Dipyrrolylquinoxaline difluoroborates with intense red solid-state fluorescence

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摘要 (English): A set of organic fluorescent dyes of dipyrrolylquinoxalines (PQs 4-6) and their BF₂ complexes (BPQs 1-3) were synthesized from commercial reagents, and were characterized by their X-ray structural analysis, and optical and electrochemical properties. BPQs 1-3 showed intense broad absorption in the visible region in the solution-state. In comparison with that of PQs 4-6, there is an over 110 nm red-shift of the absorption maximum in the BPQs 1-3 (up to 583 nm). Interestingly, dyes 1-6 all exhibit red solid-state fluorescence with moderate to high fluorescence quantum yields except for PQ 4 which showed bright yellow solid-state fluorescence. X-ray structures of BPQs 2-3 showed the planar structure of quinoxaline with one pyrrole unit via the BF₂ chelation and the almost perpendicular orientation of the uncoordinated pyrrole to the NBN core plane (the dihedral angle of 70-73°). The extended π-conjugation was in good agreement with the observed red-shift of the spectra. These dyes formed well-ordered intermolecular packing structures via the intermolecular hydrogen bonding between the N atoms of quinoxaline moieties and the NH units of adjacent pyrroles. The lack of π-π stacking in their crystal packing structures may explain the interestingly intense solid-state fluorescence of these dyes.

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主题: Crystal atomic structure (主要); Aromatic compounds; Dihedral angle; Doppler effect; Fluorescence; Hydrogen bonds; Potassium compounds; Quantum theory; Synthesis (chemical)

分类: 741.1: Light and Optics; 801.4: Physical Chemistry; 802.2: Chemical Reactions; 804.1: Organic Compounds; 931.3: Atomic and Molecular Physics; 931.4: Quantum Theory

标识符 (关键字): Crystal packing structures, Fluorescence quantum yield, Intermolecular hydrogen bonding, Intermolecular packing, Organic fluorescent dyes, Perpendicular orientation, Solid-state fluorescence, X ray structural analysis

标题: Dipyrrolylquinoxaline difluoroborates with intense red solid-state fluorescence

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语言: 英文

摘要语言: English

文档类型: Article

出版物名称: Dalton Transactions
Mild Cu(OAc)$_2$·H$_2$O-catalyzed synthesis of multi-substituted 1,2,4-triazoles from amidines with nitriles via a N-N/C-N coupling

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**Publication Information:** RSC Advances 5.96 (Sep 3, 2015): 78422-78426.

**Abstract (English):** A simple and efficient Cu(OAc)$_2$·H$_2$O-catalyzed aerobic oxidation of amidines with nitriles for the synthesis of multi-substituted 1,2,4-triazoles has been achieved. The procedure constructs multi-substituted 1,2,4-triazoles and has the advantages of operational simplicity, broad substrate scope, and no need for
prefunctionalized reagents. A possible mechanism has been proposed via the cascade N-H functionalization and N-N/C-N bond formation.
Synthesis, characterization, and reactivity of lanthanide amides incorporating neutral pyrrole ligand.

Isolation and characterization of active catalyst for cyanosilylation of ketones

作者: Wang, Fenhua 1; Wei, Yun 2; Wang, Shaowu 3; Zhu, Xiancui 2; Zhou, Shuangliu 2; Yang, Gaosheng 2; Gu, Xiaoxia 2; Zhang, Guangchao 2; Mu, Xiaolong 2
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出版物信息: Organometallics 34.1 (Jan 12, 2015): 86-93.

摘要 (English): A series of lanthanide amido complexes incorporating a neutral pyrrole ligand were synthesized and characterized, and their catalytic activities were studied. Treatment of [(Me$_3$Si)$_2$N]$_3$Ln(μ-Cl)Li(THF)$_3$ with 1 equiv of [(2,5-Me$_2$C$_6$H$_4$N)CH$_2$CH$_2$]$_2$NH (1) in toluene afforded the corresponding lanthanide amides with the formula [η$_5$:η$_1$:η$_3$-(2,5-Me$_2$C$_6$H$_4$N)CH$_2$CH$_2$]$_2$NLn[N(SiMe$_3$)$_2$]$_2$ (Ln = La (2), Nd (3)). Reaction of 2 or 3 with N,N-dicyclohexylcarbodiimide (CyN=C=NCy) gave the carbodiimide selectively inserted into the appended Ln-N bond products formulated as CyNC[N,N-(2,5-Me$_2$C$_6$H$_4$N)CH$_2$CH$_2$]N]NCyLn[N(SiMe$_3$)$_2$]$_2$ (Ln = La (4), Nd (5)). Reactions of the lanthanide amides with Me$_3$SiCN were also examined. A mixed reaction of [(Me$_3$Si)$_2$N]$_3$La(μ-Cl)Li(THF)$_3$, [(2,5-Me$_2$C$_6$H$_4$N)CH$_2$CH$_2$]$_2$NH (1), and Me$_3$SiCN in toluene at room temperature produced the novel cyano bridged dinuclear lanthanum complex η$_5$:η$_1$:η$_3$-[2,5-Me$_2$C$_6$H$_4$NCH$_2$CH$_2$]$_2$NLn[N(SiMe$_3$)$_2$](μ-CN)La[N(SiMe$_3$)$_2$]$_3$ (6). The stoichiometric reactions of lanthanide amides 2 or 3 with Me$_3$SiCN produced the novel trinuclear lanthanum and neodymium complexes η$_5$:η$_1$:η$_3$-[2,5-Me$_2$C$_6$H$_4$NCH$_2$CH$_2$]$_2$NLn[N(SiMe$_3$)$_2$](μ-CN)La[N(SiMe$_3$)$_2$]$_3$ (Ln = La (7), Nd (8)) through selective σ-bond metathesis reaction of the terminal Ln-N (N(SiMe$_3$)$_2$) bond with the Si-C bond of Me$_3$SiCN. On the basis of the stoichiometric reactions of complexes 2, or 3 with Me$_3$SiCN, complexes 2, 3, 4, 5, 7, and 8 as catalysts for cyanosilylation of ketones were investigated. Results indicated that these complexes displayed a high catalytic activity on addition of Me$_3$SiCN to ketones, and the activity of the complexes has the order of 7 ~ 8 > 2 ~ 3 ~ 4 ~ 5. Thus, complex 7 or 8 was proposed as the active catalyst in the catalytic reaction for the precatalysts of 2 and 3.

链接: Check for full text via 360 Link, Order Full Text from Infotrieve?
A simple label-free electrochemical method for the detection of polynucleotide kinase activity by a peroxidase mimic: TiO$_2$ nanotube array

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**Publication Information:** Analytical Methods 7.24 (Dec 21, 2015): 10345-10349.

**Abstract (English):** Phosphorylation of DNA by polynucleotide kinase (PNK) plays an important role in a variety of cellular processes, such as nucleic acid metabolism and DNA damage repair. Strategies for a simple and effective PNK assay are in urgent need. Here we report the development of a simple label-free electrochemical method for a PNK assay based on the mimic peroxidase character of a prepared TiO$_2$ nanotube array (NTA) and its specific attachment to phosphorylated DNA. The concentration of T4 PNK was successfully detected by the TiO$_2$ NTA electrode with a detection limit of 0.15 U mL$^{-1}$. In the process, only a one-step incubation process was used and no labeling processes were involved. In addition, the treated TiO$_2$ foil was anodized into the nanotube array and it was directly used as the electrode without any other complex modification processes which avoided the leakage of an electrode modifier, and so the TiO$_2$ nanotube array with excellent stability and flexibility is worthy of use in real time monitoring.

**Keywords:** Cellular process, Detection limits, Electrochemical methods, Modification process, Nucleic acid metabolism, Peroxidase mimics, Polynucleotides, Real time monitoring

**Language:** 英文

**Abstract Language:** English

**Document Type:** Article

**Publication Name:** Analytical Methods
FeCl$_3$-mediated synthesis of β-alkynyl ketones via domino nucleophilic-substitution/intramolecular-cyclization/reverse Claisen condensation of N-cyclohexyl propargylamines and 1,3-diketones

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摘要 (English): The synthesis of β-alkynyl ketones was achieved in good to excellent yields by an iron-catalyzed domino reaction of N-cyclohexyl propargylamines and 1,3-diketones. A plausible mechanism involving nucleophilic substitution, intramolecular cyclization, and reverse Claisen condensation for this process is proposed.

链接: Check for full text via 360 Link, Order Full Text from Infotrieve?
FeCl₃-mediated synthesis of β-alkynyl ketones via domino nucleophilic-substitution/intramolecular-cyclization/reverse Claisen condensation of N-cyclohexyl propargylamines and 1,3-diketones

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Preparation, electrochemical responses and sensing application of Au disk nanoelectrodes down to 5 nm

Authors: Zhang, Yaoyao 1; Xu, Shen 1; Qian, YuanYuan 1; Yang, Xiaosong 1; Li, Yongxin 1 College of Chemistry and Materials Science, Anhui Normal University, 241000, China yongli@mail.ahnu.edu.cn

Publication information: RSC Advances 5.94 (Sep 4, 2015): 77248-77254.

Abstract (English): In this work, we report the preparation and electrochemical responses of Au disk nanoelectrodes as small as 5 nm in radii by the improvement of the laser-assisted pulling technique. A Au microwire is sealed into a bilayer capillary and pulled into an ultrasharp Au nanowire sealed in a silica tip using a laser-assisted puller. The ultrasharp tip is then sealed into a piece of glass tube, which is manually polished to expose the Au. Transmission electron microscopy, steady-state voltammetry of small redox species (e.g., ferrocene (Fc), ferrocene methanol (FcH₂OH), potassium ferricyanide (Fe(CN)₆³⁻), hexaaammineruthenium(iii)chloride (Ru(NH₃)₆³⁺), and cyclic voltammetry in a H₂SO₄ solution are utilized to characterize the nanoelectrodes. The heterogeneous electron transfer rate constants for the oxidation/reduction of Fc, FcH₂OH, Fe(CN)₆³⁻, and Ru(NH₃)₆³⁺ are determined from steady-state voltammetry using the method developed by Mirkin and Bard and found to be k° = 7.9 ± 3.6 cm s⁻¹ and α = 0.41 ± 0.04 for Fc, k° = 7.4 ± 7.1 cm s⁻¹ and α = 0.41 ± 0.23 for FcH₂OH, k° = 4.0 ± 3.6 cm s⁻¹ and α = 0.52 ± 0.17 for Fe(CN)₆³⁻, and k° = 7.2 ± 6.9 cm s⁻¹ and α = 0.53 ± 0.22 for Ru(NH₃)₆³⁺. These Au disk nanoelectrodes have been used to investigate the direct electrochemistry of ferritin molecules, which are immobilized on the Au surface by an electrostatic interaction between the cysteamine monolayer modified on the Au surface and ferritin molecules. From the voltammetric peak of ferritin on the Au nanoelectrode (200 nm in radius), the amount of ~3900 molecules or 6.1 zmol can be calculated.

Theme: Cyclic voltammetry (主要); Electrochemistry; High resolution transmission electron microscopy; Molecules; Organometallics; Rate constants; Transmission electron microscopy; Voltammetry

Class: 741.3: Optical Devices and Systems; 801.4: Physical Chemistry; 801.4.1: Electrochemistry; 804.1: Organic Compounds; 931.3: Atomic and Molecular Physics

Keywords: Direct electrochemistry, Electrochemical response, Ferritin molecules, Heterogeneous electron transfer rate constant, Oxidation/reduction, Potassium ferricyanide, Sensing applications, Steady-state voltammetry

Title: Preparation, electrochemical responses and sensing application of Au disk nanoelectrodes down to 5 nm

Corresponding author: Li, Yongxin College of Chemistry and Materials Science, Anhui Normal University, 241000, China.

Language: 英文
Composite silicon nanostructure arrays fabricated on optical fibre by chemical etching of multicrystal silicon film

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Integrating nanostructures onto optical fibers presents a promising strategy for developing new-fashioned devices and extending the scope of nanodevices’ applications. Here we report the first fabrication of a composite silicon nanostructure on an optical fiber. Through direct chemical etching using an H$_2$O$_2$/HF solution, multicrystal silicon films with columnar microstructures are etched into a vertically aligned, inverted-cone-like nanorod array embedded in a nanocone array. A faster dissolution rate of the silicon at the void-rich boundary regions between the columns is found to be responsible for the separation of the columns, and thus the formation of the nanostructure array. The morphology of the nanorods primarily depends on the microstructure of the columns in the film. Through controlling the microstructure of the as-grown film and the etching parameters, the structural control of the nanostructure is promising. This fabrication method can be extended to a larger length scale, and it even allows roll-to-roll processing.
Hierarchical NiMn$_2$O$_4$@CNT nanocomposites for high-performance asymmetric supercapacitors

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出版物信息: RSC Advances 5.31 (Jan 1, 2015): 24607-24614.

摘要 (English): Miniaturized energy storage devices have attracted considerable research attention due to their promising applications in various smart electronic devices. In this work, a high performance asymmetric supercapacitor (ASC) device was designed and fabricated wherein a novel nanocomposite consisting of manganese oxide (NiMn$_2$O$_4$) nanosheets with carbon nanotubes (CNTs) was used as the active material. High capacitance of 151 F g$^{-1}$ and energy density of 60.69 W h kg$^{-1}$ were achieved for the CNT@NiMn$_2$O$_4$ nanocomposites ASC at a current density of 1 A g$^{-1}$, which attributing to the widen operation voltage window ranging from 0 to 1.7 V. Moreover, the CNT@NiMn$_2$O$_4$ nanocomposites ASC also showed remarkable cycling stability with 96.3% energy density retention after 5000 cycles. As a result, the CNT@NiMn$_2$O$_4$ nanocomposite is a possible contender materials for next generation supercapacitors in high energy density storage systems.
Construction of unique Co$_3$O$_4$@CoMoO$_4$ core/shell nanowire arrays on Ni foam by the action exchange method for high-performance supercapacitors
In this work, hierarchical Co$_3$O$_4$@CoMoO$_4$ core/shell nanowire arrays on nickel foam are fabricated by a facile hydrothermal ion exchange method. The Co$_3$O$_4$ nanowires are fully covered by ultrathin mesoporous CoMoO$_4$ nanosheets. A possible growth mechanism for the CoMoO$_4$ involves the capturing of the part of the cobalt ions of the Co$_3$O$_4$ nanowires by the molybdenum acid radical without annealing. When investigated as binder-free electrodes for supercapacitors (SCs), such unique Co$_3$O$_4$@CoMoO$_4$ core/shell hybrid electrodes exhibited ultrahigh areal capacitances, which are several times larger than the pristine Co$_3$O$_4$ electrode. The electrode exhibits a high specific capacitance of 1040 F g$^{-1}$ at a current density of 1 A g$^{-1}$ and an excellent cycling stability (5000 cycles). The remarkable electrochemical performance is attributed to the rational combination of two electroactive materials and the array configuration.
High-throughput and rapid fluorescent visualization sensor of urinary citrate by CdTe quantum dots

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Abstract (English): In this paper, we have presented a novel CdTe quantum dots (QDs) based fluorescent sensor for visual and turn-on sensing of citrate in human urine samples. The europium ion (Eu³⁺) can lead to the fluorescence quenching of thioglycollic acid (TGA) modified CdTe QDs due to photoinduced electron transfer accompanied by the change of emission color from yellow to orange. Next, addition of citrate breaks the preformed assembly because citrate can replace the CdTe QDs, based on the fact that the Eu³⁺ ion displays higher affinity with citrate than the CdTe QDs. Thus the photoinduced electron transfer is switched off, and the fluorescence emission of CdTe QDs is rapidly (within 5 min) recovered, simultaneously, the orange emission color restores to yellow. Such proposed strategy may conveniently discriminate the patient of renal stone from normal person by naked eyes. In addition to visualization detection, the fluorescence responses can be used for well quantifying citrate in the range of 0.67-133 μM. So, the present, simple, low-cost and visualized citrate fluorescence sensor has great potential in the applications for earlier screening in clinical detection.

Theme: Semiconductor quantum dots; Cadmium telluride; Citrus fruits; Electron transitions; Europium; Fluorescence; Nanocrystals; Quenching; Sensors; Visualization
Folate mediated self-assembled phytosterol-alginate nanoparticles for targeted intracellular anticancer drug delivery

**Authors:** Wang, Jianting 1; Wang, Ming 2; Zheng, Mingming 3; Guo, Qiong 1; Wang, Yafan 4; Wang, Heqing 4; Xie, Xiangrong 4; Huang, Fenghong 3; Gong, Renmin 1 1 College of Life Science, Anhui Normal University, 241000, China rmgong.nju@163.com 2 Anhui Province Key Laboratory of Biological Macro-molecules Research, Wannan Medical College, 241002, China, Department of Biochemistry and Molecular Biology, Wannan Medical College, 241002, China 3 Oil Crops Research Institute, Chinese Academy of Agricultural Science, 430062, China hfh.oilcrops@163.com 4 Department of Biochemistry and Molecular Biology, Wannan Medical College, 241002, China

**Publication Information:** Colloids and Surfaces B: Biointerfaces 129 (May 1, 2015): 63-70.

**Abstract (English):** It was found that DOX release from FPA NPs was pH-sensitive and more rapid in an acidic environment. Self-assembled core/shell nanoparticles (NPs) were synthesized from water-soluble alginate substituted by hydrophobic phytosterols. Folate, a cancer-cell-specific ligand, was conjugated to the phytosterol-alginate (PA) NPs for targeting folate-receptor-overexpressing cancer cells. The physicochemical properties of folate-phytosterol-alginate (FPA) NPs were characterized by nuclear magnetic resonance, transmission electron microscopy, dynamic light scattering, electrophoretic light scattering, and fluorescence spectroscopy. Doxorubicin (DOX), an anticancer drug, was entrapped inside prepared NPs by dialysis method. The identification of prepared FPA NPs to folate-receptor-overexpressing cancer cells (KB cells) was confirmed by cytotoxicity and folate competition assays. Compared to the pure DOX and DOX/PA NPs, the DOX/FPA NPs had lower IC$_{50}$ value to KB cells because of folate-receptor-mediated endocytosis process and the cytotoxicity of DOX/FPA NPs to KB cells could be competitively inhibited by free folate. The cellular uptake and internalization of pure DOX and DOX/FPA NPs was confirmed by confocal laser scanning microscopy image and the higher intracellular uptake of drug for DOX/FPA NPs over pure DOX was observed. The FPA NPs had the potential as a promising carrier to target drugs to cancer cells overexpressing folate receptors and avoid cytotoxicity to normal tissues.

