物理化学学报(Wuli Huaxue Xuebao) 第 26 卷第 10 期(2010 年 10 月)

	目			次					
综述									
表面活性剂水溶液的电导	率研究方法和一些特	持征数据的	提取 …	••••••••••••••••••••••••••••••••••••••	••••••	• • • • • • •	••••	赵剑	曦(2589)
热力学、热化学和溶液(と学								
D-和 L-丙氨酸的低温磁相]变磁场变化下的		I流磁化 率	₫	·王文清	沈亲	f春	龚	䶮(2597)
抗抑郁化合物 SIPI5358 与			吐 塚	1 to	一儿口	公士	- علد	木油	# (0(04)
KDNBF 形貌控制及其对规			陈 珠	储艳秋	1 传光	翁き	。活	子廷	其(2604)
			张建国	张同来	李志敏	杨	利	王绍	宗(2613)
化学动力学和分子动态		55.00 庄光 5	.		10 /- +	312	-#¥	r*	12/0/10)
C₂(a³∏₂)自由基与若干不依	型和恢氢化合物及应用	的温度效应	<u>v</u>	•••••	胡仁志	烋	杆	陈	旸(2619)
电化学									
柠檬酸盐体系铜电沉积及									
1 A Bill of the A = 0 - 1 to 1 to 1 to 1									民(2625)
水合肼对锂离子正极材料									伟(2633)
再生水环境中304不锈钢 Schiff 碱基过渡金属镍络						学久	义	焦	迪(2638)
SCHIII 侧茎过便壶偶保增了						韩村	梅	干新	东(2647)
聚乙烯醇/聚乙烯吡咯烷酮			123	114.14.10	11- 1111 1/2	A 10.173	-1-7		A(2011)
			林 瑞	吕 洪	王晓蕾	马建	新	乔锦	丽(2653)
外电场作用下水化聚全氟									
	••••••		朱素华	严六明	纪晓波	邵士	乐	陆文	聪(2659)
胶体及界面化学									
催化剂对乳液模板法制备	碳材料形貌的影响。		甘礼华	刘明贤	陈龙武	胡	军	刘洪	来(2666)
催化和表面结构	ᅏᄼᇎᇎ	• - + 	n####################################			-117	-11	}# L	¥ (2.552)
基于光波导分光光谱技术									
NO _x 分子在[Ag]-MAPO-5 隧道结电场辅助下叔丁胺			• • • • • • • • • •	刈冶柳	依皖尤	换竹	乐	刈吮	莉(2679)
<u>定进习它勿而以了从</u>			仇 君	袁秉凯	邓珂	杨	蓉	裘晓	辉(2686)
萘在贵金属 Pd、Pt 及 Pd-P				• • •				•	
	•••••	·张小菲	邵正锋	毛国强	何德民	张利	民	梁长	海(2691)
酯加氢反应中影响羧基活		and the second second	周娅芬	付海燕	陈华	李贤	内均	李瑞	祥(2699)
5,7-二溴-8 羟基喹啉锰配合			3.1 or 1.6	11 F7 12	士人从	L 1		-2 //	11 (0505)
毛州贮极始的郑其游龙万					秦金纬	何多	恢	尹马	林(2705)
手性胺修饰的羟基磷灰石					李瑞祥	陈	华	李紧	均(2711)
负载型非晶态 Co-B 催化剂									
					-	•			下转封三)
								`	,

