lithium metal anode will unlock the full energy capability of Li-O₂ batteries.

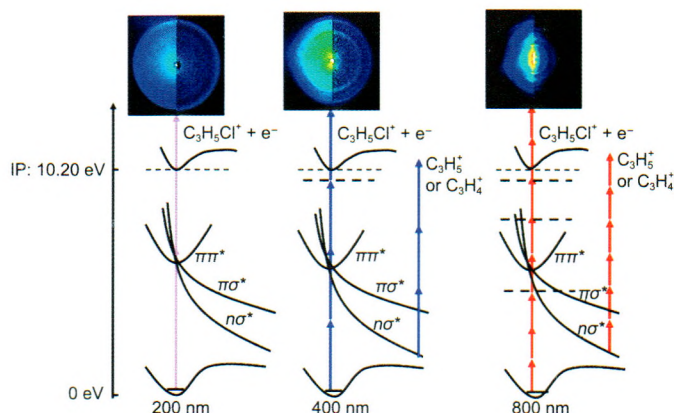
论文 ARTICLE

飞秒脉冲作用下氯丙烯的多光子解离和电离动力学

刘宁亮 沈 环

Multiphoton Dissociation and Ionization Dynamics of Allyl Chloride Using Femtosecond Laser Pulses

LIU Ning-Liang SHEN Huan



Acta Phys. -Chim. Sin. **2017**, 33 (3), 500–505

The dissociation/ionization dynamics of allyl chloride were studied by femtosecond laser pulses and wavelength-dependent behaviors were observed.

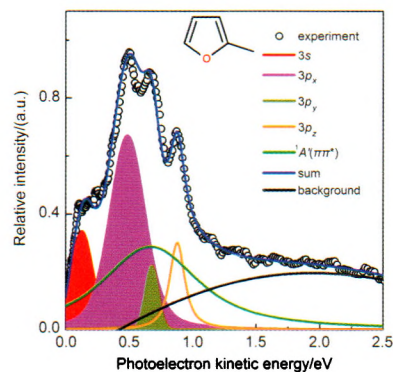
2-甲基呋喃分子激发态超快非绝热动力学

龙金友 刘志明 邱学军 张 冰

Ultrafast Nonadiabatic Dynamics of Electronically Excited 2-Methyl Furan

LONG Jin-You LIU Zhi-Ming

QIU Xue-Jun ZHANG Bing



Acta Phys. -Chim. Sin. **2017**, 33 (3), 506–512

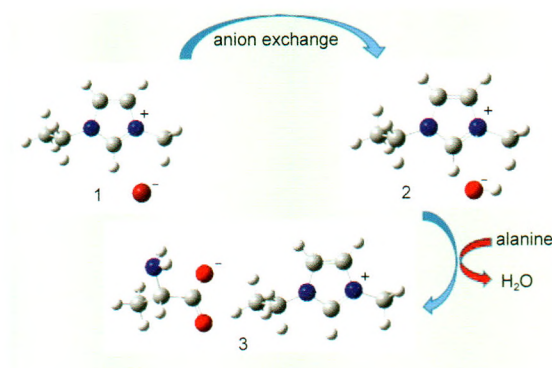
Excited-state dynamics of 2-methyl furan has been snapshotted by femtosecond time-resolved photoelectron imaging. This system represents an excellent prototype for identifying nonadiabatic interactions involving strong Rydberg-valence mixings.

[C₂mim][Ala]丙氨酸离子液体水溶液粘滞流动的活化参数

佟 静 刘 璐 张 朵 郑 煦 陈 霞
杨家振

Parameters of the Activation of Viscous Flow of Aqueous [C₂mim][Ala]

TONG Jing LIU Lu
ZHANG Duo ZHENG Xu
CHEN Xia YANG Jia-Zhen



A new semi-empirical method to estimate the viscosity of aqueous [C₂mim][Ala] was proposed that provided estimated values consistent with the corresponding experimental ones.

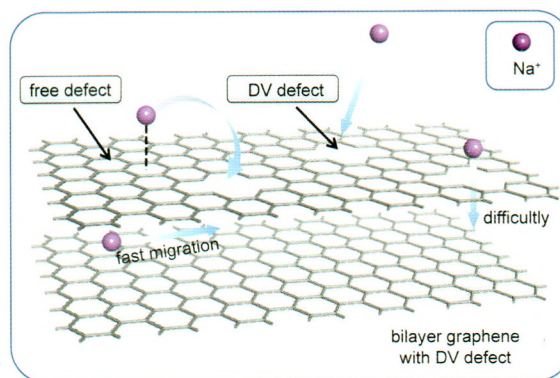
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杨绍斌 李思南 沈 丁 唐树伟 孙 闻
陈跃辉

First-Principles Study of Na Storage in Bilayer Graphene with Double Vacancy Defects

YANG Shao-Bin LI Si-Nan
SHEN Ding TANG Shu-Wei
SUN Wen CHEN Yue-Hui



Na-ion diffusion towards and storage around the double-vacancy defects of BLG are favorable. An increased defects concentration can enhance stable Na capacity.