**Keywords:** Anticancer drug, Folate receptor, Phytosterol, Self assembled nanoparticles, Targeted delivery, Self-assembled nanoparticles

**Title:** Folate mediated self-assembled phytosterol-alginate nanoparticles for targeted intracellular anticancer drug delivery
Three-dimensional NiCo$_2$O$_4$@NiMoO$_4$ core/shell nanowires for electrochemical energy storage

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Integrated nanodevices with the capability of storing energy are widely applicable and thus have been studied extensively. To meet the demand for flexible integrated devices, asymmetric supercapacitors that simultaneously realize energy storage were fabricated by growing NiCo$_2$O$_4$@NiMoO$_4$ hybrid nanowires on nickel foam, thus obtaining the positive electrode, and employing active carbon as the negative electrode. The as-assembled integrated systems were characterized by their improved energy storage (areal specific capacitance of 6.30 F cm$^{-2}$ at 60 mA cm$^{-2}$ and specific capacitance up to 1242 F g$^{-2}$ at a current density of 10 mA cm$^{-2}$), enhanced power density and energy density by increasing the potential window from 0 V to 1.6 V. Such flexible integrated devices might be used in smart and self-powered sensory, wearable, and portable electronics.
Chemical fractions and phytoavailability of copper to rape grown in the polluted paddy soil

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Abstract (English): This paper focuses on the phytoaccumulation and translocation of copper (Cu) in rape grown in the Cu-polluted paddy soil. Pot experiments were conducted in greenhouse conditions to examine the Cu availability and uptake by rape in a paddy soil. The soil was spiked with different concentrations of Cu (0, 100, 300, 500 and 1,000 mg kg⁻¹ soil, added as CuSO₄) to simulate soil Cu contamination. After 8 months of growth, plant shoots, stems, pod shells and rapeseeds were harvested for analysis. The concentrations of Cu in the roots and aerial parts of the rape and available Cu in soils were then extracted and determined. Chemical fractions of Cu in the paddy soil of rape were also investigated by sequential extraction techniques. The findings showed that Cu in the clean paddy soil was mainly distributed in residual fractions. However, the most drastic increase was observed in Fe–Mn oxides-bound fractions and organic-bound fractions with increasing soil Cu concentrations. Exchangeable fractions played a more important role than other fractions in controlling the mobility and phytoavailability of Cu. Rape growth was stimulated by low concentrations of Cu, but inhibited by high concentrations. Compares to the aerial parts, the roots were more sensitive to Cu toxicity. The correlation analysis showed that Cu in exchangeable fractions made the greatest contribution on the accumulation of Cu in rapes. The factor analysis results showed that the exchangeable fractions in roots can be indicator of Cu availability. Meanwhile, the bio-concentration factors and the translocation factors of Cu in rape were determined and the results showed that Cu had lower accumulation in the edible parts of the rape.
Effects of Myriophyllum spicatum L. on the migration and conversion of exogenous 15N at the water-sediment interface

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出版物信息: Zhongguo Huanjing Kexue/China Environmental Science 35.6 (Jan 1, 2015): 1855-1862.

摘要 (English): Simulated indoor experiments were conducted to investigate the fate of excess exogenous nitrate nitrogen and the effects of growing Myriophyllum spicatum on the migration and conversion of exogenous 15N by using the isotope labelling technology in microcosm. The results suggested that in a twelve-day experiment the percentage of exogenous nitrate nitrogen removed by denitrification, microorganism, submerged plants, dissimilatory nitrate reduction to ammonium (DNRA) and conversion to dissolvable organic nitrogen (DON) was 47.54%, 25.24%, 12.76%, 0.52% and 1.21%, respectively. In the treatment group (planted group), while in the unplanted group (control group), the percentage of exogenous nitrate nitrogen removed by denitrification, microorganism, DNRA and DON was 32.74% 30.79%, 0.54% and 5.83%, respectively. About 87.24% and 69.90% of the exogenous 15N was transformed in planted and unplanted groups, respectively during the twelve-day experiment. According to our finding, denitrification is the main pathway for nitrate nitrogen removal, followed by microorganism immobilization. M. spicatum also plays an important role in the removal of nitrate nitrogen, but the effects of DNRA and DON is relatively poor. To sum up M. spicatum promotes denitrification, accelerates the migration and conversion of nitrate nitrogen, which directly or indirectly accelerates the removal of exogenous nitrate nitrogen in the microcosm.

链接: Check for full text via 360 Link, Order Full Text from Infotrieve?

主题: Nitrogen removal (主要); Denitrification; Isotopes; Nitrates; Nitrogen

分类: 802.2: Chemical Reactions; 804: Chemical Products Generally; 804.2: Inorganic Compounds

标识符 (关键字): Dissimilatory nitrate reduction, Indoor experiment, Isotope labelling, Microorganism immobilizations, Myriophyllum spicatum, Plant wptake, Stable isotopes, Water sediment interface, Migration and conversion, Stable isotope labelling

标题: Effects of Myriophyllum spicatum L. on the migration and conversion of exogenous 15N at the water-sediment interface

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语言: 英文

摘要语言: English

文档类型: Article

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卷: 35

期: 6
Graphene quantum dots: Highly active bifunctional nanoprobes for nonenzymatic photoluminescence detection of hydroquinone

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Publication: Biosensors and Bioelectronics 74 (Dec 5, 2015): 418-422.

Abstract (English): In this paper, a simple and sensitive photoluminescence method is developed for the hydroquinone quantitation by using graphene quantum dots which simultaneously serve as a peroxidase-mimicking catalyst and a photoluminescence indicator. In the presence of dissolved oxygen, graphene quantum dots with intrinsic peroxidase-mimicking catalytic activity can catalyze the oxidation of hydroquinone to produce p-benzoquinone, an intermediate, which can efficiently quench graphene quantum dots' photoluminescence. Based on this effect, a novel fluorescent platform is proposed for the sensing of hydroquinone, and the detection limit of 5 nM is found.

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**Electrochemical sensor for paracetamol recognition and detection based on catalytic and imprinted composite film**

**Authors:** Teng, Ying 1; Fan, Limei 1; Dai, Yunlong 1; Zhong, Min 1; Lu, Xiaojing 1; Kan, Xianwen 1 1 College of Chemistry and Materials Science, Anhui Normal University, 241000, China, The Key Laboratory of Functional Molecular Solids, Ministry of Education, Anhui Laboratory of Molecule-Based Materials, Anhui Key Laboratory of Chemo-Biosensing, Anhui Key Laboratory of Functional Molecular Solids, China kanxw@mail.ahnu.edu.cn

**Publication Information:** Biosensors and Bioelectronics 71 (Sep 5, 2015): 137-142.

**Abstract (English):** A new strategy for a composite film based electrochemical sensor was developed in this work. A layer of conductive film of poly(p-aminobenzene sulfonic acid) (pABSA) was electropolymerized onto glassy carbon electrode surface and exhibited a high electrocatalytic active for paracetamol (PR) redox. The subsequent formation of a layer of molecular imprinted polymer (MIP) film on pABSA modified electrode endowed the sensor with plentiful imprinted cavities for PR specific adsorption. The advantages of the composite film made the prepared sensor display high sensitivity and good selectivity for PR detection and recognition. Under the optimal conditions, the sensor could recognize PR from its interferents. A linear ranging from $5.0 \times 10^{-8}$ to $1.0 \times 10^{-4}$ mol/L for PR detection was obtained with a detection limit of $4.3 \times 10^{-8}$ mol/L. The sensor has been applied to analyze PR in tablets and human urine samples with satisfactory results. The simple, low cost, and efficient strategy reported here can be further used to prepare electrochemical sensors for other compounds recognition and detection.

**Links:** Check for full text via 360 Link, Order Full Text from Infotrieve?

**Keywords:** Conductive Polymer, Glassy carbon electrodes, Human urine samples, Imprinted composites, Molecular imprinted polymer (MIP), Molecular imprinted polymers, P-aminobenzene sulfonic acid, Paracetamol, Electrochemical sensor, Molecular imprinted polymer

**Title:** Electrochemical sensor for paracetamol recognition and detection based on catalytic and imprinted composite film

**Corresponding Author:** Kan, Xianwen College of Chemistry and Materials Science, Anhui Normal University, 241000, China.

**Language:** English
Copper(I)-catalyzed kinetic resolution of N-sulfonylaziridines with indoles: Efficient construction of pyrroloindolines

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The first Lewis acid catalyzed [3 + 2] annulation of indoles and 2-aryl-N-tosylaziridines was realized by using copper(I)/chiral diphosphine complexes as a catalyst. With this method, a variety of uniquely substituted chiral pyrroloindolines bearing multiple contiguous stereogenic centers were facilely accessed in a straightforward, high-yielding, and highly stereoselective way under mild conditions.
Imprinted propyl gallate electrochemical sensor based on graphene/single walled carbon nanotubes/sol-gel film

作者: Xu, Guilin; Chi, Yu; Li, Lu; Liu, Shouhua; Kan, Xianwen 1 College of Chemistry and Materials Science, Anhui Normal University, Wuhu 241000, PR China, The Key Laboratory of Functional Molecular Solids, Ministry of Education, PR China, Anhui Laboratory of Molecule-Based Materials, Anhui Key Laboratory of Chemo-Biosensing, Anhui Key Laboratory of Functional Molecular Solids, PR China

摘要 (English): A novel imprinted sol-gel electrochemical sensor for the determination of propyl gallate (PG) was developed based on a composite of graphene and single walled carbon nanotubes (GR-SWCNTs). It was fabricated by stepwise modifying GR-SWCNTs and molecularly imprinted polymers and stored in 0.10 mol L⁻¹ phosphate buffer solution pH 6.0, which endowed the sensor good sensitivity and selective recognition towards template molecules. The morphology and specific adsorption capacity of the sensor was characterized by scanning electron microscope and electrochemical methods, respectively. Under the optimized conditions, a linear range of the sensor to PG was 8.0 × 10⁻⁸-2.6 × 10⁻³ mol L⁻¹ with a limit of detection of 5.0 × 10⁻⁸ mol L⁻¹ (S/N = 3). The sensor exhibited specificity and selectivity towards template molecules as well as excellent reproducibility, regeneration and stability. Furthermore, the sensor could be applied to determine PG in edible oils, instant noodles and cookies with satisfactory results.

主题: Single-walled carbon nanotubes (SWCN) (主要); Carbon; Electrochemical sensors; Graphene; Molecules; Scanning electron microscopy; Sol-gel process; Sol-gels; Yarn

分类: 761: Nanotechnology; 801: Chemistry; 804: Chemical Products Generally; 813.1: Coating Techniques; 819.4: Fiber Products; 931.2: Physical Properties of Gases, Liquids and Solids; 931.3: Atomic and Molecular Physics

标识符 (关键字): Electrochemical methods, Limit of detection, Molecularly Imprinted Polymer, Optimized conditions, Phosphate buffer solutions, Propyl gallate, Selective recognition, Specific adsorption capacities, Imprinted sol-gel electrochemical sensor, Single walled carbon nanotubes
Simultaneous fluoroimmunoassay of two tumor markers based on CdTe quantum dots and gold nanocluster coated-silica nanospheres as labels

作者: Li, Lihua 1 ; Feng, Dexiang 1 ; Zhao, Junqing 2 ; Guo, Zilin 2 ; Zhang, Yuzhong 2 1 College of Chemistry and Materials Science, Key Laboratory of Functional Molecular Solids, Ministry of Education, Anhui Laboratory
In this study, a novel fluoroimmunoassay protocol for simultaneous detection of two tumor markers is described. The new approach employed magnetic beads as a carrier for the antibody immobilization, while CdTe quantum dots (CdTe QDs) and gold nanoclusters (Au NCs) coated-silica nanospheres were used as labels. Carcinoembryonic antigen (CEA) and alpha-fetoprotein (AFP) were adopted as model proteins. After a typical sandwich-type immunoreaction, the immunocomplex exhibited two distinguishable fluorescence peaks at 550 nm and 655 nm corresponding to CdTe QDs and Au NCs, respectively. Under optimal conditions, fluorescence intensities were linearly increased to the concentration of CEA and AFP in the range of 0.1-400 ng mL\(^{-1}\), the detection limit of fluoroimmunoassay is 0.04 ng mL\(^{-1}\) for CEA and 0.08 ng mL\(^{-1}\) for AFP, respectively. The proposed method was evaluated with human serum, and the determination values obtained were in accordance with reference methods reported. These results demonstrated that the new method can be applied to the determination of two tumor markers in clinical samples.
Fast electrodeposition, influencing factors and catalytic properties of dendritic Cu-M (M = Ni, Fe, Co) microstructures

作者: Zhang, Huying 1; Ni, Yonghong 1; Zhong, Yiman 1; Wu, Hao 1; Zhai, Muheng 1

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ProQuest 文档链接

摘要 (English): The rapid electrochemical deposition of dendritic Cu-M (M = Ni, Fe, Co) microstructures with excellent catalytic activity is reported here. Simple Cu\(^{2+}\) and M\(^{2+}\) salts were employed as the initial metal sources and boric acid was used as the buffer solution. The electrodeposition process was carried out at a deposition current of 10 mA for 5 min in air at room temperature. The phase and morphology of the as-prepared products were characterized by field emission scanning electron microscopy (FESEM), powder X-ray diffraction (XRD), energy dispersive spectrometry (EDS) and transmission electron microscopy (TEM). It was found that the formation of dendritic Cu-M microstructures could be affected by some factors including the amounts of M\(^{2+}\) salts and boric acid, and the deposition current and time. Cu-Ni dendrites were used as a model and their
performance was studied. The investigations showed that the as-deposited Cu-Ni dendrites exhibited good electrochemical responses in 0.1 M KOH solution and could be used as an electrochemical catalyst for the reduction of nitrate and the oxidation of glucose. Also, the as-deposited Cu-M dendrites exhibited excellent catalytic activities for the reduction of 4-nitrophenol (4-NP) to 4-aminophenol (4-AP) in excess NaBH₄ solution.
Asymmetric Addition of Pyridyl Aluminum Reagents to Aldehydes Catalyzed by a Titanium(IV) Catalytic System of (R)-H$_8$-BINOLate

作者: Zhang, Lijun 1; Tu, Bing 1; Ge, Min 1; Li, Yimei 1; Chen, Liangyu 1; Wang, Wei 1; Zhou, Shuangliu 1

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摘要 (English): The asymmetric addition of pyridyl aluminum reagents to aldehydes has been successfully developed by employing a titanium(IV) catalytic system of (R)-H$_8$-BINOLate, which affords a series of valuable optically active diarylmethanols containing various pyridyl groups in high yields with excellent enantioselectivities of up to 98% ee.

链接: Check for full text via 360 Link. Order Full Text from Infotrieve?

主题: Titanium (主要); Aldehydes; Aluminum

分类: 541.1: Aluminum; 542.3: Titanium and Alloys; 804.1: Organic Compounds

标识符 (关键字): Asymmetric addition, Catalytic system, High yield, Optically Active, Pyridyl, Pyridyl groups

标题: Asymmetric Addition of Pyridyl Aluminum Reagents to Aldehydes Catalyzed by a Titanium(IV) Catalytic System of (R)-H$_8$-BINOLate

通讯作者: Zhang, Lijun Laboratory of Functional Molecular Solids, Ministry of Education, Anhui Laboratory of Molecule-Based Materials, College of Chemistry and Materials Science, Anhui Normal University, 241000, China.