复合半导体光催化剂 p-CoO/n-CdS 的制备、表征及光催化性能	(上接封二)		
N 掺杂 TiO, 纳米粒子表面光生电荷特性与光催化活性	复合半导体光催化剂 p-CoO/n-CdS 的制备、表征及光催化性能		
		卢南	刘福生(2726)
ACo ₂ O ₂ /HZSM-5 催化剂上 N ₂ O 的直接分解			
		,何冬青	王徳军(2733)
一氧化量外来晶溶胶内渗透电极对染料酸化太阳能电池的光伏性能的提高 基于蓝黄磷光二元互补色的高效聚合物白光器件			
二氧化钛纳米晶溶胶内渗透电极对染料敏化太阳能电池的光伏性能的提高	王 虹 王军利 李翠清 宋永吉	迟姚玲	王 焘(2739)
二氧化钛纳米晶溶胶内渗透电极对染料敏化太阳能电池的光伏性能的提高	ルルト データン薬		
基于蓝黄磷光二元互补色的高效聚合物白光器件 —— 李艳虎 方 図 邹建华 王 彪 吴宏滨 彭俊彪(2752) NaCl 对琼脂糖凝胶电泳法分离单壁碳纳米管的影响 —— 温晓南 张 静 顾文秀 金赫华 李红波 李清文(2757) 量子化学及计算化学 双螺旋金属(II)卟啉的结构、电子光谱及其反应活性 —— "			
基于蓝黄磷光二元互补色的高效聚合物白光器件 李艳虎 方 因 邹建华 王 彪 吴宏滨 彭俊彪(2752) NaCl 对琼脂糖凝胶电泳法分离单壁碳纳米管的影响		本經剛	エ安士(9745)
□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□	· · · · · · · · · · · · · · · · · · ·	于难则	工本心(2143)
NaCl 对琼脂糖凝胶电泳法分离单壁碳纳米管的影响 温晓南 张 静 顾文秀 金赫华 李红波 李清文(2757) 量子化学及计算化学 双螺旋金属(II)卟啉的结构、电子光谱及其反应活性		呈安治	彭伦敏(9759)
■子化学及计算化学 双螺旋金属(II)卟啉的结构、电子光谱及其反应活性		,入丛庆	2) 13C112(2132)
量子化学及计算化学 双螺旋金属(II)卟啉的结构、电子光谱及其反应活性		奏红油	泰涛文(9757)
双螺旋金属(II)卟啉的结构、电子光谱及其反应活性	·····································	于红夜	子用又(2131)
双螺旋金属(II)卟啉的结构、电子光谱及其反应活性	量子化学及计算化学		
一 一 一 一 一 一 一 一 一 一 一 一 一 一 一 一 一 一 一			
气相中疏水氨基酸的单电子氧化还原性质 李伟伟 侯若冰 孙彦丽(2772) 海萤荧光素衍生物发光反应关键步骤的理论研究 孙 颖 任爱民 闰春刚 邹陆一 任雪峰(2779) 叠氮化氰的光解离机理		. 蒋华江	刘述斌(2763)
海萤荧光素衍生物发光反应关键步骤的理论研究	•		
型额化氰的光解离机理	•		,
叠氮化氰的光解离机理		邹陆一	任雪峰(2779)
用第一性原理方法获取周期体系中原子的部分电荷 —— 李亚娜 吕 洋 周立川 陈 理 李慎敏(2793)基于第一性原理的 Mn-AlN 和 Cr-AlN 的半金属性质 —— 樊玉勤 何阿玲(2801)流体力学半径对估算胶体微球聚集速率常数的影响 —— 杜 媛 徐升华 孙祉伟 阿 燕(2807)生物物理化学 渗透剂的分子体积和极性表面积分率对胰凝乳蛋白酶抑制剂 2 热稳定性的影响 —— 刘夫锋 纪 绛 董晓燕(2813)硅基芯片表面化学性质对蛋白质固定化的影响 —— 周稳稳 廉 洁 胡科家 高云华 徐 百(2821)典型蛋白质折叠中阳离子— 和互作用的特异性 —— 乔 辉 李晓琴 徐海松 孔令强 彭 宇(2828) A,腺苷受体的同源模建及其结构验证 —— 柯艳蓉 金宏威 刘振明 张亮仁(2833)材料物理化学 Sn 掺杂 ZnO 纳米针的结构及其生长机制 —— 王 杰 庄惠照 薛成山 李俊林 徐 鹛(2840)双亲性光敏感遥爪聚合物 C-PNIPAAm 的合成与性能 —— 舒巧珍 陈 欣 陈开花 江金强 倪忠斌 张红武 刘晓亚 陈明清(2845)	•••		
基于第一性原理的 Mn-AlN 和 Cr-AlN 的半金属性质 类玉勤 何阿玲(2801)流体力学半径对估算胶体微球聚集速率常数的影响 杜 埭 徐升华 孙祉伟 阿 燕(2807)生物物理化学 渗透剂的分子体积和极性表面积分率对胰凝乳蛋白酶抑制剂 2 热稳定性的影响 刘夫锋 纪 终 董晓燕(2813)硅基芯片表面化学性质对蛋白质固定化的影响 周稳稳 廉 洁 胡科家 高云华 徐 百(2821)典型蛋白质折叠中阳离子—π相互作用的特异性 乔 辉 李晓琴 徐海松 孔令强 彭 宇(2828)A,腺苷受体的同源模建及其结构验证 柯艳蓉 金宏威 刘振明 张亮仁(2833)材料物理化学 Sn 掺杂 ZnO 纳米针的结构及其生长机制	· · · · · · · · · · · · · · · · · ·		,