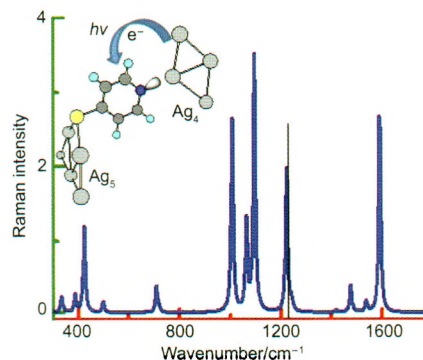
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Density Functional Theoretical Study on SERS Chemical Enhancement Mechanism of 4-Mercaptopyridine Adsorbed on Silver

WU Yuan-Fei LI Ming-Xue
ZHOU Jian-Zhang WU De-Yin
TIAN Zhong-Qun



A charge transfer mechanism contributes to the chemical enhancement of 4-mercaptopyridine on silver nanostructures in a two-end adsorption configuration.

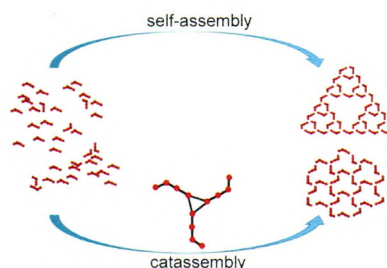
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基于卤键的谢尔宾斯基三角分形自组装的模拟研究

张 珍 谢文俊 杨 奕 孙 耿 高毅勤

Simulation Studies of the Self-Assembly of Halogen-Bonded Sierpiński Triangle Fractals

ZHANG Zhen XIE Wen-Jun
YANG Yi Isaac SUN Geng
GAO Yi-Qin



Acta Phys. -Chim. Sin. **2017**, 33 (3), 539–547

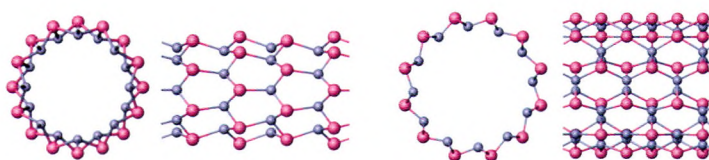
Unstable porous network was constructed through catassembly.

单壁 AlAs(111)纳米管结构和电子性质的密度泛函理论研究

王 玮 谭 凯

Structure and Electronic Properties of Single Walled Nanotubes from AlAs(111) Sheets: A DFT Study

WANG Wei TAN Kai



DFT investigations show that the strain energies (E_s) of armchair and zigzag AlAs nanotubes are negative and gradually decrease with increasing tube diameter, indicating that AlAs nanotubes might be formed by rolling up two dimensional periodic (111) single layer sheets.

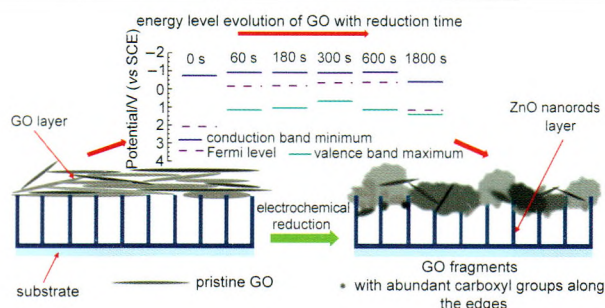
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氧化石墨烯在氧化锌衬底上的电化学还原及其光电性能

李一鸣 陈 肖 刘晓军 李文有 贺蕴秋

Electrochemical Reduction of Graphene Oxide on ZnO Substrate and Its Photoelectric Properties

LI Yi-Ming CHEN Xiao
LIU Xiao-Jun LI Wen-You
HE Yun-Qiu



After elimination of oxygen groups, the next stage in the electrochemical reduction of graphene oxide (GO) on ZnO leads to fragmentation of GO flakes, which increases the amount of carboxyl groups along the GO edges. The energy level structure of GO varies with reduction time and modulates the photoelectric behavior of the resulting composites.