语言: 英文

摘要语言: English

文档类型: Article
Reactivity of functionalized indoles with rare-earth metal amides. Synthesis, characterization and catalytic activity of rare-earth metal complexes incorporating indolyl ligands

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The reactivity of several functionalized indoles 2-(RNHCH$_2$)$_8$H$_5$NH (R = C$_6$H$_5$ (1), t-Bu (2), 2,6-i-Pr$_2$C$_6$H$_3$ (3)) with rare-earth metal amides is described. Reactions of 1 or 2 with [(Me$_3$Si)$_2$N]$_3$RE(μ-Cl)Li(THF)$_3$ (RE = Eu, Yb) respectively produced the europium complexes [2-(C$_6$H$_5$NCH)$_8$H$_5$N]$_2$Eu[N(SiMe$_3$)$_2$] (4) and [2-(t-BuNCH)$_8$H$_5$N]Eu[N(SiMe$_3$)$_2$]$_2$ (5), and the ytterbium complex [2-(t-BuNCH)$_8$H$_5$N]$_2$Yb[N(SiMe$_3$)$_2$] (6), containing bidentate anionic indolyl ligands via dehydrogenation of the amine to the imine. In contrast, reactions of the more sterically bulky indole 3 with [(Me$_3$Si)$_2$N]$_3$RE(μ-Cl)Li(THF)$_3$ afforded complexes [2-(2,6-i-Pr$_2$C$_6$H$_3$NCH)$_8$H$_5$N]RE[N(SiMe$_3$)$_2$] (THF)$_2$ (RE = Yb (7), Y (8), Er (9), Dy (10)) with the deprotonated indolyl ligand. While reactions of 3 with yttrium and ytterbium amides in refluxing toluene respectively gave the complexes [2-(2,6-i-Pr$_2$C$_6$H$_3$NCH)$_8$H$_5$N]$_3$Y (11) and [2-(2,6-i-Pr$_2$C$_6$H$_3$NCH)$_8$H$_5$N]$_2$Yb(THF)$_2$ (12), along with transformation of the amino group to the imino group, and also with a reduction of Yb$^{3+}$ to Yb$^{2+}$ in the formation of 12. Reactions of 3 with samarium and neodymium amides provided novel dinuclear complexes [μ-η$_5$:$η^1$:$η^1$-2-(2,6-i-Pr$_2$C$_6$H$_3$NCH)$_8$H$_5$N]RE[N(SiMe$_3$)$_2$]$_2$ (RE = Sm (13), Nd (14)) having indolyl ligands in μ-η$_5$:$η^1$:$η^1$ hapticities. The pathway for the transformation of the amino group to the imino group is proposed on the basis of the experimental results. The new complexes displayed excellent activity in the intramolecular hydroamination of aminoalkenes.
Dinuclear rare-earth metal alkyl complexes supported by indolyl ligands in $\mu$-$\eta^2: \eta^1: \eta^1$ hapticities and their high catalytic activity for isoprene 1,4-cis-polymerization

作者: Zhang, Guangchao 1 ; Wei, Yun 1 ; Guo, Liping 1 ; Zhu, Xiancui 1 ; Wang, Shaowu 2 ; Zhou, Shuangliu 1 ; Mu, Xiaolong 1

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摘要 (English): Two series of new dinuclear rare-earth metal alkyl complexes supported by indolyl ligands in novel $\mu$-$\eta^2: \eta^1: \eta^1$ hapticities are synthesized and characterized. Treatment of $[\text{RE}(\text{CH}_2\text{SiMe}_3)_3(\text{thf})]_2$ with 1 equivalent of 3-$(\text{tBuN}=\text{CH})C\text{H}_5 \text{NH}$ (L1) in THF gives the dinuclear rare-earth metal alkyl complexes trans-$[\mu(\mu-\eta^2: \eta^1: \eta^1-3\text{-tBuNCH}-(\text{CH}_2\text{SiMe}_3))\text{Ind}]\text{RE}(\text{thf})(\text{CH}_2\text{SiMe}_3)]_2$ (Ind=indolyl, RE=Y, Dy, or Yb) in good yields. In the process, the indole unit of L1 is deprotonated by the metal alkyl species and the imino C=N group is transferred to the amido group by alkyl CH$_2$SiMe$_3$ insertion, affording a new dianionic ligand that bridges two metal alkyl units in $\mu$-$\eta^2: \eta^1: \eta^1$ bonding modes, forming the dinuclear rare-earth metal alkyl complexes. When L1 is reduced...
to 3-(tBuNHCH$_2$)$_2$C$_8$H$_7$NH (L$_2$), the reaction of [Yb(CH$_2$SiMe$_3$)$_3$(thf)$_2$] with 1 equivalent of L$_2$ in THF, interestingly, generated the trans-[(μ-η$_2$-η$_1$-η$_1$-3-(tBuNCH$_2$)Ind)- Yb(thf)(CH$_2$SiMe$_3$)$_2$]$_2$ (major) and cis-[(μ-η$_2$-η$_1$-η$_1$-3-(tBuNCH$_2$)Ind)Yb(thf)(CH$_2$SiMe$_3$)$_2$]$_2$ (minor) complexes. The catalytic activities of these dinuclear rare-earth metal alkyl complexes for isoprene polymerization were investigated; the yttrium and dysprosium complexes exhibited high catalytic activities and high regio- and stereoselectivities for isoprene 1,4-cis-polymerization.

主题: Ytterbium (主要); Catalyst activity; Dysprosium; Dysprosium compounds; Isoprene; Ligands; Metals; Polymerization; Rare earth compounds; Rare earth elements; Rare earths; Reaction kinetics; Synthesis (chemical); Uranium mines

分类: 531: Metallurgy and Metallography; 547: Minor, Precious and Rare Earth Metals and Alloys; 547.2: Rare Earth Metals; 801.4: Physical Chemistry; 802.2: Chemical Reactions; 804.1: Organic Compounds; 804.2: Inorganic Compounds; 815.2: Polymerization

标识符 (关键字): Alkyl complexes, Bonding modes, Dianionic ligands, Dysprosium complexes, Homogeneous catalysis, Isoprene polymerizations, Ligand effect, Rare earth metals, Ligand effects, Rare-earth metals

标题: Dinuclear rare-earth metal alkyl complexes supported by indolyl ligands in μ-η$_2$-η$_1$-η$_1$ hapticities and their high catalytic activity for isoprene 1,4-cis-polymerization

通讯作者: Wang, Shaowu Anhui Laboratory of Molecule-Based Materials, School of Chemistry and Materials Science, Anhui Normal University, 241000, China.

语言: 英文

摘要语言: English

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Combined Experimental and ab Initio Study of Site Preference of Ce$^{3+}$ in SrAl$_2$O$_4$

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摘要 (English): Low-temperature photoluminescence properties of Sr$_{1-2x}$Ce$_x$Na$_x$Al$_2$O$_4$ ($x = 0.001$) synthesized by a solid-state reaction method are measured with excitation energies in the vacuum ultraviolet (VUV) to ultraviolet (UV) range. Two distinct activator centers with different emission and excitation intensities are observed and attributed to Ce$^{3+}$ occupying the Sr1 and Sr2 sites of SrAl$_2$O$_4$ with different probabilities. Hybrid density functional theory (DFT) calculations within the supercell model are then carried out to optimize the local structures of Ce$^{3+}$ located at the two Sr sites of SrAl$_2$O$_4$, on which wave function-based CASSCF/CASPT2 embedded cluster calculations with the spin-orbit effect are performed to derive the Ce$^{3+}$ 4f$^1$ and 5d$^1$ energy levels. On the basis of the observed relative spectral intensities, the calculated DFT total energies, and the comparison between experimental and calculated 4f $\rightarrow$ 5d transition energies, we conclude that, in SrAl$_2$O$_4$:Ce$^{3+}$, the dopant Ce$^{3+}$ prefers to occupy the slightly smaller Sr2 site, rather than the larger Sr1 site as proposed earlier. Furthermore, by using an established linear relationship between the lowest 4f $\rightarrow$ 5d transition energies of Ce$^{3+}$ and Eu$^{2+}$ located at the same site of a given compound, we find that, in SrAl$_2$O$_4$:Eu$^{2+}$, the dominant green emission observed at room temperature arises from Eu$^{2+}$ located at the Sr2 site of SrAl$_2$O$_4$.

主题: Density functional theory (主要); Calculations; Europium; Europium compounds; Excited states; Solid state reactions; Temperature; Wave functions

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Combined Experimental and ab Initio Study of Site Preference of Ce$^{3+}$ in SrAl$_2$O$_4$

通讯作者: Ning, Lixin Center for Nano Science and Technology, Department of Physics, Anhui Normal University, 241000, China.

摘要语言: English

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第一个可用: 2015-08-30
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An amplified electrochemical aptasensor based on hybridization chain reactions and catalysis of silver nanoclusters

作者: Chen, Ling 1; Sha, Liang 1; Qiu, Yuwei 1; Wang, Guangfeng 1; Jiang, Hong 1; Zhang, Xiaojun 1 1 Key Laboratory of Chem-Biosensing, Anhui Province, College of Chemistry and Materials Science, Anhui Normal University, 241000, China, State Key Laboratory of Chemo/Biosensing and Chemometrics, Hunan University, 410082, China wangyuz@mail.ahnu.edu.cn; xjzhang@mail.ahnu.edu.cn

出版信息: Nanoscale 7.7 (Jan 1, 2015): 3300-3308.

摘要 (English): In the present study, based on the mimic oxidase catalytic character of nucleic-acid-stabilized silver nanoclusters (DNA/AgNCs) and hybridization chain reactions for signal amplification, the fabrication of a label-free sensitive "turn-on" electrochemical aptasensor for the amplified determination of lysozyme was demonstrated. First, the designed DNA duplex was modified on the electrode. With the specific binding of the target, lysozyme and its aptamer, the lysozyme-binding DNA sequence was liberated, exposing the induced DNA sequence, which in turn triggered the formation of the supersandwich DNA structure. Because the cytosine-rich sequence was designed ingeniously on the DNA sequence, DNA/AgNCs were formed on the supersandwich DNA structure. The peroxidase-like character of DNA/AgNCs produced detectable electrochemical signals for the lysozyme aptasensor, which showed a satisfying sensitive detection of lysozyme with a low detection limit of 42 pM and a wide linear range of 10^{-10} M to 10^{-5} M.

主题: DNA (主要); Chains; DNA sequences; Enzymes; Nanoclusters; Nucleic acids; Signal detection; Silver

分类: 461.2: Biological Materials; 547.1: Precious Metals; 602.1: Mechanical Drives; 716.1: Information and Communication Theory; 761: Nanotechnology; 804.1: Organic Compounds; 933: Solid State Physics

标识符 (关键字): Electrochemical aptasensor, Electrochemical signals, Hybridization chain reactions, Low detection limit, Sensitive detection, Signal amplifications, Silver nanoclusters, Wide-linear range

主题: An amplified electrochemical aptasensor based on hybridization chain reactions and catalysis of silver nanoclusters

通讯作者: Wang, Guangfeng Key Laboratory of Chem-Biosensing, Anhui Province, College of Chemistry and Materials Science, Anhui Normal University, 241000, China.

语言: 英文

摘要语言: English

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High gas-sensor and supercapacitor performance of porous Co$_3$O$_4$ ultrathin nanosheets

Authors: Wang, Xiuhua 1; Yao, Shangwu 1; Wu, Xiaoxiu 1; Shi, Zhijie 1; Sun, Hongxia 1; Que, Ronghui 1 1
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Abstract (English): Highly porous Co$_3$O$_4$ ultrathin nanosheets were synthesized by a facile two-step approach, including a hydrothermal technique without any surfactant and subsequent calcination of the precursor. The as-synthesized materials belonged to the cubic spinel Co$_3$O$_4$ phase according to X-ray diffraction and transmission electron microscopy; and Brunauer-Emmett-Teller measurements showed that the surface area was about 97.2 m$^2$ g$^{-1}$. Owing to the unique porous ultrathin structural features, the pseudocapacitor capacitance of porous nanosheets was as high as 378 F g$^{-1}$ at a current density of 1 A g$^{-1}$, and the cycling stability remained about 78.5% after 2000 cycles. In addition, the porous Co$_3$O$_4$ ultrathin nanosheets based sensor exhibited good sensitivity and selectivity to ethanol. These results demonstrated that the porous Co$_3$O$_4$ ultrathin nanosheets were excellent candidates for electrochemical supercapacitor devices and ideal gas-sensor to ethanol. This journal is
Luminescence energy transfer detection of PSA in red region based on Mn\textsuperscript{2+}-enhanced NaYF\textsubscript{4}:Yb, Er upconversion nanorods

**Authors:** Zhang, Jianguo 1; Wang, Shaozhen 1; Gao, Ni 1; Feng, Dexiang 1; Wang, Lun 1; Chen, Hongqi 1 1

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**Abstract (English):** A new turn-on luminescence energy transfer (LET) system has been designed for the detection of prostate specific antigen (PSA, a cancer marker) that utilizes Mn\textsuperscript{2+}-enhanced long wavelength luminescence NaYF\textsubscript{4}:Yb, Er upconversion nanorods as the donor and gold nanorods as the acceptor. The Mn\textsuperscript{2+}-doped NaYF\textsubscript{4}:Yb,Er upconversion luminescence nanorods with an emission peak located in the red region were synthesized. The presence of Mn\textsuperscript{2+} markedly increased the luminescence intensity over that of the NaYF\textsubscript{4}:Yb, Er upconversion nanomaterials (excited by a 980nm continuous wavelength laser). The surfaces of Mn\textsuperscript{2+}-doped NaYF\textsubscript{4}:Yb, Er upconversion nanorods were modified with poly(acrylic acid). Antibodies against prostate specific antigen were bound to the surface of the carboxyl-functionalized upconversion nanorods, which acted as the energy donor in this LET system. Gold nanorods with an absorption band at ~666nm were synthesized by the seed growth method, acted as the energy acceptor. The emission band of the upconversion nanorods overlapped well with the absorption band of the gold nanorods. The luminescence was quenched because of the electrostatic interactions that shortened the distance between the donor (negatively charged) and the acceptor (positively charged). When the PSA antigen was added into the system, the energy acceptor and the energy donors were separated because the binding affinity between PSA and anti-PSA was greater than the electrostatic interactions, and thereby the luminescence was recovered. The linear range of detecting PSA was from 0.1172 to 18.75ng/mL (R=0.995), with a limit of detection for PSA as low as 0.1129ng/mL. The method was successfully applied to the sensing of PSA in human serum samples.
标题: Luminescence energy transfer detection of PSA in red region based on Mn²⁺-enhanced NaYF₄:Yb, Er upconversion nanorods

通讯作者: Wang, Lun Anhui Key Laboratory of Chemo-Biosensing, Key Laboratory of Functional Molecular Solids, Ministry of Education, College of Chemistry and Materials Science, Anhui Normal University, 241000, China.

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Fabrication of nanogap film for electronic DNA sensing by sandwich hybridization

作者: Gu, Cuiping 1 ; Guan, Wenmei 1 ; Huang, Huanhuan 1 ; Shim, Jae-Jin 2 ; Huang, Jiarui 2 1 College of Chemistry and Materials Science, Center for Nano Science and Technology, Anhui Normal University, 241000, China 2 School of Chemical Engineering, Yeungnam University, 712749, South Korea jjshim@yu.ac.kr ; jrhuang@mail.ahnu.edu.cn


摘要 (English): A sandwich hybridization process was applied to the fabrication of gold nanoparticle nanogap films and the electronic detection of DNA. The gold nanoparticle nanogap films were formed via a first step hybridization reaction and the distance between the neighboring gold nanoparticles was generally less than the length of probe DNA. The target DNA was detected via the second hybridization reaction by measuring the different current voltage curves before and after hybridization. The electronic DNA biosensor showed high sensitivity and good selectivity. These results suggest that the present approach is a very effective method for fabricating gold nanoparticle nanogap films and the detection of DNA.

主题: DNA (主要); Fiber optic sensors; Gold; Metal nanoparticles; Nanoparticles; Nanostructures

分类: 461.2: Biological Materials; 547.1: Precious Metals; 732.2: Control Instrumentation; 761: Nanotechnology


标题: Fabrication of nanogap film for electronic DNA sensing by sandwich hybridization

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语言: 英文

摘要语言: English

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Nonclassical properties of nonlocal coherent photon-added two-mode squeezed thermal states

作者: Wang, Zhongjie 1; Fang, Xu 1 1 College of Physics and Electronic Information, Anhui Normal University, 241000, China wuliwzj@mail.ahnu.edu.cn


摘要 (English):  We investigate theoretically the nonclassical properties of the nonlocal coherent two-mode photon-added squeezed thermal state such as cross correlation function, antibunching effect, and inseparability. The results show the excitation number has significant effect on these properties. The cross anticorrelation effect will strengthen with decreasing of the excitation number but the cross correlation effect will weaken with decreasing of the excitation number. The antibunching effect of two-mode optical fields can be observed only if the excitation number S <2. The entanglement between two modes of optical fields can be observed only if s ≤ 2.

主题: Quantum entanglement (主要); Photons

标识符 (关键字): Antibunching effects, Anticorrelation, Cross correlations, Cross-correlation function, Entanglement, Nonclassical properties, Optical field, Squeezed thermal state, Antibunching effect, Cross correlation function

标题: Nonclassical properties of nonlocal coherent photon-added two-mode squeezed thermal states

通讯作者: Wang, Zhongjie College of Physics and Electronic Information, Anhui Normal University, 241000, China.

语言: 英文
Pollution distribution and health risk assessment of heavy metals in indoor dust in Anhui rural, China

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Publication Information: Environmental Monitoring and Assessment 187.9 (Sep 12, 2015)
Zn, Pb, Cu, Cr, V, Ni, Co, and As concentrations of indoor dust in Anhui rural were determined by inductively coupled plasma–optical emission spectroscopy (ICP-OES). The degrees of metal pollution in indoor dust ranked as follows: Zn > Pb > Cr > Cu > V > Ni > Co > As, on average. The arithmetic means of Zn, Pb, Cu, Cr, V, Ni, Co, and As were 427.17, 348.73, 107.05, 113.68, 52.64, 38.93, 10.29, and 4.46 mg/kg, respectively. These were higher than background values of Anhui soil for Zn, Pb, Cu, Cr, and Ni, especially for Pb with the mean value of 13.21 times the background value. Heavy metal concentrations of indoor dust were different from different rural areas. House type (bungalows or storied house), sweeping frequency, and external environment around the house (such as the road grade) affected heavy metal concentrations in indoor dust. The results of factor analysis and correlation analysis indicated that Cu, Cr, Ni, Zn, and Co concentrations were mainly due to interior paint, metal objects, and building materials. Pb and As concentrations were due to vehicle emissions. V concentration was mainly of natural source. Average daily doses for the exposure pathway of the studied heavy metals decreased in children in the following order: hand-to-mouth ingestion > dermal contact > inhalation. The non-carcinogenic risks of heavy metals ranked as Pb > V > Cr > Cu > Zn > As > Ni, and the carcinogenic risks of metals decreased in the order of Cr > Co > As > Ni. The non-carcinogenic hazard indexes and carcinogenic risks of metals in indoor dust were both lower than the safe values.
Hydrogen Activation on the Promoted and Unpromoted ReS$_2$(001) Surfaces under the Sulfidation Conditions: A First-Principles Study

作者: Huang, Yucheng 1 ; Liu, Hai 1 ; Ling, Chongyi 1 ; Chen, Xi 1 ; Zhou, Danmei 1 ; Wang, Sufan 1 1 Center for Nano Science and Technology, College of Chemistry and Material Science, Key Laboratory of Functional Molecular Solids, Ministry of Education, Anhui Laboratory of Molecule-Based Materials, Anhui Normal University, 241000, China huangyc@mail.ahnu.edu.cn


摘要 (English): Hydrogen activation on the promoted and promoter-free ReS$_2$(001) surfaces under the sulfidation conditions is studied by means of periodic density function theory (DFT) calculations within the generalized gradient approximation. First, surface-phase diagrams are investigated by plotting the surface free energy as a function of the chemical potential of S ($\mu_S$) on the unpromoted and promoted ReS$_2$(001) surfaces with different loadings of nickel, cobalt, tungsten, and tantalum. The results show that on the unpromoted surface sulfur coverage of 25% and on the promoted surfaces sulfur coverage of 25% as well as 25% promoter modification are the most stable conditions, respectively, under hydrodesulfurization (HDS) reaction conditions. Second, hydrogen adsorption and dissociation are explored on these preferred surfaces. It is found that hydrogen adsorbs weakly on all the surfaces studied. The physical adsorption character makes its diffusion
favorable, resulting in various adsorption sites and dissociation pathways, i.e., dissociation at surface Re or promote atom, at the interlayer, as well as at the adsorbed S atom. Calculated results show that hydrogen dissociation at the surface Re site is always kinetically favorable. All of the studied dopants can largely activate the adsorbed S but display distinct roles toward the activity of the nearest Re atom; i.e., Co/Ni dopant passivates the nearest surface Re while W/Ta activates it. The activity difference is found to be closely associated with the difference in the bond strength of metal-S and the resultant difference in the induced surface geometry. Moreover, promoter effect is localized because it seems nominal when the reaction occurs at a Re atom with one dopant atom separation. The present results provide a rational understanding of the activity difference between the promoter-free and the promoted surfaces, which would be helpful to further understand the mechanism of HDS and to enhance the development of highly active and selective hydrotreating catalysts.
Au/Pt co-loaded ultrathin TiO$_2$ nanosheets for photocatalyzed H$_2$ evolution by the synergistic effect of plasmonic enhancement and co-catalysis

**Authors:** Chen, Changyu 1; Kuai, Long 1; Chen, Yanjun 1; Wang, Qing 1; Kan, Erjie 1; Geng, Baoyou 1 1
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**Publication Information:** RSC Advances 5.119 (Jan 1, 2015): 98254-98259.

