

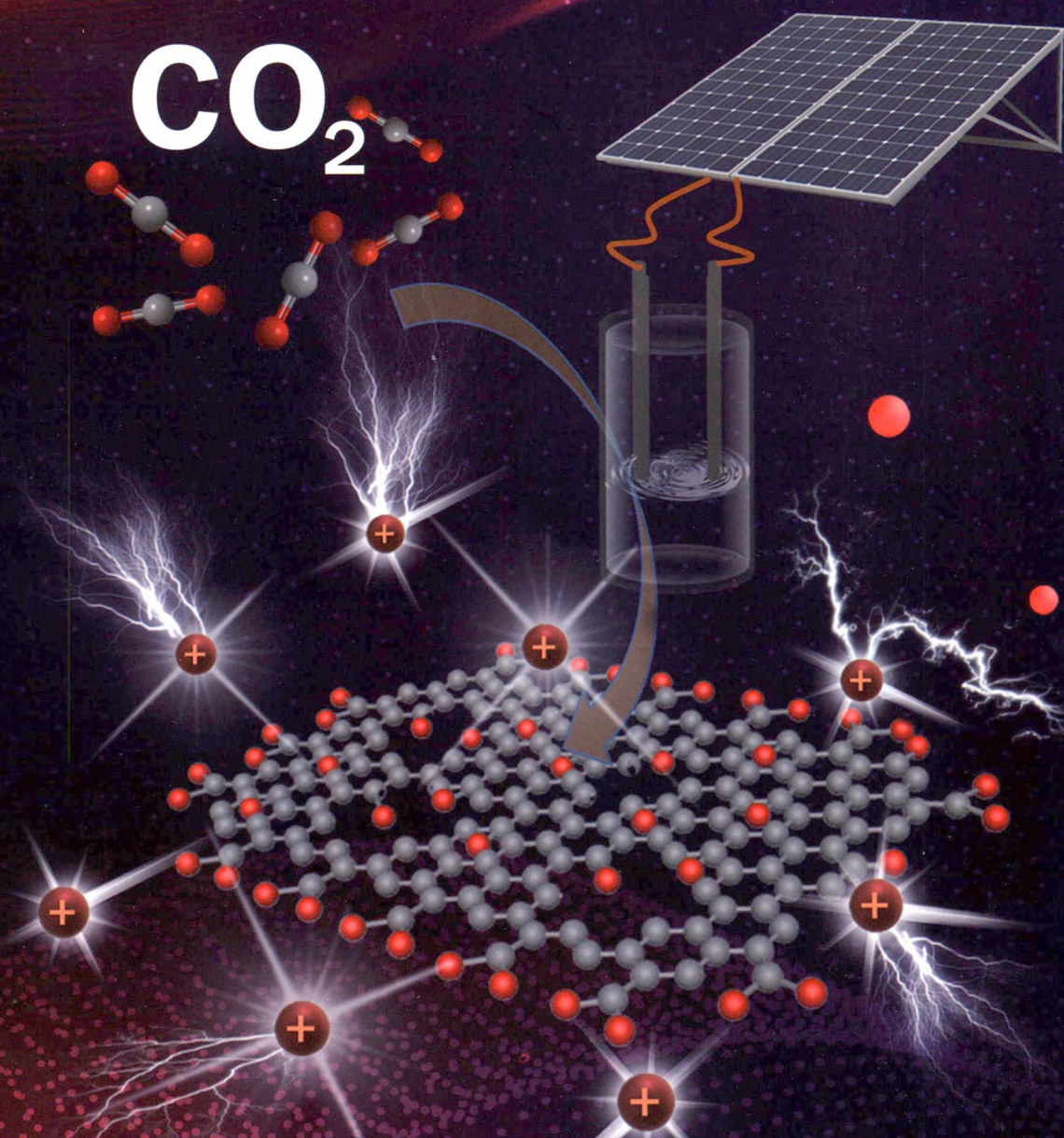


物理化学学报

ACTA PHYSICO-CHIMICA SINICA

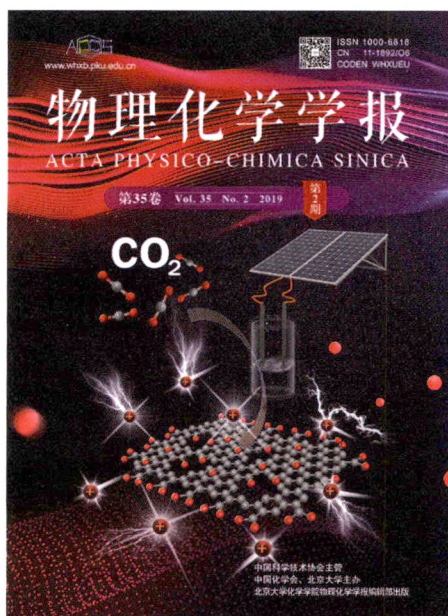
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中国化学会、北京大学主办
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COVER