流体力学半径对估算胶体微球聚集速率常数的影响		陈理	李慎敏(2793)
生物物理化学 渗透剂的分子体积和极性表面积分率对胰凝乳蛋白酶抑制剂 2 热稳定性的影响	基于第一性原理的 Mn-AlN 和 Cr-AlN 的半金属性质	·· 樊玉勤	何阿玲(2801)
渗透剂的分子体积和极性表面积分率对胰凝乳蛋白酶抑制剂 2 热稳定性的影响			阿 燕(2807)
渗透剂的分子体积和极性表面积分率对胰凝乳蛋白酶抑制剂 2 热稳定性的影响			
建基芯片表面化学性质对蛋白质固定化的影响 ······· 周稳稳 廉 洁 胡科家 高云华 徐 百(2821) 典型蛋白质折叠中阳离子-π相互作用的特异性 ····· 乔 辉 李晓琴 徐海松 孔令强 彭 宇(2828) A ₁ 腺苷受体的同源模建及其结构验证 ······ 柯艳蓉 金宏威 刘振明 张亮仁(2833) 材料物理化学 Sn 掺杂 ZnO 纳米针的结构及其生长机制 ···· 王 杰 庄惠照 薛成山 李俊林 徐 鹏(2840) 双亲性光敏感遥爪聚合物 C-PNIPAAm 的合成与性能 ······ 舒巧珍 陈 欣 陈开花 江金强 倪忠斌 张红武 刘晓亚 陈明清(2845)	生物物理化学		
硅基芯片表面化学性质对蛋白质固定化的影响 周稳稳 廉 洁 胡科家 高云华 徐 百(2821) 典型蛋白质折叠中阳离子—π相互作用的特异性 乔 辉 李晓琴 徐海松 孔令强 彭 字(2828) A,腺苷受体的同源模建及其结构验证 柯艳蓉 金宏威 刘振明 张亮仁(2833) 材料物理化学 Sn 掺杂 ZnO 纳米针的结构及其生长机制 王 杰 庄惠照 薛成山 李俊林 徐 鹏(2840) 双亲性光敏感遥爪聚合物 C-PNIPAAm 的合成与性能 舒巧珍 陈 欣 陈开花 江金强 倪忠斌 张红武 刘晓亚 陈明清(2845)			
典型蛋白质折叠中阳离子-π 相互作用的特异性 ······· 乔 辉 李晓琴 徐海松 孔令强 彭 宇(2828) A ₁ 腺苷受体的同源模建及其结构验证 ·········· 柯艳蓉 金宏威 刘振明 张亮仁(2833) 材料物理化学 Sn 掺杂 ZnO 纳米针的结构及其生长机制 ······ 王 杰 庄惠照 薛成山 李俊林 徐 鵬(2840) 双亲性光敏感遥爪聚合物 C-PNIPAAm 的合成与性能 ····································	- "		董晓燕(2813)
A ₁ 腺苷受体的同源模建及其结构验证 ····································	硅基芯片表面化学性质对蛋白质固定化的影响 周稳稳 廉 洁 胡科家	. 高云华	徐 百(2821)
材料物理化学 Sn 掺杂 ZnO 纳米针的结构及其生长机制 ··········· 王 杰 庄惠照 薛成山 李俊林 徐 鵬(2840) 双亲性光敏感遥爪聚合物 C-PNIPAAm 的合成与性能 ··························· 舒巧珍 陈 欣 陈开花 江金强 倪忠斌 张红武 刘晓亚 陈明清(2845)			
Sn 掺杂 ZnO 纳米针的结构及其生长机制 ··········· 王 杰 庄惠照 薛成山 李俊林 徐 鵬(2840) 双亲性光敏感遥爪聚合物 C-PNIPAAm 的合成与性能 ··············· 舒巧珍 陈 欣 陈开花 江金强 倪忠斌 张红武 刘晓亚 陈明清(2845)	A ₁ 腺苷受体的同源模建及其结构验证 柯艳蓉 金宏威	,刘振明	张亮仁(2833)
Sn 掺杂 ZnO 纳米针的结构及其生长机制 ··········· 王 杰 庄惠照 薛成山 李俊林 徐 鵬(2840) 双亲性光敏感遥爪聚合物 C-PNIPAAm 的合成与性能 ··············· 舒巧珍 陈 欣 陈开花 江金强 倪忠斌 张红武 刘晓亚 陈明清(2845)	I I shall de seem 21. M		
双亲性光敏感遥爪聚合物 C-PNIPAAm 的合成与性能 舒巧珍 陈 欣 陈开花 江金强 倪忠斌 张红武 刘晓亚 陈明清(2845)		* 14 11	/A mb (00.40)
舒巧珍 陈 欣 陈开花 江金强 倪忠斌 张红武 刘晓亚 陈明清(2845)		学俊林	徐 鹏(2840)
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大然宗贝对内特·// 电丁珀构和于守体性贝的影响 ··········· 陈 呼 陈是华 郑 近(2851)			
	人然宋贝刈内详》 电丁结构和于守护性贝的影响	· 陈廷平	和 近(2851)
《物理化学学报》征订启事 (2762)	《物理化学学报》征订启事	• • • • • • • • • • • • • • • • • • • •	(2762)