**Abstract (English):** Co-catalysis and plasmonic enhancement are two efficient ways to improve the photocatalytic performance of semiconductors. In this work, we systematically investigate their synergistic functions by photo-depositing Au and Pt nanoparticles on the surface of ultrathin TiO$_2$ nanosheets, where Au stimulates the plasmonic effect and Pt acts as the co-catalyst. It was found that both Au and Pt deposition can increase the H$_2$ production rate. More importantly, faster H$_2$ production can be obtained with the co-loading of Au and Pt. Furthermore, a suitable Au loading was important for the photocatalytic performance. As a consequence, the highest H$_2$ rate of 7.19 mmol g$^{-1}$ h$^{-1}$ was achieved by depositing 0.75% Pt and 0.5% Au on TiO$_2$. Therefore, this work presents the synergistic effect between the plasmonic enhancement of Au and the co-catalysis of Pt for photocatalytic H$_2$ production, which contributes some guidance to catalyst design and preparation.

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**Themes:** Gold (主要); Catalysis; Catalysts; Nanosheets; Plasmons; Platinum; Titanium dioxide

**Classification:** 547.1: Precious Metals; 761: Nanotechnology; 802.2: Chemical Reactions; 803: Chemical Agents and Basic Industrial Chemicals; 804: Chemical Products Generally; 804.2: Inorganic Compounds; 931.3: Atomic and Molecular Physics; 933: Solid State Physics
Au/Pt co-loaded ultrathin TiO$_2$ nanosheets for photocatalyzed H$_2$ evolution by the synergistic effect of plasmonic enhancement and co-catalysis.

通讯作者: Geng, Baoyou Center for Nano Science and Technology, College of Chemistry and Materials Science, Key Laboratory of Functional Molecular Solids, Ministry of Education, Anhui Laboratory of Molecular-Based Materials, Anhui Normal University, 241000, China.
Low cost visible light driven plasmonic Ag-AgBr/BiVO$_4$ system: Fabrication and application as an efficient photocatalyst

**Authors:** Sang, Yan 1 ; Huang, Yan 2 ; Wang, Wu 1 ; Fang, Zhen 1 ; Geng, Baoyou 1 1 Anhui Laboratory of Molecular-Based Materials, Ministry of Education, Anhui Normal University, 241000, China 2 Library of Anhui Normal University, 241000, China

**Publication Information:** RSC Advances 5.50 (Jan 1, 2015): 39651-39656.

**Abstract (English):** In this work, visible light driven plasmonic photocatalyst, Ag-AgBr/BiVO$_4$ nanostructures have been facilely prepared by a hydrothermal process, the deposition precipitation method with surfactant and subsequent light driven route. As a low cost and efficient visible light driven photocatalyst, BiVO$_4$ is chosen as an ideal support. Cetyltrimethylammonium bromide (CTAB) was used as both of the surfactant, template directing reagent and the Br source. The obtained Ag-AgBr/BiVO$_4$ photocatalyst shows excellent visible light driven photocatalytic performance. It can decompose Rhodamine B (RhB) within 16 min under visible light irradiation. Meanwhile, compared with other VLD (visible light driven) photocatalysts such as Ag-AgBr, Ag-TiO$_2$ and AgBr-Ag-TiO$_2$ composite, the amount of Ag needed as well as the cost decrease significantly. Moreover, the possible photocatalytic mechanism of the Ag-AgBr/BiVO$_4$ nanostructures was investigated.

**Themes:** Light (主要); Costs; Nanostructures; Photocatalysts; Photodegradation; Plasmons; Precipitation (chemical); Silver; Silver alloys; Silver halides; Surface active agents

**Classification:** 547.1: Precious Metals; 712.1: Semiconducting Materials; 741.1: Light and Optics; 761: Nanotechnology; 802.3: Chemical Operations; 803: Chemical Agents and Basic Industrial Chemicals; 804: Chemical Products Generally; 911: Cost and Value Engineering; Industrial Economics; 933: Solid State Physics

**Keywords:** Cetyltrimethylammonium bromide, Deposition precipitation methods, Hydrothermal process, Photocatalytic performance, Plasmonic photocatalysts, Visible light driven photocatalysts, Visible-light irradiation, Visible-light-driven

**Title:** Low cost visible light driven plasmonic Ag-AgBr/BiVO$_4$ system: Fabrication and application as an efficient photocatalyst

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**Language:** English

**Document Type:** Article

**Publication Name:** RSC Advances

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Preparation, crystal structures and properties of zinc complexes containing Bis(oxazoline) ligand

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**Abstract (English):** Three zinc complexes \(\text{[(DMOX)}\text{ZnX}_2\text{]}\), \(X = \text{Cl} (1), \text{Br} (2) \text{or} \text{I} (3))\), where DMOX is 4,5-dihydro-2-(4,5-dihydro-4,4-dimethylloxazol-2-yl)-4,4-dimethylloxazole), have been fully characterized by single crystal X-ray diffraction, UV-vis, NMR and IR spectroscopy. Moreover, all zinc complexes showed activities in catalyzing hydrolysis of 4-nitrophenyl acetate (4-NA). And active species have been determined by pH titrations of \(\text{[(DMOX)}\text{ZnI}_2\text{]}\) in catalyzing hydrolysis of 4-NA.
Preparation, crystal structures and properties of zinc complexes containing Bis(oxazoline) ligand.

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Copper-Catalyzed Electrophilic Amination of Organoaluminum Nucleophiles with O-Benzoyl Hydroxylamines

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摘要 (English): A copper-catalyzed electrophilic amination of aryl and heteroaryl aluminums with N,N-dialkyl-O-benzoyl hydroxylamines that affords the corresponding anilines in good yields has been developed. The catalytic reaction proceeds very smoothly under mild conditions and exhibits good substrate scope. Moreover, the developed catalytic system is also well suited for heteroaryl aluminum nucleophiles, providing facile access to heteroarylamines.

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主题: Amines (主要); Aluminum; Catalysis; Copper; Nucleophiles

分类: 541.1: Aluminum; 544.1: Copper; 802.2: Chemical Reactions; 803: Chemical Agents and Basic Industrial Chemicals; 804.1: Organic Compounds

标识符 (关键字): Catalytic reactions, Catalytic system, Copper catalyzed, Electrophilic amination, Facile access

标题: Copper-Catalyzed Electrophilic Amination of Organoaluminum Nucleophiles with O-Benzoyl Hydroxylamines

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SnS\textsubscript{2} nanosheet-based microstructures with high adsorption capabilities and visible light photocatalytic activities

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**Publication Information:** RSC Advances 5.31 (Jan 1, 2015): 24640-24648.

**Abstract (English):** The engineering of semiconductors with high adsorption and visible light-driven photocatalytic activity is of growing interest in the removal of environmental pollutants. Herein, SnS\textsubscript{2} nanosheet-based microstructures of flower-like, nanosheet-like, nest-like and nanoplate-like morphologies with high adsorption capacities and visible light photocatalytic activities were experimentally achieved by a facile solution-phase approach based on a simple reaction of SnCl\textsubscript{4}·5H\textsubscript{2}O and three hydration sodium diethyldithiocarbamate (C\textsubscript{5}H\textsubscript{10}NS\textsubscript{2}Na·3H\textsubscript{2}O) in a solvent of ethylene glycol with or without the addition of acetic acid, where C\textsubscript{5}H\textsubscript{10}NS\textsubscript{2}Na·3H\textsubscript{2}O served as both a sulfur source and a coordination agent. The negatively charged nature of the as-prepared SnS\textsubscript{2} products is responsible for the superior absorptive and visible light photocatalytic performances of cationic dyes. The revelation of the charged nature of the surface of SnS\textsubscript{2} nanosheet-based microstructures leads to a
new possibility for the design of adsorptive photocatalysts.

主题: Light (主要); Adsorption; Coordination reactions; Ethylene; Ethylene glycol; Microstructure; Nanosheets; Organic solvents; Photocatalysis; Photocatalysts


标题: SnS$_2$ nanosheet-based microstructures with high adsorption capabilities and visible light photocatalytic activities

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摘要语言: English

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文档 URL: [http://search.proquest.com/professional/docview/1665002069?accountid=131175](http://search.proquest.com/professional/docview/1665002069?accountid=131175)
Photoinduced electron transfer (PET) based label-free aptasensor for platelet-derived growth factor-BB and its logic gate application

作者: Wang, Guangfeng 1 ; Zhu, Yanhong 2 ; Chen, Ling 2 ; Zhang, Xiaojun 1 1 Anhui Key Laboratory of Chem-Biosensing, College of Chemistry and Materials Science, Center for Nanoscience and Nanotechnology, Anhui Normal University, Wuhu 241000, China, State Key Laboratory of Chemo/Biosensing and Chemometrics, Hunan University, Changsha 410082, China wangyuz@mail.ahnu.edu.cn ; xjzhang@mail.ahnu.edu.cn 2 Anhui Key Laboratory of Chem-Biosensing, College of Chemistry and Materials Science, Center for Nanoscience and Nanotechnology, Anhui Normal University, Wuhu 241000, China


摘要 (English): Platelet-derived growth factor-BB (PDGF-BB) is often overexpressed in human malignant tumors as an indicator for tumor angiogenesis. Here by the photoinduced electron transfer (PET) between DNA-Ag fluorescent nanoclusters (NCs) and G-quadruplex/hemin complexes, we present a sensitive label-free fluorescent sensor for PDGF-BB. In the presence of PDGF-BB, the specific conjugation with its aptamer induced the conformational change of the duplex-like DNA sequence, releasing the G-quadruplex sequence part. Then in the presence of hemin and K+, the horseradish peroxidase mimicking DNAzyme (HRP-DNAzyme) was formed. With the electron transfer between the DNA-Ag NCs to the hemin Fe (III) center of HRP-DNAzyme, the PET occurred with a decrease in the fluorescence intensity of the DNA-Ag NCs. The detection performance such as selectivity, linear dynamic range, sensitivity, and the quenching capability of HRP-DNAzyme were estimated. The detection range for PDGF-BB is from $5 \times 10^{-13}$ to $1 \times 10^{-8}$ M and the detection limit is $1 \times 10^{-13}$ M. The experimental results confirmed that the novel fluorescent aptasensor possessed a good sensitivity and high selectivity for PDGF-BB. In addition, the developed probe is nontoxic, label-free only involving one-step hybridization without sophisticated fabrication process. Furthermore, based on this quenching mode occurred by PDGF-BB and hemin, using PDGF-BB and hemin as inputs and the fluorescence signal as an output, a logic gate has been fabricated. © 2014 Elsevier B.V.

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主题: Quenching (主要); DNA; Electron transitions; Fluorescence; Logic gates; Nanoclusters; Platelets; Silver; Tumors


标识符 (关键字): Fluorescence intensities, Fluorescent nanoclusters, Hemin/G-quadruplex complex, Horseradish peroxidase, Pdgf bb's, Photo-induced electron transfer, Silver nanoclusters, Specific conjugations, Logic gate, PDGF-BB, Photoinduced electron transfer
Technologies for detecting data conflicts in distributed situation
Data conflicts are one of the key problems in a distributed situation. When the data of the database is divided horizontally or vertically and are distributed across different nodes, the test data will be faced with greater challenges of conflict which often need to move data from one site to another site. In this paper, an algorithm for detecting conditional functional dependencies conflicts in distributed database is presented which not only can detect the conflicts of conditional functional dependencies in horizontally divided data, but also reduce effectively the data transmission. Experimental results demonstrated that the algorithms are effective.
Tandem Regioselective Substitution and Palladium-Catalyzed Ring Fusion Reaction for Core-Expanded Boron Dipyrromethenes with Red-Shifted Absorption and Intense Fluorescence

作者: Zhou, Xin 1 ; Wu, Qinghua 1 ; Feng, Yuanmei 1 ; Yu, Yang 1 ; Yu, Changjiang 1 ; Hao, Erhong 1 ; Wei, Yun 1 ; Mu, Xiaolong 1 ; Jiao, Lijuan 1 1 Key Laboratory of Functional Molecular Solids, Ministry of Education, School of Chemistry and Materials Science, Anhui Normal University, 241000, China jiao421@mail.ahnu.edu.cn


摘要 (English): A selective method for the core-extension of boron dipyrromethene (BODIPY) with two annulated indole rings with exclusive syn-connectivity is reported. The method is based on a regioselective nucleophilic substitution reaction of 2,3,5,6-tetrabromoBODIPY with aryl amines, followed by palladium-catalyzed intramolecular C-C coupling ring fusion. The unsymmetrical core-expanded BODIPY with annulated indole and benzofuran rings was also synthesized by stepwise and regioselective nucleophilic substitution and palladium-catalyzed intramolecular C-C coupling reaction. The diindole-annulated BODIPY was unambiguously characterized by single-crystal X-ray analysis. The optical properties of the present core-expanded BODIPYs were studied, revealing clearly red-shifted absorption and emission bands and enhanced absorption coefficients upon annulation. Green to Red: Regioselective tetrabromination and nucleophilic substitution reactions of boron dipyrromethene (BODIPY) and aryl amines followed by palladium-catalyzed ring fusion extends the BODIPY core by two annulated indole rings with exclusive syn-connectivity. These core-expanded BODIPYs show clearly red-shifted absorption and emission bands and enhanced absorption coefficients.
Synthesis of thermo- and pH-responsive Ag nanoparticle-embedded hybrid microgels and their catalytic activity in methylene blue reduction

Authors: Tang, Yecang 1; Wu, Ting 1; Hu, Botao 1; Yang, Qian 1; Liu, Li 1; Yu, Bo 1; Ding, Yi 1; Ye, Shiyong 1

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Publication Information: Materials Chemistry and Physics 149 (Jan 1, 2015): 460-466.

Abstract (English): Ag nanoparticles (AgNPs)-containing hybrid microgels were prepared by in situ reduction of Ag⁺ ions pre-dispersed in copolymer microgels of poly (N-isopropylacrylamide-co-2-(dimethylamino)ethyl methacrylate) (P(NIPAM-co-DMA)). The prepared hybrid microgels possess excellent thermo- and pH-responsive properties and exhibit a responsive swelling and shrinking behavior. The increase in pH can induce a decrease in the absorption intensity and a blue shift of the surface plasmon band of AgNPs, which is attributed to a reduction in the polarity of AgNPs surroundings as a result of the conformational change of PDMA segments. Furthermore, the hybrid microgel was found to be an active catalyst for the reduction of methylene blue by NaBH₄ in aqueous solution. The effects of temperature and the amount of catalyst on the reduction rate were investigated using UV-vis spectrophotometry. Kinetic studies indicate that the apparent reaction rate constant kₚ follows the typical Arrhenius-type dependence on temperature in the range of 25 ~ 40 °C and the activation energy is 62.0 kJ mol⁻¹. The AgNPs embedded in hybrid microgels show good thermal and chemical stability and the catalytic activity remains unchanged after storage for 40 days at room temperature. Such hybrid microgels, with the merits of good thermal and chemical stability as well as the catalytic activity, have a potential application in the field of heterogenous catalysis.

Theme: Catalyst activity (主要); Acrylic monomers; Activation energy; Aromatic compounds; Chemical stability; Composite materials; Gels; Nanoparticles; Nanostructures; pH; Polymers; Rate constants; Silver; Surface properties; Synthesis (chemical); Temperature

Identification (Keywords): Absorption intensity, Conformational change, Effects of temperature, Heterogenous catalysis, N-isopropylacrylamide, Surface plasmon band, Thermal and chemical stabilities, UV-vis spectrophotometry

Title: Synthesis of thermo- and pH-responsive Ag nanoparticle-embedded hybrid microgels and their catalytic activity in methylene blue reduction

Corresponding Author: Tang, Yecang Key Laboratory of Functional Molecular Solids, Anhui Normal University, Ministry of Education, 241000, China.