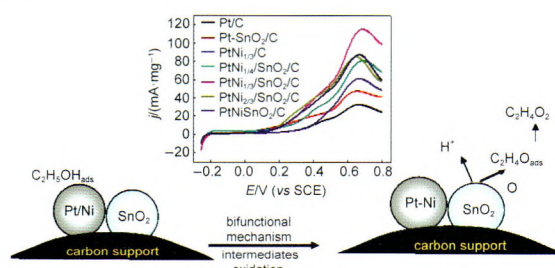
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PtNiSnO₂/C 的制备、表征及其电催化氧化乙醇活性

黄明辉 金碧瑶 赵莲花 孙世刚

Preparation and Characterization of Pt-Ni-SnO₂/C for Ethanol Oxidation Reaction

HUANG Ming-Hui JIN Bi-Yao
ZHAO Lian-Hua SUN Shi-Gang



Activity of Pt-Ni-SnO₂/C for EOR was found to be higher than that of Pt/C, Pt-Ni/C and Pt-SnO₂/C catalysts. Incorporation of Ni and SnO₂ improved the oxidation of acetaldehyde to generate the acetic acid at low potentials (0.1 V vs SCE).

Acta Phys. -Chim. Sin. **2017**, 33 (3), 563–572

氧化钯作为电位型传感器中敏感电极的工作机理

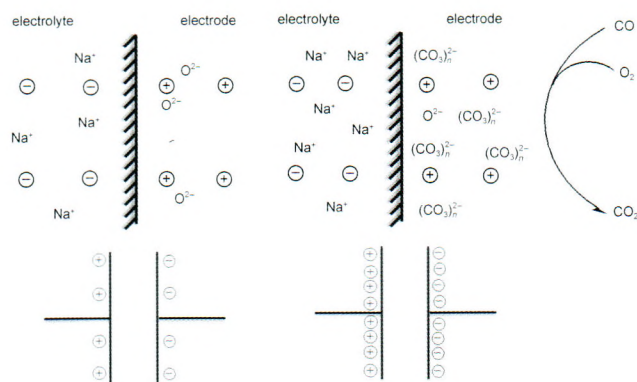
郑雁公 朱丽娜 李晗宇 简家文 杜海英

Operating Mechanism of Palladium Oxide as a Potentiometric Sensing Electrode

ZHENG Yan-Gong ZHU Li-Na

LI Han-Yu JIAN Jia-Wen

DU Hai-Ying



Alteration of an electrochemical double layer is attributed to the capacitance behavior of a potentiometric sensor with a PdO electrode.

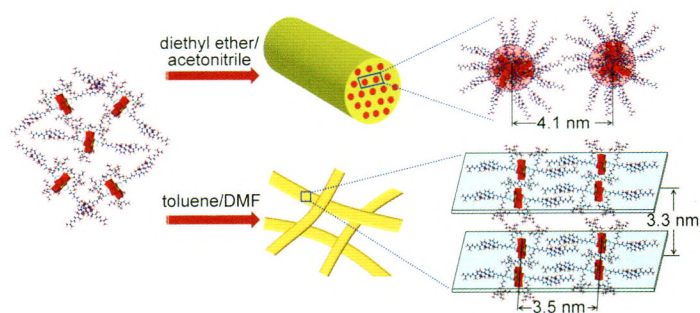
Acta Phys. -Chim. Sin. **2017**, 33 (3), 573–581

溶液自组装法构筑超分子杂化功能材料

杨海宽

A Solution-Based Self-Assembly Approach to Preparing Functional Supramolecular Hybrid Materials

YANG Hai-Kuan



A hybrid molecule can self-assemble into hexagonally packed cylinders in a bulk sample and long fibers in mixed DMF/toluene solvents.

Acta Phys. -Chim. Sin. **2017**, 33 (3), 582–589

水热法制备 $p\text{-CoFe}_2\text{O}_4/n\text{-CdS}$ 及其光催化制氢性能

胡海龙 王 晟 侯美顺 刘福生 王田珍

李天龙 董乾乾 张 鑫

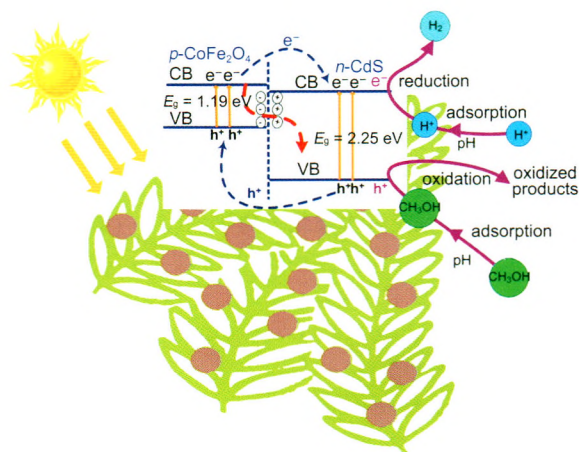
Preparation of $p\text{-CoFe}_2\text{O}_4/n\text{-CdS}$ by Hydrothermal Method and Its Photocatalytic Hydrogen Production Activity