The cover image presents the electrolytic-carbon (EC) prepared by molten salt electro-reduction of CO₂ and its specific cations adsorption features. On page 208, GU *et al.* demonstrate that EC behaves an unusual hysteresis of the charge/discharge current response in the negative potential region which is related to the specific adsorption of cations.

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- 过渡金属与主族重元素多重键: Fe≡A三重键(A = As, Sb, Bi) (Multiple Bonding between Transition Metal and Heavier Main-Group Elements: The Fe≡A Triple Bonds (A = As, Sb, Bi)) 方维海(FANG Weihai) (131)
- 基于有机半导体TIPS-Pentacene晶态薄膜的超灵敏NO₂气体传感器(An Ultra-Sensitive NO₂ Sensor Based on Organic Semiconductor Crystalline Films) 刘忠范(LIU Zhongfan) (133)

当期推荐 RECOMMENDATION

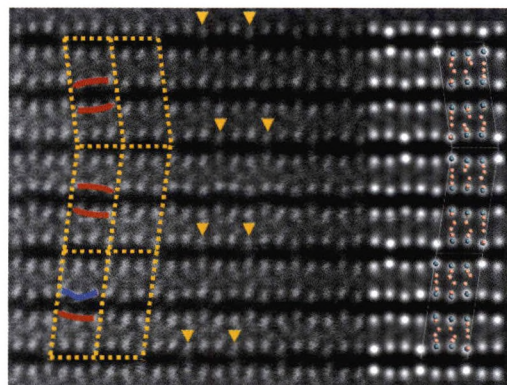
- 硫化镉纳米晶的表面缺陷及钯修饰对光催化制氢性能的影响(Influence of Surface Defects and Pd Modification on the Activity of CdS Nanocrystals for Photocatalytic Hydrogen Production) 吴凯(WU Kai) (135)
- α-Cu₂Se 有序起伏结构的原子级分辨率表征(Atomic Resolution Characterization of Ordered Fluctuation Structure in α-Cu₂Se) 彭海琳(PENG Hailin) (137)

α -Cu₂Se 精细结构的球差校正扫描透射电镜表征

陈陆, 刘军, 王勇, 张泽

Characterization of α -Cu₂Se Fine Structure by Spherical-Aberration-Corrected Scanning Transmission Electron Microscope

CHEN Lu, LIU Jun, WANG Yong, ZHANG Ze



Direct atomic-resolution observation using spherical-aberration (C_s)-corrected scanning transmission electron microscopy (STEM) reveals structural details of α -Cu₂Se.

Acta Phys. -Chim. Sin. **2019**, 35 (2), 139–144

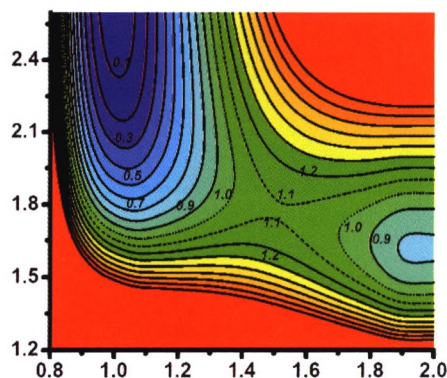
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多原子反应体系的高精度拟合势能面

傅碧娜, 陈俊, 刘天辉, 邵科杰, 张东辉

Highly Accurately Fitted Potential Energy Surfaces for Polyatomic Reactive Systems

FU Bina, CHEN Jun, LIU Tianhui, SHAO Kejie, ZHANG Dong H.



Using a neural-network approach, the potential energy surfaces for selected polyatomic reactions in the gas phase and the dissociation of gas-phase molecules on metal surfaces are fitted to unprecedented levels of accuracy; the potential energy surfaces were rigorously tested using quantum dynamics calculations.