Language: English

Abstract Language: English

Document Type: Article

Publication Name: Materials Chemistry and Physics
Colorimetric detection of dopamine based on silver nanoparticles

作者: Feng, Juanjuan 1; Zhao, Yiman 1; Wang, Haiyan 1 1 Anhui Key Laboratory of Chemo-Biosensing, College of Chemistry and Materials Science, Anhui Normal University, 241000, China
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摘要 (English): A simple and sensitive colorimetric method for the detection of dopamine was proposed based on the redox reaction between silver ion and dopamine, which was catalyzed by silver nanoparticles (AgNPs), causing the color change. The increase of dopamine concentration led to red shift of absorption peak and increase of the absorbance. Meanwhile, the color of the solution changed from pale yellow and deep yellow. Under optimal conditions, a linear range of 0.05-16 μmol/L between the absorbance and dopamine concentration and a detection limit of 0.04 μmol/L was obtained. The proposed method was sensitive, simple, low-cost and selective, which could be applied for the detection of dopamine in human serum.
Compressed sensing based on doubly-selective slow-fading channel estimation in OFDM systems

作者: Ye, Xin-Rong 1; Zhu, Wei-Ping 2; Zhang, Ai-Qing 1; Meng, Qing-Min 2 1 Institute of Signal Processing and Transmission, Nanjing University of Posts and Telecommunications, 210003, China, The College of Physics and Electronic Information, Anhui Normal University, 241000, China 20100126@njupt.edu.cn 2 Institute of Signal Processing and Transmission, Nanjing University of Posts and Telecommunications, 210003, China


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摘要 (English): In order to improve the reconstruction accuracy of smoothed $\ell_0$-norm ($S\ell_0$) algorithm in the presence of noise, a modified algorithm named smoothed $\ell_0$-norm regularized least-square ($\ell_2$-$S\ell_0$) is proposed in this paper, which permits a small perturbation. Further, through placing a finite grid in the planar time-frequency bounded region, the problem of doubly-selective slow-fading channel estimation in OFDM system is modeled as the problem of sparse signal reconstruction in compressed sensing framework, and then the $\ell_2$-$S\ell$ algorithm is applied to reconstruct the channel parameters. A number of computer-simulation-based experiments show that reconstruction accuracy of the $\ell_2$-$S\ell$ algorithm is improved by approximately 10 dB as compared with the $0\ S\ell$ algorithm in the presence of noise. The performance of the proposed doubly-selective slow-fading channel estimation method using $\ell_2$-$S\ell$ algorithm is nearly close to that of the ideal Least Square (ideal-LS) method. Moreover, the proposed method has higher estimation accuracy well in the case of low SNR.

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主题: Frequency selective fading (主要); Algorithms; Channel capacity; Channel estimation; Compressed sensing; Fading channels; Frequency estimation; Least squares approximations; Multiuser detection; Orthogonal frequency division multiplexing; Signal reconstruction; Signal to noise ratio


标识符 (关键字): Channel parameter, Modified algorithms, Reconstruction accuracy, Regularized least squares, Slow fading channel, Slow-time, Small perturbations, Sparse signal reconstruction, OFDM, Slow time-varying channel

标题: Compressed sensing based on doubly-selective slow-fading channel estimation in OFDM systems

通讯作者: Ye, Xin-Rong Institute of Signal Processing and Transmission, Nanjing University of Posts and Telecommunications, 210003, China.
A standardized design methodology for complex digital logic components of cyber-physical systems

Authors: Chen, F. 1 ; Ye, H. 1 ; Yang, J. 1 ; Huang, Y. 2 ; Zhang, J. 3 ; Qi, X. 1 ; Zhao, C. 1 ; Zhu, J. 1 ; Zhou, W. 4
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As an important part of cyber-physical systems, the digital logic system's complexity are rapidly increasing, and its design flows become more and more tedious. A modeling and verification methodology for complex digital logic components is presented to improve the development quality and efficiency. In order to help developer to understand the design intent preferably and speed up the development process, design activities are carried out under a convenient modeling methodology and a precise verification solution for completing the design cycle. Its calculus system offers a theoretic way to connect components via connectors, and then provides a theoretical basis for further verification. A washing machine controller design shows that the modeling can reflect the design intent of the designers effectively, detect some design errors which maybe result in modeling failures in implementation as soon as possible, and avoid the negligence and errors in modeling for complex digital systems.

A standardized design methodology for complex digital logic components of cyber-physical systems

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Revised
β-cyclodextrin functionalized CdTe quantum dots for electrochemiluminescent detection of benzo[a]pyrene

作者: Yang, Miao 1 ; Wang, Yan 1 ; Wang, Haiyan 1 Anhui Key Laboratory of Chemo-biosensing, College of Chemistry Materials Science, Anhui Normal University, 241000, China hywang@mail.ahnu.edu.cn


摘要 (English): β-cyclodextrin (β-CD) functionalized CdTe quantum dots (QDs) were prepared with β-CD and mercaptopropionic acid (MPA) as the stabilizers (denoted as β-CD-MPA-CdTe). The QDs capped with the dual stabilizers, β-CD and MPA, not only showed improved electrochemiluminescence (ECL) efficiency and higher ECL intensity due to the effective removal of the nonradiative surface state and deep surface trap of the QDs, but also exhibited selective response toward benzo[a]pyrene (BaP) as a consequence of specific host-guest interaction between the β-CD and BaP, resulting in decreased ECL of the QDs. On the basis of the quenching effect of BaP on the ECL of β-CD-MPA-CdTe QDs, a sensitive and selective method for the determination of BaP was developed. Under optimal conditions, a linear range from 87 pM to 10 nM with a detection limit of 29 pM (S/N = 3) was obtained for the detection of BaP.

主题: Semiconductor quantum dots (主要); Cadmium telluride; Charge trapping; Cyclodextrins; Nanocrystals; Pyrene


标识符 (关键字): Benzo [a] pyrene, CdTe quantum dots, Cdtue quantum dots (QDs), Electrochemiluminescence, Electrochemiluminescent, Host guest interactions, Mercaptopropionic acid, Selective response, Benzo[a]pyrene, β-cyclodextrin

标题: β-cyclodextrin functionalized CdTe quantum dots for electrochemiluminescent detection of benzo[a]pyrene

通讯作者: Wang, Haiyan Anhui Key Laboratory of Chemo-biosensing, College of Chemistry Materials Science, Anhui Normal University, 241000, China.
One-pot preparation of Au-RGO/PDDA nanocomposites and their application for nitrite sensing

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Sensors and Actuators, B: Chemical 208 (Mar 1, 2015): 36-42.
In this paper, we demonstrate that Au-reduced graphene oxide/PDDA nanocomposites (Au-RGO/PDDA) can be rapidly synthesized through a facile, cost-effective, one-pot method with the use of poly(diallyldimethylammonium chloride) (PDDA) as both reducing and stabilizing agents. The prepared Au-RGO/PDDA nanocomposites film endowed the modified electrode fast electron transfer rate and high electrocatalytic activity toward nitrite oxidation. Under the optimal conditions, the oxidation current increased linearly with increasing the concentration of nitrite in the range 0.05-8.5 μM with the correlation coefficient of 0.9964 and the detection limit of 0.04 μM at a ratio of signal to noise of 3 using differential pulse voltammograms (DPV). The presented sensor was also demonstrated for the determination of nitrite ion in lake water, meat and dairy products samples with satisfactory results.

Title: One-pot preparation of Au-RGO/PDDA nanocomposites and their application for nitrite sensing

Author: Wang, Lun Anhui Key Laboratory of Chemo/Biosensing, College of Chemistry and Materials Science, Anhui Normal University, 241000, China.

Language: English

DOI: http://dx.doi.org/10.1016/j.snb.2014.11.020

PII: S0925400514013902
Unusual spectroscopic and photophysical properties of meso-tert-butylBODIPY in comparison to related alkylated BODIPY dyes

作者: Jiao, Lijuan 1; Yu, Changjiang 1; Wang, Jun 1; Briggs, Edward A. 2; Besley, Nicholas A. 2; Robinson, David 2; Ruedas-Rama, María J. 3; Orte, Angel 3; Crovetto, Luis 3; Talavera, Eva M. 3; Alvarez-Pez, Jose M. 3; Van Der Auweraer, Mark 4; Boens, Noël 4 1 Laboratory of Functional Molecular Solids, Ministry of Education, Anhui Laboratory of Molecule-Based Materials, School of Chemistry and Materials Science, Anhui Normal University, 241000, China jiao421@mail.ahnu.edu.cn 2 School of Chemistry, University of Nottingham, University Park, NG7 2RD, United Kingdom 3 Department of Physical Chemistry, Faculty of Pharmacy, University of Granada, Cartuja Campus, 18701, Spain 4 Department of Chemistry, Katholieke Universiteit Leuven (KU Leuven), Celestijnenlaan 200f, 3001, Belgium


摘要 (English): Five alkyl-substituted difluoroboron dipyrrin (BODIPY) dyes have been synthesized: three with a methyl, isopropyl or tert-butyl group at the meso-position of the BODIPY core and two substituted with one or two tert-butyl functions at the 3/5-positions. X-Ray structural analysis, UV-vis absorption spectroscopy and fluorescence (steady-state and time-resolved) techniques have been used to study the structures and the spectroscopic/photophysical properties of these dyes. All but one of these BODIPYs are highly fluorescent in all the solvents tested, the exception being meso-tert-butylBODIPY (2). Derivative 2 differs from the other alkylated boron dipyrrins as it exhibits a broad and red-shifted fluorescence band with a large Stokes shift. In addition, very low fluorescence quantum yields and short fluorescence lifetimes characterize 2. Quantum chemical calculations indicate that 2 has a distorted, nonplanar geometry in the S_1 excited state due to the rotation of 8-tert-butyl group. Our results lead us to the conclusion that the torsional rotation about the bond connecting the meso-C and the quatermary C of the tert-butyl group of 2 plays a crucial role in the fast radiationless deactivation of this isomer.

链接: Check for full text via 360 Link, Order Full Text from Infotrieve?
Reduced graphene oxide modified flower-like BiOCOOH architectures with enhanced photocatalytic activity

作者: Xia, Shan-Hui 1 ; Dong, Chao 1 ; Wei, Xian-Wen 1 ; Wang, Jing 1 ; Wu, Kong-Lin 1 ; Hu, Yu 1 ; Ye, Yin 1

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摘要 (English): A series of reduced graphene oxide - flower-like BiOCOOH (RGO-BiOCOOH) composites with different weight addition ratios of reduced graphene oxide have been prepared for the first time by a two-step solvothermal approach, which showed higher photocatalytic activity than BiOCOOH toward degradation of rhodamine B (RhB) in water under simulated sunlight irradiation. The RGO-BiOCOOH composite with 2 wt% RGO content exhibited the highest photocatalytic degradation efficiency of RhB, which was about 2 times of pure BiOCOOH microflower. The enhanced photocatalytic activity of RGO-BiOCOOH composite could be attributed to the synergetic effects of enhanced adsorption capacity, narrower band gap, and more efficient separation of photogenerated electron-hole pairs and effective interfacial hybridization between RGO and flower-like BiOCOOH architecture.

标签: Bismuth oxides, Interfacial hybridization, Optical materials and properties, Photocatalytic degradation, Photocatalytic activities, Photogenerated electrons, Reduced graphene oxides, Solvothermal approach, Bismuth oxide formate, Reduced graphene oxide, Semiconductors

主题: Graphene (主要); Complexation; Composite films; Composite materials; Degradation; Energy gap; Materials properties; Photocatalysis; Semiconductor materials


链接: Check for full text via 360 Link, Order Full Text from Infotrieve

语言: 英文
摘要语言: English
Ge@C core-shell nanostructures for improved anode rate performance in lithium-ion batteries

作者: Qiang, Tingting; Fang, Jiaxin; Song, Yixuan; Ma, Qiuyang; Ye, Ming; Fang, Zhen; Geng, Baoyou

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出版物信息: RSC Advances 5.22 (Jan 1, 2015): 17070-17075.

摘要 (English): Ge@C core-shell nanostructures were successfully synthesized by a facile n-hexane pyrogenation-reducing process. The Ge@C core-shell nanostructures exhibit excellent cycling performance and
rate capability in comparison with pure Ge nanoparticles when used as an anode material for a lithium ion battery. The thin carbon shell endows the obtained Ge@C nanostructures with a high specific capacity of 985 mA h g⁻¹ at a current density of 500 mA g⁻¹ after 50 cycles. Furthermore, a discharge capacity of 850 mA h g⁻¹ was observed at a current density of 4000 mA g⁻¹. The excellent lithium storage performance can be attributed to the unique carbon shell structure. The carbon shell not only acts as the buffer layer to maintain structural stability during lithiation, but also increases electrical conductivity during the charge/discharge processes. The high rate capacity of the Ge@C nanostructures demonstrates it a promising anode material for high power lithium-ion batteries.

主题: Lithium batteries (主要); Anodes; Carbon; Electric batteries; Electrodes; Germanium; Hexane; Ions; Lithium; Lithium alloys; Lithium compounds; Lithium-ion batteries; Nanostructures; Secondary batteries; Shells (structures); Stability


标识符 (关键字): Core shell nano structures, Cycling performance, Discharge capacities, Electrical conductivity, High specific capacity, High-power lithium-ion batteries, High-rate capacities, Structural stabilities

标题: Ge@C core-shell nanostructures for improved anode rate performance in lithium-ion batteries

通讯作者: Fang, Zhen Key Laboratory of Functional Molecular Solids, Ministry of Education, Anhui Normal University, 241000, China.

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Effects of straw return on C$_2$-C$_5$ non-methane hydrocarbon (NMHC) emissions from agricultural soils

作者: Wang, Ran 1 ; Wu, Ting 2 ; Dai, WanHong 1 ; Liu, Hui 1 ; Zhao, Juan 1 ; Wang, XinMing 3 ; Huang, FeiYu 4 ; Wang, Zhe 1 ; Shi, ChengFei 1 1 College of Environmental Sciences and Engineering, Anhui Normal University, 241000, China 2 College of Environmental Sciences and Engineering, Anhui Normal University, 241000, China, State Key Laboratory of Organic Geochemistry, Guangzhou Institute of Geochemistry, Chinese Academy of Sciences, 510640, China wuting19@mail.ahnu.edu.cn 3 State Key Laboratory of Organic Geochemistry, Guangzhou Institute of Geochemistry, Chinese Academy of Sciences, 510640, China wangxm@gig.ac.cn 4 Huangshan Meteorological Administration Office, 245800, China


摘要 (English): The effect of crop straw return on C$_2$-C$_5$ non-methane hydrocarbon (NMHC) emissions from agricultural soils is investigated using a laboratory-controlled incubation of agricultural soils amended with crop straw for a period of 56 days. The average emission fluxes of total C$_2$-C$_5$ NMHCs from amended agricultural soils are 304 and 173ngkg$^{-1}$h$^{-1}$ under non-flooded and flooded conditions, respectively. Alkenes are the principal emitted C$_2$-C$_5$ NMHCs from amended agricultural soils, where a predominance of ethene, propene and 1-butene together shared 65% and 59% of the total C$_2$-C$_5$ NMHCs under non-flooded and flooded conditions, respectively. The emissions rates of the above top three alkenes and the total C$_2$-C$_5$ alkenes from amended agricultural soils under non-flooded conditions are one to four times those under flooded conditions, and these average values are 14-89 and 5-34 times those in their corresponding control treatments, respectively. These results imply that straw return contributes substantially to the emissions of light alkenes from agricultural soils, particularly under non-flooded conditions. The high correlation between microorganisms and C$_2$-C$_5$ NMHC fluxes from amended agricultural soils suggest that microbes play an important role in C$_2$-C$_5$ NMHC emissions from straw-amended agricultural soils. A rough estimate indicates that crop straw return could contribute insignificantly to global C$_2$-C$_5$ hydrocarbon budgets.
Synthesis of Ni-riched NiO-Co$_3$O$_4$ sheet-like nanocomposites and their application in supercapacitors

作者: Wang, Xian-Wen 1; Wu, Kong-Lin 1; Zhang, Zai-Xian 1; Yue, Yao-Xiang 1; Zhao, Meng-Li 1; Cheng, Juan 1; Wei, Xian-Wen 2 1 College of Chemistry and Materials Science, Key Laboratory of Functional Molecular Solids, Anhui Normal University, 241000, China konglin@mail.ahnu.edu.cn 2 College of Chemistry and Materials Science, Key Laboratory of Functional Molecular Solids, Anhui Normal University, 241000, China, College of Chemical and Engineering, Anhui University of Technology, 243002, China


摘要 (English): In this reported work Ni-riched NiO-Co$_3$O$_4$ sheet-like nanocomposites (SNCs) were obtained through a facile solvothermal method in a mixed solvent and subsequently calcinated in air. Galvanostatic charge-discharge measurement revealed that the Ni-riched NiO-Co$_3$O$_4$ SNCs electrode has an impressive specific capacitance as high as 836 F g$^{-1}$ at 4 A g$^{-1}$ in 3 M KOH solution. The as-obtained Ni-riched NiO-Co$_3$O$_4$ SNCs product showed a weak cycling stability, but the higher capacitance (424 F g$^{-1}$) was retained after 1000 cycles at 4 A g$^{-1}$.