HU Hai-Long WANG Sheng

HOU Mei-Shun LIU Fu-Sheng

WANG Tian-Zhen LI Tian-Long

DONG Qian-Qian ZHANG Xin



$p\text{-CoFe}_2\text{O}_4/n\text{-CdS}$ exhibits higher photocatalytic activity and resistance against cadmium leakage because of strong light absorption, formation of a “forest-like” CdS structure, and rapid electron transfer.

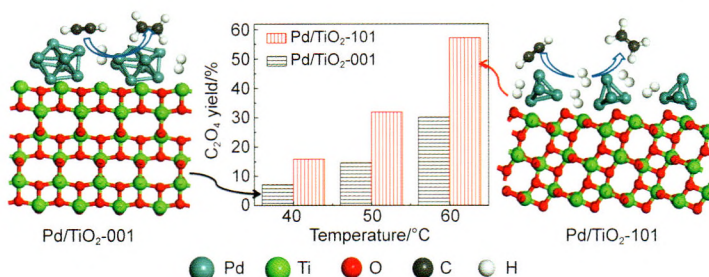
Acta Phys. -Chim. Sin. **2017**, 33 (3), 590–601

锐钛矿型 TiO₂ 负载的 Pd 催化剂用于乙炔选择加氢的催化性能及其表征

高晓平 郭章龙 周亚男 敬方梨 储 伟

Catalytic Performance and Characterization of Anatase TiO₂ Supported Pd Catalysts for the Selective Hydrogenation of Acetylene

GAO Xiao-Ping GUO Zhang-Long
ZHOU Ya-Nan JING Fang-Li
CHU Wei



Acta Phys. -Chim. Sin. **2017**, 33 (3), 602–610

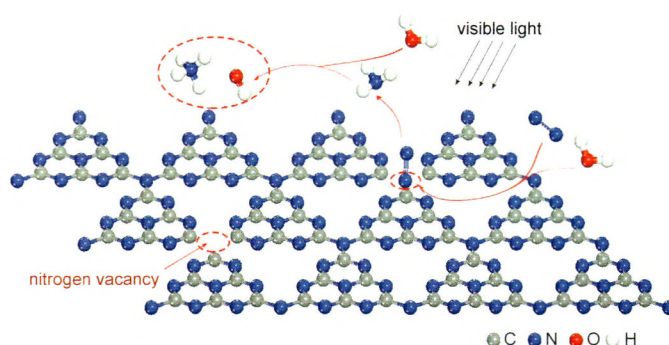
Smaller Pd particle size and better dispersion of Pd/TiO₂-101 catalyst provide more active sites to promote catalysis.

溶剂热后处理对石墨相氮化碳光化学固氮产氨性能的影响

白金 陈鑫 奚兆毅 王翔 李强
胡绍争

Influence of Solvothermal Post-Treatment on Photochemical Nitrogen Conversion to Ammonia with g-C₃N₄ Catalyst

BAI Jin CHEN Xin
XI Zhao-Yi WANG Xiang
LI Qiang HU Shao-Zheng



Acta Phys. -Chim. Sin. **2017**, 33 (3), 611–619

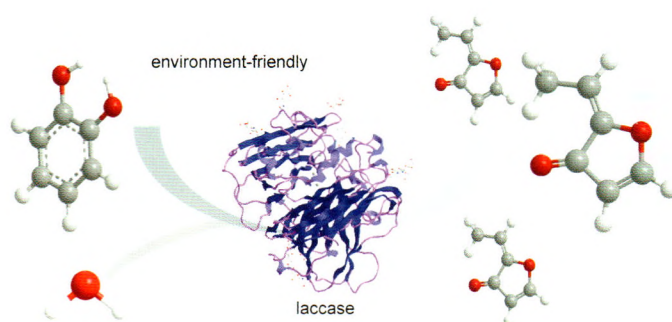
Nitrogen vacancy doped g-C₃N₄ with outstanding nitrogen photofixation ability under visible light is prepared by introducing ionic liquid [Bmim]Br solvent.