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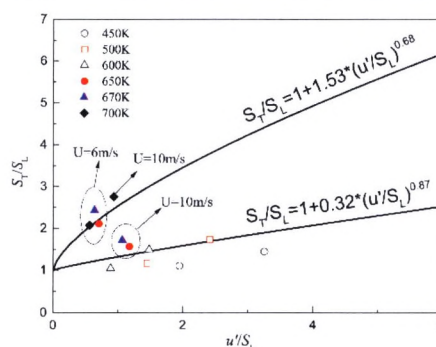
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低温燃料化学特性对湍流预混火焰传播的影响

张帆, 任哲, 钟生辉, 尧命发, 彭志军

Role of Low-Temperature Fuel Chemistry on Turbulent Flame Propagation

ZHANG Fan, REN Zhe, ZHONG Shenghui, YAO Mingfa, PENG Zhijun



Two branches of turbulent burning velocity show the upper and lower limits indicating the flame is in low-temperature ignition regime and chemically-frozen-flow regime, respectively.

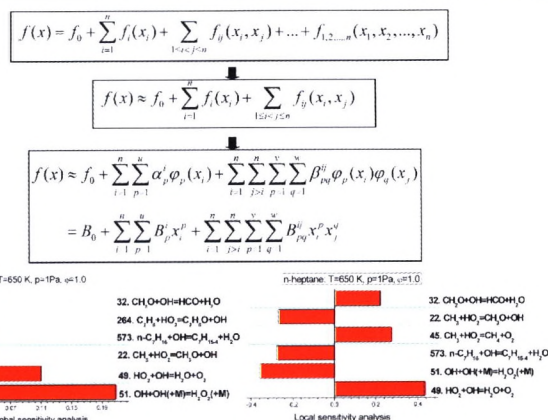
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典型燃料点火延迟时间的一阶和二阶局部和全局敏感度分析

席双惠, 王繁, 李象远

First- and Second-Order Local and Global Sensitivity Analyses on Ignition Delay Times of Four Typical Fuels

XI Shuanghui, WANG Fan, LI Xiangyuan



Two branches of turbulent burning velocity show the upper and lower limits indicating the flame is in low-temperature ignition regime and chemically-frozen-flow regime, respectively.

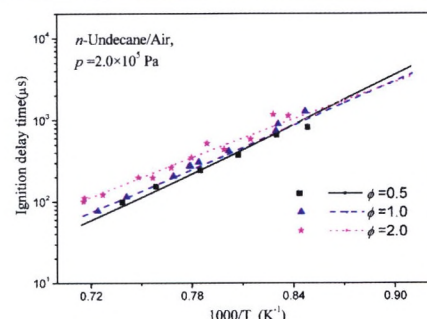
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高碳烃宽温度范围燃烧机理构建及动力学模拟

郭俊江, 唐石云, 李瑞, 谈宁馨

Mechanism Construction and Simulation for Combustion of Large Hydrocarbon Fuels Applied in Wide Temperature Range

GUO Junjiang, TANG Shiyun, LI Rui, TAN Ningxin



Comparison between simulated results of the ignition delay time for high-temperature combustion of *n*-undecane using our *n*-undecane mechanism and experimental data for different equivalence ratios.

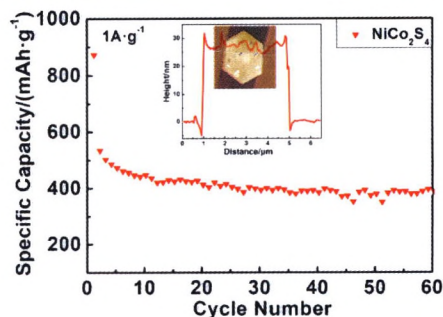
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NiCo₂S₄六角片作为钠离子电池负极材料的电化学性能及储钠动力学

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Sodium Ion Storage Performance of NiCo₂S₄ Hexagonal Nanosheets

ZHAO Mingyu, ZHU Lin, FU Bowen, JIANG Suhua, ZHOU Yongning, SONG Yun



The morphology and electrochemical performance of NiCo₂S₄ nanosheets were studied.