ACTA PHYSICO-CHIMICA SINICA

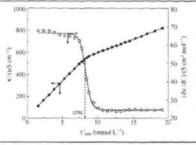
Vol. 26 No.10 (October, 2010)

CONTENTS

Review

Conductivity for the Investigation of Ionic Surfactants in an Aqueous Solution and Some Characteristic Parameters

ZHAO Jian-Xi



Conductivity is sensitive toward the behavior of ionic surfactants in aqueous solutions and it is important in the investigation of surfactant selfassembly.

Acta Phys. -Chim. Sin., 2010, 26(10): 2589-2596

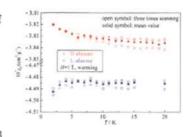
THERMODYNAMICS, THERMOCHEMISTRY AND SOLUTION CHEMISTRY

Cryogenic Magnetic Transition of D- and L-Alanine: Magnetic Field Dependence of Specific Heat and DC Magnetic Susceptibility

WANG Wen-Qing

SHEN Xin-Chun

GONG Yan



A difference in the nuclear spinelectron spin hyperfine interaction reveals the intrinsic asymmetries of D- and L-alanine crystals.

Acta Phys. -Chim. Sin., 2010, 26(10): 2597-2603

Non-Covalent Complexes of the Antidepressant Compound SIPI5358 with Cyclodextrins

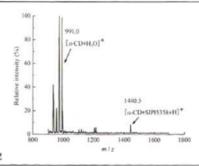
HE Xiao-Dan J CHEN Chen C

JIANG Dan CHU Yan-Qiu

DING Chuan-Fan

WENG Zhi-Jie

LI Jian-Qi



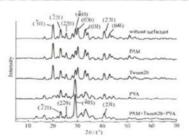
Non-covalent complexes of α -, β -, and γ -cyclodextrin with the antidepressant compound SIPI5358 were investigated by mass spectrometry, UV and fluorescence spectroscopies.

Acta Phys. -Chim. Sin., 2010, 26(10): 2604-2612

Morphology Control and Its Influence on the Decomposition Behavior and Sensitivity of KDNBF

FENG Jin-Ling ZHANG Jian-Guo ZHANG Tong-Lai LI Zhi-Min YANG Li WANG Shao-Zong

Acta Phys. -Chim. Sin., 2010, 26(10): 2613-2618



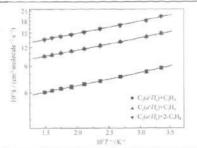
Samples of KDNBF with different morphologies were obtained by adding various surfactants in individual reaction. The decomposition behavior shows that the spherical sample has a lower decomposition temperature and higher reaction activation energy.

CHEMICAL KINETICS AND MOLECULE DYNAMICS

Temperature Dependence of Reactions of $C_2(a^3\Pi_u)$ Radical with Several Unsaturated Hydrocarbons

HU Ren-Zhi ZHANG Qun CHEN Yang

Acta Phys. -Chim. Sin., 2010, 26(10): 2619-2624



We studied a temperature dependence of the reactions of $C_2(a^3\Pi_u)$ with several unsaturated hydrocarbons (C_2H_4 , C_2H_2 , C_3H_6 , and $2-C_4H_8$).

ELECTROCHEMISTRY

Electrodeposition of Copper in a Citrate Bath and Its Application to a Micro-Electro-Mechanical System

WU Wei-Gang YANG Fang-Zu
LUO Ming-Hui TIAN Zhong-Qun

ZHOU Shao-Min

A copper coating was electrodeposited from a novel citrate bath and a planar inductor was successfully fabricated for MEMS in this bath.

Acta Phys. -Chim. Sin., 2010, 26(10): 2625–2632

Effect of Hydrazine on the Performance of LiNi_{0.5}Mn_{1.5}O₄ Cathode Materials

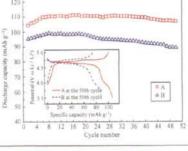
CHANG Zhao-Rong DAI Dong-Mei LI Bao TANG Hong-Wei

Acta Phys. -Chim. Sin., 2010, 26(10): 2633–2637

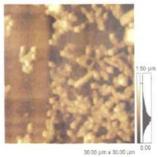
Characteristics of the Microbiologically Influenced Corrosion of 304 Stainless Steel in Reclaimed Water Environment

LI Jin XU Zhao-Yi LI Jiu-Yi JIAO Di

Acta Phys. -Chim. Sin., 2010, 26(10): 2638-2646



LiNi_{0.5}Mn_{1.5}O₄ was synthesized from a hydrazine pretreated precursor and it shows a much better electrochemical properties because of the formed pure spinel phase.



Because of the development of a biofilm on the surface of SS304, which resulted from the interactions between the SS304 surface and the biofilm, a corrosive pit appeared on the surface of SS304. This indicates that the SS304 surface suffered from microbiologically influenced corrosion.

Electropolymerization of Nickel Complexes with Schiff Bases: Effect of Sweep Rate on Anodic Polymerization

LI Jian-Ling GAO Fei
ZHANG Ya-Kun HE Li-Zhi
HAN Gui-Mei WANG Xin-Dong

nNi([I])salen $\frac{1}{2}nNi([II])$ salen $+ne^{-\frac{2}{2}}$, poly[Ni(salen)]

The active centers of poly[Ni(salen)] reach a maximum at a sweep rate of 20 mV \cdot s⁻¹ and it shows preferred diffusion kinetics.