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主题: Nickel (主要); Capacitance; Discharge (fluid mechanics); Meteorites; Nanocomposites


标识符 (关键字): Cycling stability, Galvanostatic charge discharges, KOH solution, Mixed solvent, Sheet-like, Solvothermal method, Specific capacitance, Super capacitor

标题: Synthesis of Ni-riched NiO-Co$_3$O$_4$ sheet-like nanocomposites and their application in supercapacitors

语言: 英文

摘要语言: English

文档类型: Article

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期: 1

分页: 9-11
Three-dimensional focus shaping of partially coherent circularly polarized vortex beams using a binary optic

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出版物信息: Journal of Optics (United Kingdom) 17.6 (Jun 1, 2015).
ProQuest 文档链接

摘要 (English): The three-dimensional (3D) focus shaping technique using the combination of partially coherent circularly polarized vortex beams with a binary diffractive optical element (DOE) is reported. It is found that the intensity distribution near the focus can be tailored in three dimensions by appropriately adjusting the parameters of the incident beams, numerical aperture of the objective lens, and the design of the DOE.
Numerical results show that partially coherent circularly polarized vortex beams can be used to generate several special beam patterns, such as optical chain, optical needle, optical dark channel, flat-topped field, and 3D optical cage. Furthermore, compared with the ordinary 3D optical cage, this kind of 3D optical cage generated by our method has a controllable switch; that is, it can be easy to 'open' and 'close' by controlling the coherence length of the incident beams. Our work may find valuable applications in optical tweezers, microscopes, laser processing, and so on.
Radiation forces of highly focused radially polarized hollow sinh-Gaussian beams on a Rayleigh metallic particle

Based on the vector diffraction theory, the tight focusing properties of radially polarized hollow sinh-Gaussian (HsG) beams are theoretically studied. It is found that the radially polarized HsG beams can form a longitudinally polarized sub-wavelength focal spot. Moreover, the radiation forces acting on a Rayleigh metallic particle are calculated for the case where the radially polarized HsG beams are applied. Compared with the use of conventional Gaussian beams, the high-order radially polarized HsG beams can largely enhance the radial trap stiffness and broaden the axial trap distance. The influence of the beam order \( m \) on the focusing properties and trap stiffness is investigated in detail.

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主题: Gaussian beams (主要); Focusing; Gaussian distribution; Metallic compounds; Polarization; Stiffness

标识符 (关键字): Focusing properties, Metallic particles, Radially polarized, Radiation forces, Sub-wavelength, Tight focusing, Trap stiffness, Vector diffraction theory

题目: Radiation forces of highly focused radially polarized hollow sinh-Gaussian beams on a Rayleigh metallic particle

通讯作者: Huang, Wei Institute of Physics and Materials Science, Anhui University, China.

语言: 英文

摘要语言: English
3D hollow framework of GeO$_x$ with ultrathin shell for improved anode performance in lithium-ion batteries

**Authors:** Fang, Zhen 1; Qiang, Tingting 1; Fang, Jiaxin 1; Song, Yixuan 1; Ma, Qiuyang 1; Ye, Ming 1; Qiang, Feiqiang 2; Geng, Baoyou 1 1 Key Laboratory of Functional Molecular Solids, College of Chemistry and Materials Science, Anhui Normal University, 241000, China fzfscn@mail.ahnu.edu.cn; bygeng@mail.ahnu.edu.cn 2 Department of Mechanics, Academy of Armored Force Engineering, 100072, China

**Publication Information:** Electrochimica Acta 151 (Jan 1, 2015): 453-458.

**ProQuest Document Link**
In this paper, 3D hollow framework of GeO$_x$ is synthesized using a bubble-template hydrothermal procedure. The as-obtained hollow structure exhibits excellent cycling performance and rate capability in comparison with GeO$_x$ nanoparticles when used as an anode material in lithium ion batteries. The GeO$_x$ 3D hollow framework shows a high capacity of up to 1480 mAh·g$^{-1}$ and 1109 mAh·g$^{-1}$ at 80 mA·g$^{-1}$ and 1600 mA·g$^{-1}$ current density, respectively. The excellent lithium storage performance can be attributed to the unique 3D hollow framework. The framework not only acts as the buffer layer to alleviate the strain during lithiation, but also facilitates the electron transfer during the charge/discharge processes.

3D hollows, Anode performance, Cycling performance, GeOx, Hydrothermal, Hydrothermal procedure, Lithium-ion battery, Rate capabilities, 3D hollow framework, GeOx

3D hollow framework of GeO$_x$ with ultrathin shell for improved anode performance in lithium-ion batteries

Fang, Zhen , East Beijing Road 1#, China.

Lithium batteries (主要); Anodes; Electric batteries; Electrodes; Ions; Lithium; Lithium alloys; Lithium compounds; Secondary batteries

Alkali Metals; 702: Electric Batteries and Fuel Cells; 704.1: Electric Components; 801: Chemistry; 802.1: Chemical Plants and Equipment; 804.1: Organic Compounds

3D hollows, Anode performance, Cycling performance, GeOx, Hydrothermal, Hydrothermal procedure, Lithium-ion battery, Rate capabilities, 3D hollow framework, GeOx

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New

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Anion-exchange reaction synthesized CoNi$_2$S$_4$ nanowires for superior electrochemical performances

**Authors:** Hu, Qingqing 1; Ma, Wenqin 1; Liang, Gan 1; Nan, Honghong 1; Zheng, Xiaoting 1; Zhang, Xiaojun 1

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**Publication Information:** RSC Advances 5.103 (Jan 1, 2015): 84974-84979.

**Abstract (English):** In this paper, we report CoNi$_2$S$_4$ nanowire arrays (NWAs) on 3D nickel foams based on an anion-exchange reaction which involved the pseudo Kirkendall effect. Due to the low electronegativity of sulfur, CoNi$_2$S$_4$ NWAs exhibit higher conductivity compared with Ni-Co oxide NWAs when used as active materials in supercapacitors. The electrochemistry tests show that these self-supported electrodes are able to deliver ultrahigh specific capacitance (1250 F g$^{-1}$ at a current density of 5 mA cm$^{-2}$), together with a considerable areal capacitance (2.5 F cm$^{-2}$ at a current density of 5 mA cm$^{-2}$). Furthermore, a capacitance retention of 72% after 5000 charge-discharge cycles at 5 mA cm$^{-2}$ is obtained, indicating the excellent cycling stability of the CoNi$_2$S$_4$ NWA/nickel foam electrode. The superior electrochemistry capacity demonstrates that CoNi$_2$S$_4$ NWAs are promising electrode materials for supercapacitor applications.

**Keywords:** Capacitance, Charge-discharge cycle, Electrochemical performance, Electrochemistry, Electrodes, Electrolytic capacitors, Electronegativity, Nanowires, Nickel

**Identifiers (Keywords):** Capacitance retention, Charge-discharge cycle, Electrochemical performance, Electrochemistry tests, Electrode material, Kirkendall effects, Specific capacitance, Supercapacitor application

**Title:** Anion-exchange reaction synthesized CoNi$_2$S$_4$ nanowires for superior electrochemical performances

**Corresponding Author:** Zhang, Xiaojun

Key Laboratory for Functional Molecular Solids, Education Ministry of China, College of Chemistry and Materials Science, Center for Nano Science and Technology, Anhui Normal University, 241000, China.
Synthesis of Ag₃PO₄-Bi₂O₂CO₃ composites with high visible-light photocatalytic activity

作者: Hu, Yu 1; Dong, Chao 1; Wu, Kong-Lin 1; Xia, Shan-Hui 1; Li, Xiao 1; Wei, Xian-Wen 1

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Ag$_3$PO$_4$-Bi$_2$O$_2$CO$_3$ composites were prepared by a combination of hydrothermal technique and precipitation method for the first time. Ag$_3$PO$_4$ nanoparticles with ca. 200 nm in size were attached to the surface of Bi$_2$O$_2$CO$_3$ microspheres in diameter of 1-2 μm, which had higher photocatalytic activity than Bi$_2$O$_2$CO$_3$ microspheres toward degradation of Rhodamine B (RhB) in water under visible light irradiation. The Ag$_3$PO$_4$-Bi$_2$O$_2$CO$_3$ composite with the molar ratio of Ag$_3$PO$_4$-Bi$_2$O$_2$CO$_3$=1:1 exhibited the highest photodegradation efficiency of RhB (97% in 30 min), which was about 2.2 times of pure Bi$_2$O$_2$CO$_3$ microspheres. The enhanced photoactivity could be ascribed to more light harvest and more effective separation of photo-generated electron-hole pairs.
Occurrence of Decabromodiphenyl Ethane in Captive Chinese Alligators (Alligator sinensis) from China

作者: Hong, Bing 1 ; Wu, Ting 1 ; Zhao, Guangchao 1 ; Sun, Yuxin 2 ; Wang, Xinming 3 ; Zhao, Juan 1 ; Yi, Zhigang 4 ; Wu, Xiaobing 1 ; Mai, Bixian 3 1 College of Environmental Science and Engineering, Anhui Normal University, 241003, China wuting19@mail.ahnu.edu.cn ; wuxb@mail.ahnu.edu.cn 2 Key Laboratory of Tropical Marine Bio-resources and Ecology, South China Sea Institute of Oceanology, Chinese Academy of Sciences, 510301, China 3 State Key Laboratory of Organic Geochemistry, Guangzhou Institute of Geochemistry, Chinese Academy of Sciences, 510640, China 4 College of Resources and Environment, Fujian Agriculture and Forestry University, 350002, China


摘要 (English): Decabromodiphenyl ethane (DBDPE), a replacement for decabromodiphenyl ether (deca-BDE), was investigated in captive Chinese alligators from China. DBDPE was detected in adult tissues, neonates and eggs of Chinese alligators with concentrations ranging from 4.74-192, 0.24-1.94, and 0.01-0.51 ng g^{-1} lipid weight, respectively. Compared to PBDEs and PCBs, DBDPE contamination was limited in Chinese alligators. Additionally, DBDPE concentrations in adult muscles were one to three orders of magnitude higher than those in neonates and eggs, suggesting the limited maternal transfer potential of DBDPE in Chinese alligators. This is the first study to report the occurrence of DBDPE in Chinese alligators.

主题: Ethane (主要); Organic pollutants; Polychlorinated biphenyls

分类: 804.1: Organic Compounds

标识符 (关键字): Chinese alligator, DBDPE, Decabromodiphenyl ethane, Decabromodiphenyl ethers, Maternal transfer, Reptile, Three orders of magnitude
Electrochemiluminescence properties of Tb(III) nicotinic acid complex and its analytical application

作者: Yang, Yu 1 ; Zhang, Yuqin 2 ; Shu, Guibo 1 ; Dong, Qin 1 ; Zou, Lili 1 ; Zhu, Yinggui 1 1 College of Chemistry and Material Science, Anhui Normal University, No. 1 Beijing East Road, 241000, China
A water soluble lanthanide Tb(III) complex $\text{Tb}_2(C_6\text{NO}_2\text{H}_4)(\text{H}_2\text{O})_4$ has been synthesized as luminescent material, and it is characterized by X-ray crystallography, infrared spectra and elemental analysis, respectively. This material showed excellent characterize of electrochemiluminescence (ECL) in the presence of co-reactant potassium peroxodisulfate ($K_2\text{S}_2\text{O}_8$) at glassy carbon electrode. With the increase of the concentration for nicotinic acid (NA), the ECL intensity of the complex/$K_2\text{S}_2\text{O}_8$ system in HAc-NaAc buffer solution will be decreased apparently. Novel approach for the detection of nicotinic acid (NA) was developed based on the quenching effect of NA. Furthermore, the possible mechanisms for the ECL behavior of $\text{Tb}_2(C_6\text{NO}_2\text{H}_4)(\text{H}_2\text{O})_4/K_2\text{S}_2\text{O}_8$ system are proposed. The effects of $K_2\text{S}_2\text{O}_8$ concentration, pH of the buffer on the ECL intensity have also been discussed in detail. The experiment results showed that the limit of detection for NA was $6.0 \times 10^{-7}$ M ($S/N=3$) with a linear range of $2.0 \times 10^{-6}$-2.0×10^{-4} M.
Collision dynamic behaviors of CO(X\(^1\Sigma^+\)) molecule with Mg atom in cold and ultracold temperatures

**Authors:** Han, Yu-Long 1 ; Zhang, Kan 2 ; Feng, Er-Yin 3 ; Huang, Wu-Ying 3 1 College of Physics and Electronics Information, Anhui Normal University, 241000, China, Mechanical and Electrical College, Anhui Polytechnic University, 241003, China 2 Mechanical and Electrical College, Anhui Polytechnic University, 241003, China 3 College of Physics and Electronics Information, Anhui Normal University, 241000, China

**Email:** fengbf@mail.ahnu.edu.cn

**Publication Information:** Wuli Xuebao/Acta Physica Sinica 64.10 (Jan 1, 2015).

**Abstract (English):** Sympathetic cooling is one of the most promising techniques for producing ultracold molecules from precooled molecules. The previous work has shown that it is inadequate to use the ultracold alkali-metal atoms as coolant for sympathetic cooling. Whether the ultracold alkali-earth-metal atoms can be used as coolant deserves to be investigated. In this paper, the cold collision dynamic behaviors for Mg atom and CO molecule are investigated by quantum scattering calculations. The influences of electric field on the elastic and inelastic collision cross sections of low field seeking state within cold and ultracold temperature are explored. The results show that sympathetic cooling CO molecule with ultracold Mg atom might be difficult to perform.

**Linked citations:** Check for full text via 360 Link, Order Full Text from Infotrieve

**Keywords:** Molecules (主要); Alkali metals; Atoms; Coolants; Cooling; Electric fields; High energy physics

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Collision dynamic behaviors of CO($^1\Sigma^+$) molecule with Mg atom in cold and ultracold temperatures

Feng, Er-Yin College of Physics and Electronics Information, Anhui Normal University, 241000, China.

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Quantitative analysis of thiram by surface-enhanced raman spectroscopy combined with feature extraction algorithms

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摘要 (English): Three feature extraction algorithms, such as the principal component analysis (PCA), the discrete cosine transform (DCT) and the non-negative factorization (NMF), were used to extract the main information of the spectral data in order to weaken the influence of the spectral fluctuation on the subsequent quantitative analysis results based on the SERS spectra of the pesticide thiram. Then the extracted components were respectively combined with the linear regression algorithm-the partial least square regression (PLSR) and the non-linear regression algorithm-the support vector machine regression (SVR) to develop the quantitative analysis models. Finally, the effect of the different feature extraction algorithms on the different kinds of the regression algorithms was evaluated by using 5-fold cross-validation method. The experiments demonstrate that the analysis results of SVR are better than PLSR for the non-linear relationship between the intensity of the SERS spectrum and the concentration of the analyte. Further, the feature extraction algorithms can significantly improve the analysis results regardless of the regression algorithms which mainly due to extracting the main information of the source spectral data and eliminating the fluctuation. Additionally, PCA performs best on the linear regression model and NMF is best on the non-linear model, and the predictive error can be reduced nearly three times in the best case. The root mean square error of cross-validation of the best regression model (NMF+SVR) is 0.0455 μmol·L⁻¹ (10⁻⁶ mol·L⁻¹), and it attains the national detection limit of thiram, so the method in this study provides a novel method for the fast detection of thiram. In conclusion, the study provides the experimental references the selecting the feature extraction algorithms on the analysis of the SERS spectrum, and some common findings of feature extraction can also help processing of other kinds of spectroscopy.

主题: Algorithms (主要); Chemical analysis; Discrete cosine transforms; Extraction; Factorization; Feature extraction; Linear regression; Machine components; Mean square error; Principal component analysis; Raman spectroscopy; Regression analysis; Spectrum analysis

分类: 601.2: Machine Components; 741.1: Light and Optics; 801: Chemistry; 802.3: Chemical Operations; 804: Chemical Products Generally; 921: Applied Mathematics; 921.3: Mathematical Transformations; 922.2: Mathematical Statistics

标识符 (关键字): 5-fold cross validation method, Discrete Cosine Transform(DCT), Feature extraction algorithms, Partial least square regression, SERS, Support vector machine regression (SVR), Surface enhanced Raman spectroscopy, Thiram, Feature extraction algorithm, Quantitative analysis

标题: Quantitative analysis of thiram by surface-enhanced raman spectroscopy combined with feature extraction algorithms

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语言: 英文
Research on meteorological thresholds of drought and flood disaster: a case study in the Huai River Basin, China

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摘要 (English): Together with affected areas of crops from 1978 to 2008, the daily precipitation of 110 stations located in the Huai River Basin during 1959–2008 was used to study the critical conditions when drought and...
flood occur, based on which the quantitative relationship between the critical condition and the affected area of crops was further studied. Based on the research on the hazard-formative factor of precipitation and the damage degree of crops, the spatial-temporal characteristics of disasters were analyzed, the drought and flood disaster-causing threshold was determined, and the quantitative relationship between the disaster-causing threshold and affected area of crops was established. The results are as the follows: (1) During 1959–2008, extreme precipitation levels were high in the eastern and western part of the Huai River Basin and were low in its central part; the spatial distribution of the coefficient of variation (CV) differed greatly from average extreme precipitation: the series of most stations were located in the central basin, and especially there was a positive trend in Anhui and Henan Provinces. (2) The cumulative precipitation during the disaster period of each station was divided by its mean cumulative precipitation during the same period in 1959–2008 to obtain the disaster-causing threshold, which has shown a good effect on reflecting the actual grade and affected areas in disasters. (3) The relationship among disaster grade, disaster-causing threshold and damage area of crops was established; this threshold can be used as a tool for agricultural disaster assessment and early warning, and can effectively improve the ability to prevent and mitigate disaster in the Huai River Basin. (4) The disaster-causing threshold can be an important input parameter for hazard assessment; other underlying surface indicators can be good supplements for determining the threshold in hazard assessment.
Thermodynamic properties and microstructures of the mixture of N-butylpyridinium tetrafluoroborate with acetonitrile studied by molecular dynamics simulation

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Abstract (English): The binary system of the ionic liquid (IL) N-butylpyridinium tetrafluoroborate ([BPy][BF$_4$]) and acetonitrile (MeCN) was investigated by molecular dynamics simulation method. The thermodynamic properties of the mixture were obtained by simulation including density, self-diffusion coefficients, viscosity, and vaporization enthalpy. This study focused on the relationship between the microscopic structure and the proportion of [BPy][BF$_4$] in the mixed system. Radial distribution functions (RDFs) for different components were also compared. Results showed that the first peak of the nonpolar regions of [BPy][BF$_4$] increased with increasing mole fraction $x_i$ of IL, whereas that of polar regions decreased. The coordination number as a function of distance was calculated by integrating RDFs to the first shell. Results indicated that a wide distribution of possible configurations in ion pairs formed by anions and cations of the IL in mixtures. Spatial distribution functions (SDFs) indicated that the anions [BF$_4$]$^-$ were mainly distributed around the pyridine ring of the cation [BPy]$^+$ and the methyl of MeCN. Moreover, the excess molar volume was negative and showed a minimum at $x_i = 0.3$, consistent with the change law of SDFs.
Synthesis of Bis(NHC)-Based CNC-Pincer Rare-Earth-Metal Amido Complexes and Their Application for the Hydrophosphination of Heterocumulenes

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出版物信息: Organometallics 34.18 (Sep 28, 2015): 4553-4559.