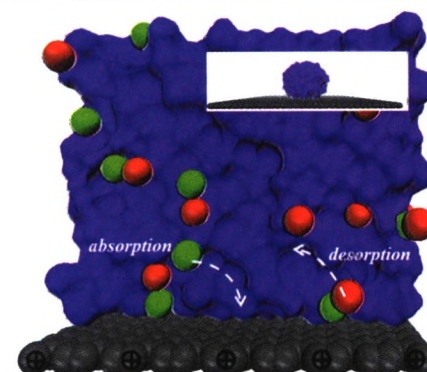
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Influence of Wettability on the Charging Dynamics of Electric Double-Layer Capacitors

YANG Huachao, BO Zheng, SHUAI Xiaorui, YAN Jianhua, CEN Kefa



Wettability plays a significant role in regulating the charge storage and charging dynamics of electric double-layer capacitors.

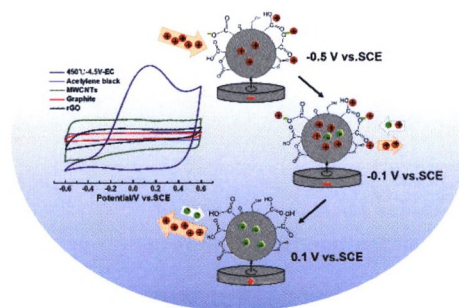
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GU Yuxing, YANG Juan, WANG Dihua



The capacitance nature of electrolytic carbon is significantly different from that of normal carbon with special ion distribution under various polarization conditions.

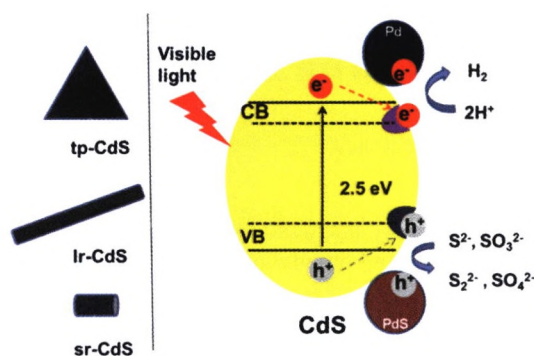
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刘志明, 刘国亮, 洪昕林

Influence of Surface Defects and Palladium Deposition on the Activity of CdS Nanocrystals for Photocatalytic Hydrogen Production

LIU Zhiming, LIU Guoliang, HONG Xinlin



Surface defects and palladium deposition promote photocatalytic hydrogen production in the case of CdS nanocrystals with different morphologies.

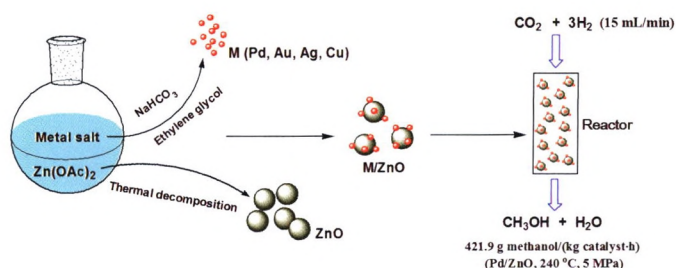
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刘艳芳, 胡兵, 尹雅芝, 刘国亮, 洪昕林

One-Pot Surfactant-Free Synthesis of Transition Metal/ZnO Nanocomposites for Catalytic Hydrogenation of CO₂ to Methanol

LIU Yanfang, HU Bing, YIN Yazhi, LIU Guoliang, HONG Xinlin



We demonstrate a facile one-pot surfactant-free synthesis of transition metal/ZnO nanocomposites for catalytic hydrogenation of CO₂ to methanol.

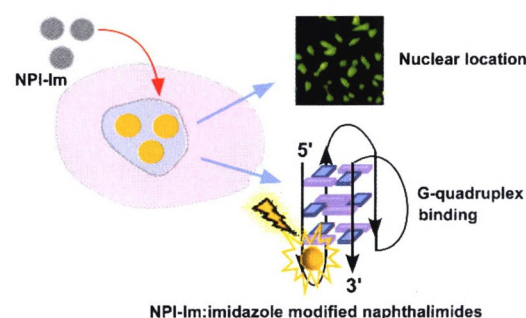
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DNA Interactions and Cytotoxicity of Imidazole-Modified Naphthalimides

GAO Yunyan, CAI Wenjiao, OU Zhize, MA Tuotuo, YI Na, LI Zhiyuan



The imidazolium-modified naphthalimides, possessing high affinity for the G-quadruplex, exhibited less cytotoxicity against non-cancerous MRC-5 cells over A549.

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