Acta Phys. -Chim. Sin., 2010, 26(10): 2647-2652

Preparation and Properties of Poly(vinyl alcohol)/Poly(vinyl pyrrolidone) Composites for Solid Alkaline Electrolyte Membranes

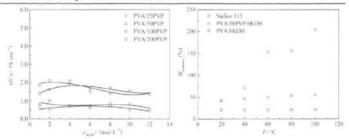
FU Jing LIN Rui LÜ Hong WANG Xiao-Lei MA Jian-Xin OIAO Jin-Li

Acta Phys. -Chim. Sin., 2010, 26(10): 2653–2658

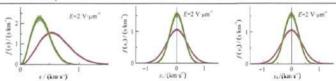
Electroosmotic Drag of Water in Hydrated Potassium Perfluorosulfonated Polymer Membrane in External Electric Fields

ZHU Su-Hua YAN Liu-Ming JI Xiao-Bo SHAO Chang-Le LU Wen-Cong

Acta Phys. -Chim. Sin., 2010, 26(10): 2659-2665



We obtained high ionic conductivity (2.01×10⁻³ S·cm⁻¹) for an alkaline PVA/ PVP membrane and it maintained good strength stability in a methanol solution at elevated temperatures.



The electroosmotic drag coefficient of water molecules in hydrated potassium perfluorosulfonate membrane is analyzed from different coordination shells of the cation and evaluated from the Maxwall velocity distribution function and molecular dynamics simulations with an external electric field applied.

COLLOID AND INTERFACE CHEMISTRY

Effect of Catalysts on the Morphologies of Carbon Materials Synthesized by an Emulsion Templating Method

GAN Li-Hua LIU Ming-Xian CHEN Long-Wu HU Jun LIU Hong-Lai Sacret from

| Confeet from | Internal index | Wormlike particles | Index | Internal Internal

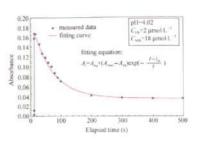
A phase inversion occurred in an O/W emulsion system and was caused by intermolecular H-bond interactions. Carbon foams and carbon materials consisting of fused microspheres or worm-like particles were prepared using NaOH and ammonia as catalysts, respectively.

Acta Phys. -Chim. Sin., 2010, 26(10): 2666-2671

CATALYSIS AND SURFACE STRUCTURE

Study of Competitive Adsorption Behavior of Protein and Methylene Blue by Optical Waveguide Spectroscopy

DENG Lin QI Zhi-Mei



The competitive coadsorption of methylene blue (MB) and protein on hydrophilic glass was monitored in situ by time-resolved optical waveguide spectroscopy and the best fit of the measured time course of absorbance with the theoretical kinetic equation reveals that the number of adsorbed MB molecules decreases exponentially with time after reaching a maximum.

Acta Phys. -Chim. Sin., 2010, 26(10): 2672-2678

NO. Molecule Adsorption in [Agl-MAP0-5 (M=Si, Ti) Molecular Sieves

LIU Jie-Xiang ZHANG Xiao-Guang DUAN Zhong-Yu LIU Xiao-Li

NO, SO2, H2O, and O2 adsorption in [Ag]-MAPO-5 (M=Si, Ti) were investigated using the density functional theory (DFT). The natural bond orbital (NBO) analysis was performed to investigate the interaction mechanism of NO, in the molecular sieves.

Acta Phys. -Chim. Sin., 2010, 26(10): 2679-2685

Electric Field Assisted Hopping of Tert-Butylamine on Cu(111) Surface

XU Yu-Qun ZHANG Jun YUAN Bing-Kai DENG Ke YANG Rong QIU Xiao-Hui

The hopping probabilities of tertbutylamine on Cu(111) surface present difference under the electric field of opposite polarity in an STM junction.

Acta Phys. -Chim. Sin., 2010, 26(10): 2686-2690

Naphthalene Hydrogenation Activity over Pd, Pt and Pd-Pt Catalysts and Their Sulfur Tolerance

ZHANG Xiao-Fei MAO Guo-Qiang ZHANG Qiu-Min

SHAO Zheng-Feng HE De-Min

LIANG Chang-Hai

without DBT naphthalene conversion decalin selectivity decalin selectivity trans-/cir-decalin ratio trans-/cis-decalin rati 80 60 Pd,Pt, Catalyst

The Pd4Pt1 catalyst has the highest naphthalene conversion and best selectivity toward decalin among the studied Pd and Pt monometallic catalysts as well as the bimetallic Pd-Pt catalysts with molar ratios of 4:1, 1: 1, and 1:4 in the presence and absence of dibenzothiophene (DBT).