摘要 (English): The bis(NHC) (NHC = N-heterocyclic carbene)-based CNC-pincer rare-earth-metal amido complexes LRE[N(SiMe\textsubscript{3})\textsubscript{2}]\textsubscript{2} (L\textsubscript{2}, R = CH\textsubscript{3}; L\textsubscript{3}, R = CH(CH\textsubscript{3})\textsubscript{2}) were synthesized and characterized, and their catalytic activities toward hydrophosphination of heterocumulenes were developed. Reactions of bis[2-(3-methylimidazolium)-4-methylphenyl]amine diiodide (H\textsubscript{3}L\textsubscript{2}I\textsubscript{2}) or bis[2-(3-isopropylimidazolium)-4-methylphenyl]amine diiodide (H\textsubscript{3}L\textsubscript{3}I\textsubscript{2}) with 5 equiv of NaN(SiMe\textsubscript{3})\textsubscript{2} followed by treatment with 1 equiv of RECl\textsubscript{3} in THF at -78 °C afforded the bis(NHC)-based CNC-pincer rare-earth-metal amido complexes LRE[N(SiMe\textsubscript{3})\textsubscript{2}]\textsubscript{2} (RE = Y (1), Eu (2), Er (3); L\textsubscript{3}, RE = Y (4), Er (5), Yb (6)). Complexes 4-6 can also be prepared by stepwise reactions of H\textsubscript{3}L\textsubscript{3}I\textsubscript{2} with n-BuLi in THF followed by reactions with [(Me\textsubscript{3}Si)\textsubscript{2}N]\textsubscript{3}RE(μ-Cl)Li(THF)\textsubscript{3}. Stepwise reactions of H\textsubscript{3}L\textsubscript{1}I\textsubscript{2} with n-BuLi in THF followed by treatment with [(Me\textsubscript{3}Si)\textsubscript{3}N]RE(μ-Cl)Li(THF)\textsubscript{3} generated the bis(NHC)-based CNC-pincer rare-earth-metal amido complexes L\textsubscript{2}RE[N(SiMe\textsubscript{3})\textsubscript{2}]\textsubscript{2} (RE = Y (1), Er (3)) together with the fused-heterocyclic compound 3,8,9-trimethyl-8a,9-dihydro-8H-benzo[4,5]imidazo[2′,1′:2,3]imidazo[1,2-a]imidazo[2,1-c]quinoxaline (7), which formed through carbene C-C and C-N coupling. Attempts to prepare complexes of the type LRE[N(SiMe\textsubscript{3})\textsubscript{2}]\textsubscript{2} by reaction of H\textsubscript{3}L\textsubscript{3}I\textsubscript{2} with [(Me\textsubscript{3}Si)\textsubscript{3}N]Yb(μ-Cl)Li(THF)\textsubscript{3} in THF, however, afforded mixed complexes of the bis(NHC)-based CNC-pincer ytterbium complex L\textsubscript{3}Yb[N(SiMe\textsubscript{3})\textsubscript{2}]\textsubscript{2} (6) and the unexpected bis(NHC)-based CNC-pincer monoamido ytterbium iodide L\textsubscript{3}YbI[N(SiMe\textsubscript{3})\textsubscript{2}] (8). Investigation of the catalytic activity of complexes 1-6 and 8 indicated that all complexes displayed high activity toward the addition of the phosphine P-H bond to heterocumulenes, producing the corresponding phosphaguanidines, phosphaureas, and phosphathioureas, which represents the first example of bis(NHC)-based CNC-pincer type rare-earth-metal amido complexes as catalysts for the catalytic addition of the phosphine P-H bond to heterocumulenes with high efficiency in the presence of a low catalyst loading at room temperature.

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Synthesis and Reactivity of Rare-Earth-Metal Monoalkyl Complexes Supported by Bidentate Indolyl Ligands and Their High Performance in Isoprene 1,4-cis Polymerization

Authors: Zhang, Guangchao 1; Wang, Shaowu 2; Zhou, Shuangliu 1; Wei, Yun 1; Guo, Liping 1; Zhu, Xiancui 1; Zhang, Lijun 1; Gu, Xiaoxia 1; Mu, Xiaolong 1 1 Key Laboratory of Functional Molecular Solids, Ministry of Education, Anhui Laboratory of Molecule-Based Materials, College of Chemistry and Materials Science, Anhui Normal University, 241000, China 2 Key Laboratory of Functional Molecular Solids, Ministry of Education, Anhui Laboratory of Molecule-Based Materials, College of Chemistry and Materials Science, Anhui Normal University, 241000, China, State Key Laboratory of Organometallic Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, 200032, China swwang@mail.ahnu.edu.cn

Publication Information: Organometallics 34.17 (Sep 14, 2015): 4251-4261.

Abstract (English): A series of novel rare-earth-metal monoalkyl complexes incorporating partially rotation restricted [N,N]-bidentate indolyl ligands were synthesized and characterized, and their reactivities and catalytic activities were investigated. Treatment of \([\text{RE}(\text{CH}_2\text{SiMe}_3)_3(\text{thf})_2]\) with 1 equiv of 2-[(N-2,6-diisopropylphenyl)iminomethyl]indole \((\text{2-(2,6-iPr}_2\text{C}_6\text{H}_3\text{N}=\text{CH})\text{C}_8\text{H}_5\text{NH})\) in toluene at room temperature afforded the rare-earth-metal monoalkyl complexes \([\eta^1:\eta^1-\text{2-(2,6-iPr}_2\text{C}_6\text{H}_3\text{N}=\text{CH})\text{Ind}]\text{RE}(\text{CH}_2\text{SiMe}_3)(\text{thf})\) \((\text{Ind} = \text{indolyl}; \text{RE} = \text{Yb (1), Er (2), Y (3), Dy (4), Gd (5)})\) and the samarium complex \([\eta^1:\eta^1-\text{2-(2,6-iPr}_2\text{C}_6\text{H}_3\text{N}=\text{CH})\text{Ind}]\text{Sm (6)}\) via alkane elimination in good yields. Treatment of complex 2 or 3 with 1 equiv of PhSiH\(_3\) in toluene at 80 °C for 12 h afforded the dinuclear complexes \([\mu-\eta^6:\eta^1:\eta^1-\text{2-(2,6-iPr}_2\text{C}_6\text{H}_3\text{NCH}_2})\text{Ind}]\text{RE}[\text{2-(2,6-iPr}_2\text{C}_6\text{H}_3\text{N}=\text{CH})\text{Ind}]\text{2 (Ind = indolyl, RE = Er (7), Y (8)})\) in good isolated yields. Treatment of complex 2 or 3 with 1 equiv of amidine \((\text{2,6-iPr}_2\text{C}_6\text{H}_3\text{N})_2\text{CH}\) produced the corresponding complexes \([\eta^1:\eta^1-\text{2-(2,6-iPr}_2\text{C}_6\text{H}_3\text{N}=\text{CH})\text{N}]\text{2 (RE = Er (9), Y (10))}\) possessing the amidinate ligand \([(\text{2,6-iPr}_2\text{C}_6\text{H}_3\text{N})_2\text{CH}]).\) The molecular structures of all complexes were determined by X-ray crystallography. The monoalkyl complexes 1-5 were tested as isoprene polymerization initiators. Among the complexes investigated, the optimum combination \(5/\text{Al}_3\text{Bu}_3/[\text{Ph}_3\text{C}][\text{B}(\text{C}_6\text{F}_5)_4]\) displayed a high catalytic activity in isoprene polymerization, producing polymers with an extremely high 1,4-cis selectivity (up to 99%), a high number-average molecular weight \((M_n = 7.2 \times 10^5)\), and a narrow molecular weight distribution \((\text{PDI} = 1.34)\) at an isoprene to initiator molar ratio of 6000:1.

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Main: Praseodymium (首要); Catalyst activity; Chelation; Crystallography; Dysprosium; Dysprosium compounds; Erbium; Erbium compounds; Gadolinium; Isoprene; Ligands; Molecular weight; Molecular weight distribution; Polymerization; Polymers; Rare earth elements; Rare earths; Samarium; Synthesis (chemical); Toluene; X ray crystallography; Ytterbium

Category: 547.2: Rare Earth Metals; 801: Chemistry; 802.2: Chemical Reactions; 804.1: Organic Compounds; 804.2: Inorganic Compounds; 815.1: Polymeric Materials; 815.2: Polymerization; 933.1: Crystalline Solids; 933.1.1: Crystal Lattice
Shape-Controlled Synthesis of NiCo$_2$O$_4$ Microstructures and Their Application in Supercapacitors

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**Publication Information:** Chemistry - An Asian Journal 10.9 (Sep 1, 2015): 1972-1978.

**Abstract (English):** The shape-controlled synthesis of NiCo$_2$O$_4$ microstructures through a facile hydrothermal method and subsequent calcinations was explored. By employing CoSO$_4$, NiSO$_4$, and urea as the starting reactants, flower-like NiCo$_2$O$_4$ microstructures were obtained at 100°C after 5 h without the assistance of any additive and subsequent calcination at 300°C for 2 h; dumbbell-like NiCo$_2$O$_4$ microstructures were prepared at 150°C after 5 h in the presence of trisodium citrate and subsequent calcination at 300°C for 2 h. The as-prepared NiCo$_2$O$_4$ microstructures were characterized by X-ray powder diffraction, field-emission scanning electron microscopy, energy-dispersive X-ray spectroscopy, and (high-resolution) transmission electron microscopy. Both the flower-like and dumbbell-like NiCo$_2$O$_4$ microstructures could be used as electrode materials for supercapacitors, and they exhibited excellent electrochemical performance, including high specific capacitance, good rate capability, and excellent long-term cycle stability. Simultaneously, the shape-dependent electrochemical properties of the product were investigated.

**Keywords:** Electrochemical performance, Energy dispersive X-ray spectroscopy, Field emission scanning electron microscopy, High specific capacitances, Hydrothermal methods, Shape controlled synthesis, Supercapacitor, Tri-sodium citrates, microstructures, shape-controlled synthesis, supercapacitors
Layer-by-layer assembly of graphene oxide on polypropylene macroporous membranes via click chemistry to improve antibacterial and antifouling performance

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Polypropylene is an extensively used membrane material; yet, polypropylene membranes exhibit extremely poor resistance to protein fouling. To ameliorate this issue, graphene oxide (GO) nanosheets were used to modify macroporous polypropylene membrane (MPPM) via layer-by-layer assembly technique through click reaction. First, alkyne-terminated GO was prepared through esterification between carboxyl groups in GO and amide groups in propargylamine; azide-terminated GO was synthesized by the ring-opening reaction of epoxy groups in GO with sodium azide. Second, GO was introduced to the membrane by click chemistry. Characterizations of infrared spectra and X-ray photoelectron spectroscopy confirmed the modification. The sharply decreasing of static water contact angle indicated the improvement of the surface hydrophilicity for GO modified membrane. Introducing GO to the membrane results in a dramatic increase of water flux, improvements in the antifouling characteristics and antibacterial property for the membranes. The pure water flux through the 5-layered GO modified membrane is 1.82 times that through the unmodified one. The water flux restores to 43.0% for the unmodified membrane while to 79.8% for the modified membrane. The relative flux reduction decreases by 32.1% due to GO modification. The antibacterial property was also enhanced by two-thirds. These results demonstrate that the antifouling and antibacterial characteristics can be raised by tethering GO to the membrane surface.

主题: Membranes (主要); Graphene; Photoelectron spectroscopy; Polypropylene oxides; Polypropylenes; Synthesis (chemical); X ray photoelectron spectroscopy

分类: 761: Nanotechnology; 801: Chemistry; 802.2: Chemical Reactions; 804: Chemical Products Generally; 815.1.1: Organic Polymers; 951: Materials Science

标识符 (关键字): Antibacterial ability, Antifouling performance, Click chemistry, Graphene oxides, Layer-by-layer assemblies, Graphene oxide, Layer-by-layer assembly

标题: Layer-by-layer assembly of graphene oxide on polypropylene macroporous membranes via click chemistry to improve antibacterial and antifouling performance

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出版物类型: Journal
Focusing properties of hypergeometric gaussian beam through a high numerical-aperture objective

作者: Peng, Ji 1 ; Shan, Zhengye 2 ; Yuan, Yangsheng 2 ; Cui, Zhifeng 2 ; Huang, Wei 3 ; Qu, Jun 2 1

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摘要 (English): The focusing properties of radially polarized hypergeometric Gaussian beam are studied using the Richards-Wolf vectorial diffraction model. Such a polarized beam is decomposed into radial and longitudinal polarization. With a proper combination of the beam order, beam size and imaginary parameter variables, the adjustably confined flat-topped focus and focal hole can be obtained in the focal region. Moreover, we got originality characteristic for the axial intensity distribution of two shaped symmetric light spots. The tight focusing of a hypergeometric Gaussian beam may find applications in data storage, laser drilling, optical trapping, etc.
SnS$_2$ nanotubes: A promising candidate for the anode material for lithium ion batteries

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First-principles calculations were employed to investigate the adsorption and diffusion of lithium atoms (Li) on various SnS$_2$ nanostructures, i.e., bulk, bilayer, monolayer, nanoribbons and nanotubes. Our results show that on the SnS$_2$ bulk and bilayer, Li adsorption is more stable than the counterparts of the monolayer, nanoribbons and nanotubes, but the diffusion is unfavorable. Although the SnS$_2$ monolayer can greatly increase the mobility of Li, its adsorption strength is relatively weak with respect to other nanostructures. When cutting the monolayer into one-dimensional zigzag nanoribbons, the binding energies of Li do not increase, leading to them being excluded as an electrode material for Li-ion batteries. Interestingly, when rolling the monolayer into one-dimensional nanotubes, the adsorption strength is enhanced and the diffusion of Li atoms becomes kinetically favorable. Therefore, SnS$_2$ nanotubes would be expected to be a very promising anode material in Li-ion batteries.
Colorimetric and Phosphorimetric Dual-Signaling Strategy Mediated by Inner Filter Effect for Highly Sensitive Assay of Organophosphorus Pesticides

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Abstract (English): We describe here a colorimetric and phosphorimetric dual-signaling strategy for sensitive assay of organophosphorus pesticides (OPPs). The principle for assay depends on the phenomenon that the phosphorescence of Mn-ZnS quantum dots (QDs) can be dramatically quenched by Au nanoparticles (AuNPs) through the inner filter effect (IFE) and the activity of acetylcholinesterase (AChE), an enzyme that catalytically hydrolyzes acetylthiocholine to thiocholine that can be inhibited by OPPs. By virtue of the variations of absorbance and phosphorescence of the analytical system, a dual-readout assay for OPPs has been proposed. The limits of detection for different OPPs including paraoxon, parathion, omethoate, and dimethyl dichlorovinyl phosphate (DDVP) are found to be 0.29, 0.59, 0.67, and 0.44 ng/L, respectively. The proposed assay was allowed to detect pesticides in real spiked samples and authentic contaminated apples with satisfactory results, suggesting its potential applications to detect pesticides in complicated samples.

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Delivery of Highly Active Noble-Metal Nanoparticles into Microspherical Supports by an Aerosol-Spray Method

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Abstract (English): Noble metal nanoparticles (NPs) with 1-5 nm diameter obtained from NaHB₄₄ reduction possess high catalytic activity. However, they are rarely used directly. This work presents a facile, versatile, and efficient aerosol-spray approach to deliver noble-metal NPs into metal oxide supports, while maintaining the size of the NPs and the ability to easily adjust the loading amount. In comparison with the conventional spray approach, the size of the loaded noble-metal nanoparticles can be significantly decreased. An investigation of the 4-nitrophenol hydrogenation reaction catalyzed by these materials suggests that the NPs/oxides catalysts have high activity and good endurance. For 1% Au/CeO₂ and Pd/Al₂O₃ catalysts, the rate constants reach 2.03 and 1.46 min⁻¹, which is much higher than many other reports with the same noble-metal loading scale. Besides, the thermal stability of catalysts can be significantly enhanced by modifying the supports. Therefore, this work contributes an efficient method as well as some guidance on how to produce highly active and stable supported noble-metal catalysts. Spraying metals: An aerosol-spray approach has been developed as an efficient way to deliver highly active noble-metal nanoparticles (NPs) into oxide supports (see scheme). This method is also applicable for the formation of other catalysts composed of noble-metal NPs on different kinds of metal oxide supports. The catalytic properties of the materials were investigated by using of 4-nitrophenol hydrogenation as a model reaction.