漆酶催化邻苯二酚开环的自由基反应机制

陈明 王林 谭天 罗学才 郑在
尹若春 苏吉虎 杜江峰

Radical Mechanism of Laccase-Catalyzed Catechol Ring-Opening

CHEN Ming WANG Lin
TAN Tian LUO Xue-Cai
ZHENG Zai YIN Ruo-Chun
SU Ji-Hu DU Jiang-Feng



Acta Phys. -Chim. Sin. **2017**, 33 (3), 620–626

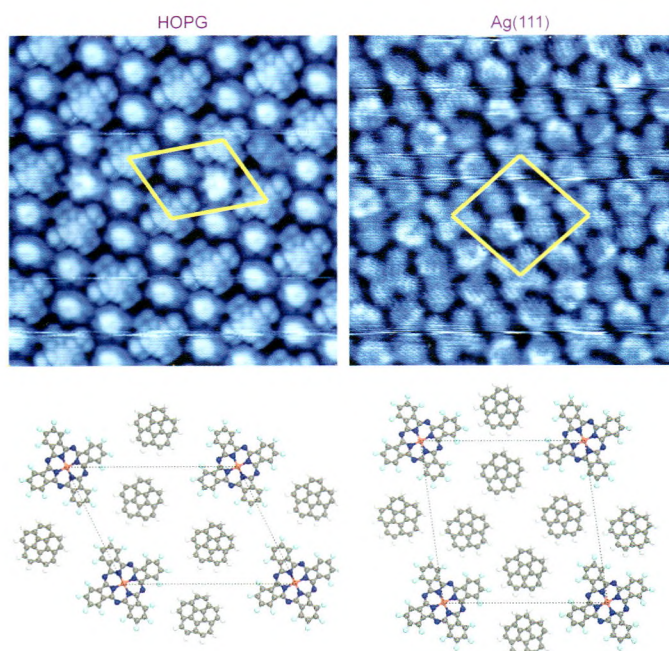
Laccase-catalyzed catechol oxidation features a ring-opening that involves radical kinetics.

基于全氟酞菁铜和碗烯双分子体系在银和石墨表面自组装行为的低温扫描隧道显微镜研究

郭 瑞 张嘉霖 赵宋焘 余小江 钟 舒
孙 硕 李震宇 陈 伟

LT-STM Investigation of the Self-Assembled $F_{16}CuPc$ -Corannulene Binary System on Ag(111) and Graphite Surfaces

GUO Rui ZHANG Jialin
ZHAO Songtao YU Xiaojiang
ZHONG Shu SUN Shuo
LI Zhenyu CHEN Wei



Binary supramolecular structures of $F_{16}CuPc$ -COR monolayer assembled on the highly oriented pyrolytic graphite (HOPG) and Ag(111) substrates were investigated via low-temperature scanning tunneling microscopy (LT-STM), with emphasis on the configuration of COR molecules.

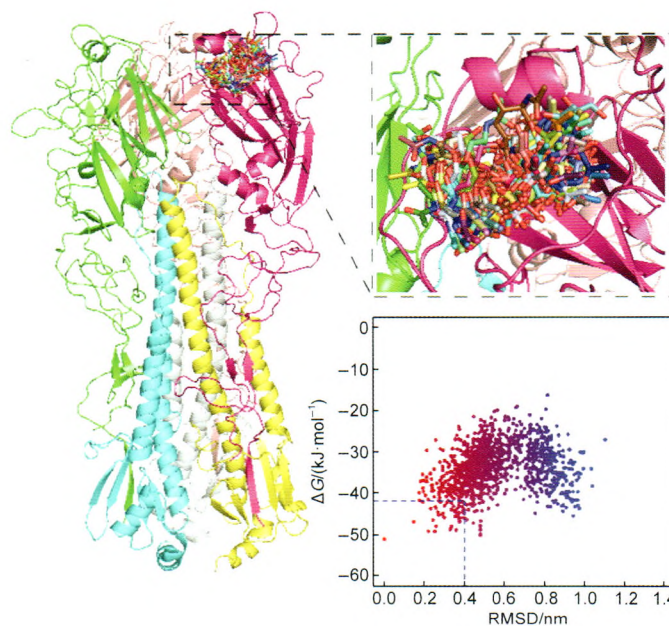
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禽流感病毒HA蛋白与人受体的分子对接

邓迎春 柳 青 黄 强

Molecular Docking of Human-Like Receptor to Hemagglutinins of Avian Influenza A Viruses

DENG Ying-Chun LIU Qing
HUANG Qiang



A high-throughput method was developed to predict the affinity of HA for human receptor rapidly.

Acta Phys. -Chim. Sin. **2017**, 33 (3), 633–641

韩德刚教授生平简介 (642)

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