Acta Phys. -Chim. Sin., 2010, 26(10): 2691-2698

Activation Factors for the Carboxyl Group in the Hydrogenation of Carboxylic Esters

ZHENG Xiao-Juan ZHOU Ya-Fen

FU Hai-Yan CHEN Hua LI Xian-Jun LI Rui-Xiang

Acta Phys. -Chim. Sin., 2010, 26(10): 2699-2704

Selective Oxidation of Ethylbenzene with Hydrogen Peroxide Catalyzed by 5,7-Dibromo-8-quinolinolato Manganese Complexes

LU Chun-Li FU Zai-Hui
LIU Ya-Chun LIU Feng-Lan
QIN Jin-Wei HE Xiang-Ling

YIN Du-Lin

Acta Phys. -Chim. Sin., 2010, 26(10): 2705-2710

Asymmetric Hydrogenation of Acetophenone Catalyzed by RuCl_z(TPP)₃ Supported on Hydroxyapatite Modified with Chiral Amine

ZHANG Ding-Lin YANG Chao-Fen

SUN Ya-Ping LI Rui-Xiang FU Hai-Yan CHEN Hua

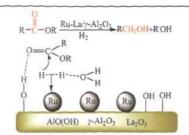
LI Xian-Jun

Acta Phys. -Chim. Sin., 2010, 26(10): 2711-2718

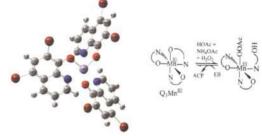
1-Octene Hydroformylation Using Supported Amorphous Co-B Catalysts

LONG Jun-Ying MA Lan HE De-Hua

Acta Phys. -Chim. Sin., 2010, 26(10): 2719-2725

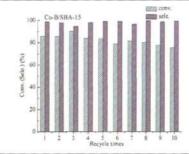


Water, Co(NO₃)₂, and an electronwithdrawing group all contributed to the activation of the carboxyl group in a carboxylic ester.



A 5,7-dibromo-8-quinolinolato manganese(III) complex (Q₃Mn^{III}) of changeable hexadentate mode, with the help of NH₄OAC and HOAc, was found to be an efficient catalyst for the selective oxidation of ethylbenzene (EB) to acetophenone (ACP) with aqueous hydrogen peroxide in environmentally benign acetone-water media.

RuCl₂(TPP)₃ supported on (1R,2R)-DPENDS modified HAP was prepared and used to catalyze the asymmetric hydrogenation of acetophenone with high activity and enantioselectivity.



Supported Co-B catalysts showed high initial activity and selectivity in 1-octene hydroformylation and Co-B/SBA-15 showed relatively high stability during catalyst recycling.

Preparation, Characterization and Photocatalytic Property of p-CoO/n-CdS Compound Semiconductor Photocatalyst

DU Huan WANG Sheng
LIU Lian-Lian LIU Zhong-Xiang
LI Zhen LU Nan
LIU Fu-Sheng

Acta Phys. -Chim. Sin., 2010, 26(10): 2726-2732

Photoinduced Charge Carrier Properties and Photocatalytic Activity of N-Doped TiO₂ Nanocatalysts

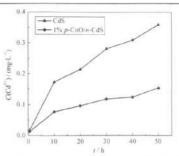
ZHANG Xiao-Ru LIN Yan-Hong ZHANG Jian-Fu HE Dong-Qing WANG De-Jun

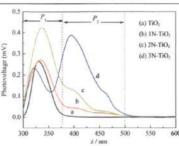
Acta Phys. -Chim. Sin., 2010, 26(10); 2733-2738

Decomposition of N₂O on ACo₂O₄/HZSM-5 Catalysts

WANG Hong
LI Cui-Qing
CHI Yao-Ling
WANG Jun-Li
SONG Yong-Ji
WANG Tao

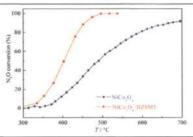
Acta Phys. -Chim. Sin., 2010, 26(10): 2739-2744





The photocatalyst CdS and CoO/CdS (p-CoO/n-CdS) compound semiconductor photocatalyst were prepared. The results of photocorrosion test showed that the photocorrosion rate of CdS was two or more times than that of p-CoO/n-CdS compound, which indicated that CoO coupled with CdS could effectively restrain the photocorrosion of CdS.

 $N\text{-}TiO_2$ photocatalysts with an appropriate amount of N doping showed a higher separation efficiency for photoinduced charge carriers than TiO_2 photocatalysts.



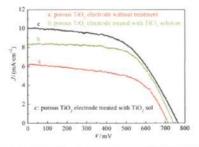
ACo₂O₄ (A=Mg, Ni, Zn) and ACo₂O₄/ HZSM-5(A=Mg, Fe, Ni, Cu, Zn, Zr, La) catalysts were synthesized and the performance of the catalysts was characterized. Compared with ACo₂O₄, the ACo₂O₄/HZSM-5 catalyst had better catalytic activity.

PHOTOCHEMISTRY AND SPECTROSCOPY

Enhancing the Photovoltaic Performance of Dye Sensitized Solar Cells with the TiO₂ Sol Infiltrated Nanocrystalline Electrode

QIAN Di-Feng ZHANG Qing-Hong WAN Jun LI Yao-Gang WANG Hong-Zhi

Acta Phys. -Chim. Sin., 2010, 26(10): 2745-2751



The overall energy conversion efficiency of the DSSCs was significantly enhanced by 64% after the low-concentration ${\rm TiO_2}$ sol infiltrated to the porous ${\rm TiO_2}$ photoanode.

Efficient Polymer White-Light-Emitting **Devices Based on Two Complementary Phosphorescent Colors**

LI Yan-Hu

FANG Yuan

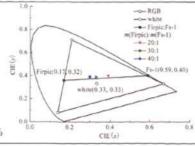
ZOU Jian-Hua

WANG Biao

WU Hong-Bin

PENG Jun-Biao

Acta Phys. -Chim. Sin., 2010, 26(10): 2752-2756



Efficient white polymer light-emitting diodes (WPLEDs) were fabricated by spin coating method using two complementary colors.

Effects of NaCl on the Separation of Single-Walled Carbon Nanotubes by Agarose Gel Electrophoresis

WEN Xiao-Nan

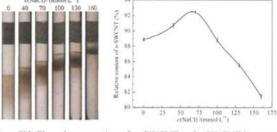
ZHANG Jing

GU Wen-Xiu

JIN He-Hua

LI Hong-Bo

LI Qing-Wen



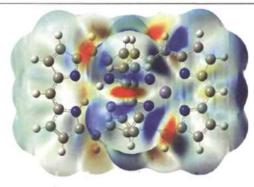
The effect of NaCl on the separation of m-SWCNT and s-SWCNT by agarose gel electrophoresis was investigated.

Acta Phys. -Chim. Sin., 2010, 26(10): 2757-2762

QUANTUM CHEMISTRY AND COMPUTATION CHEMISTRY

Structure, Spectroscopy and Reactivity Properties of Helically Chiral Metal(II)-**Bisdipyrrin Complexes**

ZHONG Ai-Guo **HUANG Ling** LI Bai-Lin JIANG Hua-Jiang LIU Shu-Bin



Knotted helical porphyrins metalated by a variety of divalent metal cations are investigated by conventional, time-dependent, and density functional theory approaches rendering a number of quantitative structure-reactivity linear relationships and other insights from structure and reactivity viewpoints.

Acta Phys. -Chim. Sin., 2010, 26(10): 2763-2771

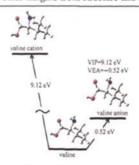
Characteristics of One Electron Redox Behavior of Hydrophobic Amino Acids in Gas Phase

LI Wei-Wei

HOU Ruo-Bing

SUN Yan-Li

Acta Phys. -Chim. Sin., 2010, 26(10): 2772-2778



The lower redox activities of hydrophobic amino acids in gas phase are attributable to their high ionization potentials and negative electron affinities.

Theoretical Investigation of the Key Reaction for the Chemiluminescence of Cypridina Luciferin Analogues

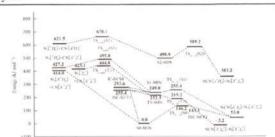
SUN Ying REN Ai-Min MIN Chun-Gang ZOU Lu-Yi REN Xue-Feng

We verify by theoretical calculations that MIPb (with 3-indolyl as the substituent) has a lower EEP and energy gap and a larger natural charge population change than other luciferin derivatives, and this is similar to cypridina luciferin in diglyme.

Acta Phys. -Chim. Sin., 2010, 26(10): 2779-2786

Photodissociation Mechanism of Cyanogen Azide

CI Cheng-Gang DUAN Xue-Mei LIU Jing-Yao SUN Chia-Chung



The photodissociation mechanism of N₃CN in the S0, T1, S1, and S2 states were investigated at the MRCI+Q//CAS(10, 9)/6-311+G(2df) level of theory.

Acta Phys. -Chim. Sin., 2010, 26(10): 2787-2792

Atomic Partial Charges for Periodic Systems from First-Principles Calculations

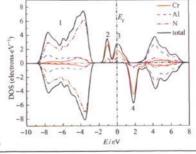
LI Ya-Na LÜ Yang ZHOU Li-Chuan CHEN Li LI Shen-Min

We proposed a method to obtain atomic partial charges rapidly for periodic systems and we carried out least squares fitting of the electrostatic potential (ESP) from first-principles calculations and used this in the Ewald summation.

Acta Phys. -Chim. Sin., 2010, 26(10): 2793-2800

Half-Metallic Properties of Mn-AlN and Cr-AlN Based on First-Principles

FAN Yu-Qin HE A-Ling



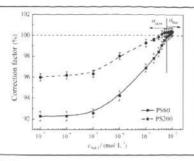
As the Mn/Cr doping concentration increases, the interaction between Mn and Mn or Cr and Cr atoms increases and the hybridization of the Mn/Cr 3d and N 2p states weakens, so the half-metallic gap is decreased.

Acta Phys. -Chim. Sin., 2010, 26(10): 2801-2806

Effect of the Hydrodynamic Radius of Colloid Microspheres on the Estimation of the Coagulation Rate Constant

DU Xuan XU Sheng-Hua SUN Zhi-Wei AA Yan

Acta Phys. -Chim. Sin., 2010, 26(10): 2807-2812



Coagulation rate constants calculated by using the hydrodynamic radius instead of the geometric radius can be lower than its theoretical value by up to 8% at low ionic strength and this difference decreases with the increase of ionic strength.

BIOPHYSICAL CHEMISTRY

Effects of Molecular Volume and Fractional Polar Surface Area of Osmolytes on the Thermal Stability of Chymotrypsin Inhibitor 2

LIU Fu-Feng JI Luo DONG Xiao-Yan 2.2 2.0 1.8 1.4 1.2 1.0 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 0.00 0.05 0.10 0.15 0.20 0.25

The molecular basis for the stabilizing effect of osmolytes was studied by molecular dynamics simulations. We found that the fractional polar surface area and the molecular volume determine their protective ability.

Acta Phys. -Chim. Sin., 2010, 26(10): 2813-2820

Effect of Surface Chemical Properties of a Silicon Chip on Antibody Immobilization

ZHOU Wen-Wen LIAN Jie HU Ke-Jia GAO Yun-Hua XU Bai

Acta Phys. -Chim. Sin., 2010, 26(10): 2821-2827

We found that the most efficient immobilization strategy was the use of glutaraldehyde as a coupling reagent to link a CEA antibody and an amino abundant surface that had been modified by a poly-L-lysine spacer-arm.

Specificity of Cation- π Interactions in Typical Protein Folds

QIAO Hui LI Xiao-Qin XU Hai-Song KONG Ling-Qiang PENG Yu

Fold type	$N_{\pi}(j)$	N(j)	$N_{\pi}(j) / N(j)$	0.68 0.05	
singly wound	4.91	326.03	1.51%		
doubly wound	1.19	206.76	0.58%		

In proteins, cation $-\pi$ interactions are formed between positively charged amino acids (Lys, Arg) and aromatic amino acids (Phe, Tyr, Trp). Cation- π interactions have existential specificity in typical protein folds.

Acta Phys. -Chim. Sin., 2010, 26(10): 2828-2832

Homology Modeling and Structure Validation of the Adenosine A₁ Receptor

KE Yan-Rong JIN Hong-Wei
LIU Zhen-Ming ZHANG Liang-Ren

Acta Phys. -Chim. Sin., 2010, 26(10): 2833-2839

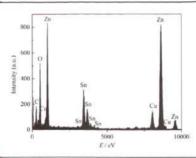


We established the adenosine A₁ receptor model based on the adenosine A_{2A} receptor crystal structure and validated the models using DOCK, VINA, and GOLD softwares for virtual screening.

PHYSICAL CHEMISTRY OF MATERIALS

Structure and Formation Mechanism of Sn-Doped ZnO Nanoneedles

WANG Jie ZHUANG Hui-Zhao XUE Cheng-Shan LI Jun-Lin XU Peng

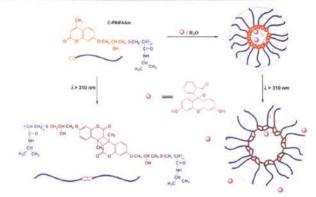


Sn-doped ZnO nanoneedles were synthesized in two steps: sputtering and thermal oxidation. These nanoneedles showed good luminescence characteristics.

Acta Phys. -Chim. Sin., 2010, 26(10): 2840-2844

Synthesis and Properties of Amphiphilic Photosensitive Telechelic Polymer C-PNIPAAm

SHU Qiao-Zhen
CHEN Kai-Hua
NI Zhong-Bin
LIU Xiao-Ya
CHEN Xin
JIANG Jin-Qiang
ZHANG Hong-Wu
CHEN Ming-Qing



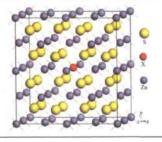
A coumarin-containing telechelic C-PNIPAAm polymer was used to form micelles in water with fluorescein as a hydrophobic agent. When irradiated by UV light (λ >310 nm), the hydrophobic coumarin unit at the end of the polymer chain was photodimerized, which resulted in a change in the micelle structure and the effective release of hydrophobic fluorescein into water.

Acta Phys. -Chim. Sin., 2010, 26(10): 2845-2850

Effect of Natural Impurities on the Electronic Structures and Semiconducting Properties of Sphalerite

CHEN Ye CHEN Jian-Hua GUO Jin

Acta Phys. -Chim. Sin., 2010, 26(10): 2851-2856



A systematic study of the electronic structures and semiconducting properties of sphalerite containing fourteen kinds of natural impurities was performed.