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Themes: Catalyst supports (主要); Aerosols; Catalysis; Catalyst activity; Catalysts; Hydrogenation; Metal nanoparticles; Metals; Nanoparticles; Palladium; Precious metals; Rate constants; Thermodynamic stability

Identifiers (keywords): 4-Nitrophenol, High activity, Homogeneous catalysis, Hydrogenation reactions, Loading amount, Metal oxide supports, Noble metal loading, Supported noble metal catalysts, aerosol sprays, noble metals, supported catalysts

Title: Delivery of Highly Active Noble-Metal Nanoparticles into Microspherical Supports by an Aerosol-Spray Method

Corresponding Author: Geng, Baoyou College of Chemistry and Materials Science, Anhui Normal University, Key Laboratory of Functional Molecular Solids, Ministry of Education, Anhui Laboratory of Molecular-Based Materials, Center
Dual-site polydopamine spheres/CoFe layered double hydroxides for electrocatalytic oxygen reduction reaction

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Development of efficient and low-cost electro-catalysts for the oxygen reduction reaction (ORR) has been a great challenge for fuel cells and metal-air batteries. Here the hybrids of CoFe layered double hydroxides (CoFe-LDHs) with polydopamine spheres (PDAS) were prepared by growing CoFe-LDHs at the surface of PDAS in situ and their catalytic activity toward the ORR was investigated in detail. The results show that the as-prepared CoFe-LDHs/PDAS hybrids exhibited higher ORR catalytic activity with 4e-route selectivity than pure CoFe-LDHs, PDAS and even calcinated CoFe-LDHs/PDAS, which displays synergistic effect between CoFe-LDHs and PDAS for ORR. Moreover, the CoFe-LDHs/PDAS hybrids demonstrated better durability than commercial Pt/C ORR catalysts. To uncover the ORR mechanism, the interaction between CoFe-LDHs and PDAS were characterized by XPS and the ORR activity of CoFe-LDHs/PDAS and CoFe-LDHs/PDAS leached with acid was compared. The catalytic behavior of CoFe-LDHs/PDAS hybrids is consistent with a dual-site ORR mechanism.
Quantitative analysis of Mn in soil samples using LIBS

作者: Zhang, Bao-Hua 1 ; Jiang, Yong-Cheng 1 ; Zhang, Xian-Yan 2 ; Cui, Zhi-Feng 2

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出版物信息: Guang Pu Xue Yu Guang Pu Fen Xi/Spectroscopy and Spectral Analysis 35.6 (Jan 1, 2015): 1715-1718.

摘要 (English): The trace element of Manganese element in the agricultural farm (Anhui Huaiyuan Nongkang) soil was quantitatively analyzed by Laser-induced breakdown spectroscopy. The line of 403.1 nm was selected as the analysis line of Mn. The matrix element of Fe in soil was chosen as the internal calibration element and the analysis line was 407.2 nm. Ten soil samples were used to construct calibration curves with traditional method and internal standard method, and four soil samples were selected as test samples. The experimental results showed that the fitting correlation coefficient (r) is 0.954 when using the traditional method, the maximum relative error of the measurement samples is 5.72%, and the detection limit of Mn in soil is 93 mg·kg⁻¹. While using the internal standard method to construct the calibration curve, the fitting correlation coefficient (r) is 0.983, the relative error of measurement samples is reduced to 4.1%, and the detection limit of Mn in soil is 71 mg·kg⁻¹. The result indicates that LIBS technique can be used to detect trace element Mn in soil. In a certain extent, the internal standard method can improve the accuracy of measurement.

主题: Soil surveys; Atomic emission spectroscopy; Calibration; Chemical analysis; Curve fitting; Error detection; Laser induced breakdown spectroscopy; Manganese; Soils; Trace elements

分类: 483.1: Soils and Soil Mechanics; 543.2: Manganese and Alloys; 721.1: Computer Theory (Includes Formal Logic, Automata Theory, Switching Theory and Programming Theory); 801: Chemistry; 804: Chemical
Quantitative analysis of Mn in soil samples using LIBS
Precious-metal-free co-fe-o/rGO synergetic electrocatalysts for oxygen evolution reaction by a facile hydrothermal route

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摘要 (English): Abundant iron group metal oxides and their composites possess great potential in the application of electrochemical energy storage and conversion. In this work, we obtained Co-Fe-O composites/reduced graphene oxides (CFO/rGO) hybrid structures, engineered their compositions, phase, and structures by a facile hydrothermal route, and studied their composition-dependent activity for electrochemical oxygen evolution reaction (OER) in alkaline media. It is found that synergetic effects bring a clear decrease in overpotential and Tafel slope for CFO/rGO catalysts in comparison with monometallic composition/rGO catalysts. OER charge-transfer resistance is significantly reduced after Fe addition, indicating that the reaction barriers of CFO/rGO are reduced. The optimal CFO/rGO with Co-Fe ratio of 2:1 was identified. Our results on the synergetic effects of CFO/rGO enrich the understanding of iron-group composites for electrocatalytic applications.

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主题: Oxygen (主要); Catalysts; Charge transfer; Composite materials; Electrocatalysis; Electrocatalysts

分类: 415: Metals, Plastics, Wood and Other Structural Materials; 802.2: Chemical Reactions; 803: Chemical Agents and Basic Industrial Chemicals; 804: Chemical Products Generally; 811: Cellulose, Paper and Wood Products; 951: Materials Science

标识符 (关键字): Charge transfer resistance, Electrochemical energy storage, Electrochemical oxygen, Hydrothermal routes, Oxygen evolution reaction, Reaction barriers, Spinel, Synergetic effect, Composites

标题: Precious-metal-free co-fe-o/rGO synergetic electrocatalysts for oxygen evolution reaction by a facile hydrothermal route

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Laser flash photolysis study on the quenching reaction of the excited triplet state of acenaphthenequinone by antioxidant vitamin C

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Abstract (English): The photo-induced reactions of acenaphthenequinone (ACQ) as well as ACQ and vitamin C (VC) in ACN-H2O (v/v, 4:1) mixed solvent have been investigated by means of laser flash photolysis technique. The reaction intermediates have been identified and the reaction mechanism has been analyzed. The self-quenching rate constant of 3ACQ by ground state ACQ and the quenching rate constant of 3ACQ by biological antioxidant VC have also been measured. The results indicate that there is a hydrogen transfer from VC to 3ACQ during the laser photolysis. VC is an effective quencher to 3ACQ and the quenching rate constant is 4.0 × 10^8 L mol^-1 s^-1.

Categories: 537.1: Heat Treatment Processes; 741: Light, Optics and Optical Devices; 741.1: Light and Optics; 801: Chemistry; 801.4: Physical Chemistry; 804: Chemical Products Generally; 931.3: Atomic and Molecular
Title: Laser flash photolysis study on the quenching reaction of the excited triplet state of acenaphthenequinone by antioxidant vitamin C

Authors: Xu, Xinsheng
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Abstract: This study investigates the quenching reaction of the excited triplet state of acenaphthenequinone using antioxidant vitamin C through laser flash photolysis techniques. The transient absorption spectroscopies were employed to analyze the reaction dynamics.
Homogeneous core-shell NiCo$_2$S$_4$ nanostructures supported on nickel foam for supercapacitors

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**Abstract (English):** In this study, we report the fabrication of NiCo$_2$S$_4$ with a homogeneous core-shell nanostructure in which NiCo$_2$S$_4$ nanotubes are wrapped by NiCo$_2$S$_4$ nanosheets. The core-shell structured NiCo$_2$S$_4$ was in situ grown on nickel foam and can be directly applied as a supercapacitor electrode. Electrochemical tests demonstrate that the NiCo$_2$S$_4$ electrode achieved a high specific capacitance of 1948 mF cm$^{-2}$ at a current density of 1 mA cm$^{-2}$, a good rate capability, and an excellent cycling stability. The outstanding performance of the NiCo$_2$S$_4$ electrode can be attributed to its core-shell architecture with good mechanical and electrical contact and rich redox reactions, as well as high transport rate for both electrolyte ions and electrons. By applying NiCo$_2$S$_4$ as the positive electrode and porous carbon as the negative electrode, an asymmetric supercapacitor device was fabricated and it exhibited an excellent electrochemical performance. These results demonstrate that the homogeneous core-shell NiCo$_2$S$_4$ nanostructure is promising for supercapacitor applications.
Mediatorless glucose biosensor and direct electron transfer type glucose/air biofuel cell enabled with carbon nanodots

Authors: Zhao, Mei 1; Gao, Yue 1; Sun, Junyong 1; Gao, Feng 1 1 Laboratory of Functionalized Molecular Solids, College of Chemistry and Materials Science, Anhui Normal University, 241000, China fgao@mail.ahnu.edu.cn

Abstract (English): Utilization of carbon nanodots (CNDs), newcomers to the world of carbonaceous nanomaterials, in the electrochemistry realm has rarely been reported so far. In this study, CNDs were used as immobilization supports and electron carriers to promote direct electron transfer (DET) reactions of glucose oxidase (GOx) and bilirubin oxidase (BOD). At the CNDs electrode entrapped with GOx, a high rate constant (k_s) of 6.28 ± 0.05 s⁻¹ for fast DET and an apparent Michaelis-Menten constant (K_M app) as low as 0.85 ± 0.03 mM for affinity to glucose
were found. By taking advantage of its excellent direct bioelectrocatalytic performances to glucose oxidation, a DET-based biosensor for glucose detection ranging from 0 to 0.64 mM with a high sensitivity of 6.1 μA mM⁻¹ and a limit of detection (LOD) of 1.07 ± 0.03 μM (S/N = 3) was proposed. Additionally, the promoted DET of BOD immobilized on CNDs was also observed and effectively catalyzed the reduction of oxygen to water at the onset potential of +0.51 V (vs Ag/AgCl). On the basis of the facilitated DET of these two enzymes at CNDs electrodes, a mediator-free DET-type glucose/air enzymatic biofuel cell (BFC), in which CNDs electrodes entrapped with GOx and BOD were employed for oxidizing glucose at the bioanode and reducing oxygen at the biocathode, respectively, was successfully fabricated. The constructed BFC displayed an open-circuit voltage (OCV) as high as 0.93 V and a maximum power density of 40.8 μW cm⁻² at 0.41 V. These important features of CNDs have implied to be promising materials for immobilizing enzymes and efficient platforms for elaborating bioelectrochemical devices such as biosensors and BFCs.

主题: Glucose oxidase (主要); Biofuels; Biological fuel cells; Biosensors; Carbon; Diamonds; Electrodes; Electron transitions; Enzymatic fuel cells; Enzyme electrodes; Enzymes; Glucose; Glucose sensors; Open circuit voltage; Oxygen; Rate constants

分类: 461: Bioengineering; 482.2.1: Gems; 523: Liquid Fuels; 524: Solid Fuels; 701.1: Electricity, Basic Concepts and Phenomena; 704.1: Electric Components; 711.1: Electromagnetic Waves in Different Media; 801.2: Biochemistry; 801.4: Physical Chemistry; 804: Chemical Products Generally; 804.1: Organic Compounds

标识符 (关键字): Bioelectrochemical devices, Direct electron transfer, Glucose oxidases (GOx), Immobilization support, Immobilizing enzymes, Maximum power density, Michaelis-Menten constant, Reduction of oxygen

标题: Mediatorless glucose biosensor and direct electron transfer type glucose/air biofuel cell enabled with carbon nanodots

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Facile synthesis of porous TiO$_2$ nanospheres and their photocatalytic properties

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**Abstract (English):** Uniform and monodisperse porous TiO$_2$ nanospheres were synthesized by a hydrothermal method. Techniques of X-ray diffraction, scanning electron microscopy, Brunauer-Emmett-Teller (BET) nitrogen adsorption-desorption, UV-vis absorption spectroscopy, and transmission electron microscopy were used to characterize the structure and morphology of the products. The BET surface area of the porous TiO$_2$ nanospheres was calculated to be 26.1 cm$^2$ g$^{-1}$. In addition, the obtained porous TiO$_2$ nanospheres were used as catalyst to photodegrade methylene blue, Rhodamine B, methyl orange, p-nitrophenol, and eosin B. Compared to commercial TiO$_2$ powder, the as-prepared porous TiO$_2$ nanospheres exhibited higher catalytic activities due to their large surface areas and porous nanostructures. The photocatalytic reaction rate constant of the porous TiO$_2$ nanospheres in photocatalytic decomposition of methylene blue and Rhodamine B under simulated solar light were calculated as 0.0545 min$^{-1}$ and 0.0579 min$^{-1}$, respectively. Moreover, the catalyst was demonstrated to have good stability and reusability.

**Links:** Check for full text via 360 Link, Order Full Text from Infotrieve?
Facile synthesis of porous TiO$_2$ nanospheres and their photocatalytic properties

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New

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Fabrication of defect-rich MoS\textsubscript{2} ultrathin nanosheets for application in lithium-ion batteries and supercapacitors

作者: Wu, Zhengcui 1 ; Li, Baor 1 ; Xue, Yejing 1 ; Li, Jingjing 1 ; Zhang, Yali 1 ; Gao, Feng 1 1 Anhui Key Laboratory of Molecule-Based Materials, Key Laboratory of Functional Molecular Solids, Ministry of Education, College of Chemistry and Materials Science, Anhui Normal University, 241000, China
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摘要 (English): Defect-rich MoS\textsubscript{2} ultrathin nanosheets with abundant unsaturated sulfur atoms are constructed using a stoichiometric ratio of Mo(vi) and l-cysteine in the presence of 1,6-hexanediamine. The as-prepared MoS\textsubscript{2} ultrathin nanosheets exhibit excellent electrochemical activities in lithium-ion batteries and supercapacitors with a high reversible capacity and good cycling stability. The construction of defects with abundant unsaturated sulfur atoms in the MoS\textsubscript{2} ultrathin nanosheets provided active sites for improving the electrochemical performance in lithium-ion batteries and supercapacitors. This work provides an accessible foundation for engineering more sophisticated defect-rich MoS\textsubscript{2} ultrathin nanosheet-based composites for further optimization across a range of possible domains of application.

主题: Lithium-ion batteries (主要); Amino acids; Capacitors; Defects; Electric batteries; Ions; Lithium; Lithium alloys; Lithium compounds; Molybdenum compounds; Nanosheets; Secondary batteries; Sulfur


标识符 (关键字): 1,6-Hexanediamine, Cycling stability, Electrochemical activities, Electrochemical performance, High reversible capacities, Stoichiometric ratio, Super capacitor, Ultrathin nanosheets

标题: Fabrication of defect-rich MoS\textsubscript{2} ultrathin nanosheets for application in lithium-ion batteries and supercapacitors

通讯作者: Zhang, Yali Anhui Key Laboratory of Molecule-Based Materials, Key Laboratory of Functional Molecular Solids, Ministry of Education, College of Chemistry and Materials Science, Anhui Normal University, 241000, China.
Teleportation for atomic state based on disentanglement-free state

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Publication Information: Guangxue Xuebao/Acta Optica Sinica 35.3 (Jan 1, 2015).
Quantum teleportation is easily effected by noisy environment. In order to decrease this adverse effect induced by the amplitude-damping noisy environment, a scheme for quantum teleportation is proposed based on disentanglement-free state and quantum error-avoiding codes. In this scheme, a kind of disentanglement-free four-qubit state is used as the quantum entanglement channel, and single qubit of the teleportated quantum information is encoded into two qubits. This scheme has the advantages that quantum teleportation has full fidelity and the success probability for this teleportation scheme is 100%. The study has important applications in improvement of quantum communication.
The fractional fourier transform of hypergeometric-gauss beams through the hard edge aperture

作者: Qu, Jun 1 ; Fang, Mengyao 1 ; Peng, Ji 1 ; Huang, Wei 2 1 Department of Physics, Anhui Normal University, 241000, China qujun70@mail.ahnu.edu.cn 2 School of Environmental Science and Optoelectronic Technology, University of Science and Technology of China, 230026, China


ProQuest文档链接

摘要 (English): Based on the Collins integral formula and Lohmann optical system, we expand the hard edge aperture into complex Gauss function and derive an approximate analytic expression of intensity distribution theoretically for Hypergeometric-Gauss beams through the fractional Fourier transform (FRT) optical systems with hard edge aperture. The influences of FRT order, aperture size and other optical parameters on the light intensity distribution of Hypergeometric-Gauss beams passing through the FRT optical systems are discussed in detail. The results show that the FRT is an excellent beam-shaping method.

链接: 指向全文文献的链接

主题: Optical systems (主要); Gaussian distribution

分类: 741.3: Optical Devices and Systems; 922.1: Probability Theory

标识符 (关键字): Analytic expressions, Collins integral formula, Fractional Fourier transforms, Hard-edge aperture, Hypergeometric, Intensity distribution, Light intensity distribution, Optical parameter

标题: The fractional fourier transform of hypergeometric-gauss beams through the hard edge aperture

通讯作者: Qu, Jun Department of Physics, Anhui Normal University, 241000, China.

语言: 英文

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Ammonia cation-assisted bubble template for synthesizing hollow TiO$_2$ nanospheres and their application in lithium ion storage

Authors: Long, Liuyang; Zhang, Hui; Ye, Ming; Fang, Zhen

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Abstract (English): Hollow TiO$_2$ nanospheres are promising anode materials for lithium ion batteries. The synthesis of such nanostructures was achieved by an ammonia cation-assisted oxygen bubble template strategy in the present work. The formation of other transition metal-based hollow spheres also validates the proposed ammonia cation-assisted oxygen bubble template method. The formation mechanism was proposed on the basis of an investigation of the time dependency as well as the effect of H$_2$O$_2$ and NH$_4$Cl on the morphology. The discharge capacity of the prepared hollow TiO$_2$ nanospheres is 131 mA h g$^{-1}$ after 30 cycles.

Theme: Lithium batteries (主要); Ammonia; Anodes; Lithium; Lithium alloys; Lithium compounds; Lithium-ion batteries; Nanospheres; Oxygen; Positive ions; Titanium dioxide; Transition metals
Ammonia cation-assisted bubble template for synthesizing hollow TiO$_2$ nanospheres and their application in lithium ion storage

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The potential energy surface and microwave spectra of the Xe-CO$_2$ complex

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摘要 (English): The first potential energy surface for the Xe-CO$_2$ complex has been generated using the CCSD(T) method. The basis sets employed are: aug-cc-pVQZ for the C and O atoms, and aug-cc-pVQZ-PP for the Xe atom, with an additional (3s3p2d2f1g) set of midbond functions. The surface has a global minimum of -258.805 cm$^{-1}$ at T-shaped with $R_e = 7.15\text{a}_0$. Bound state energies have been calculated for seven Xe-CO$_2$ isotopologues. Calculated microwave transition frequencies for the various isotopologues are in good agreement with the experimental data.

摘要语言: English

主题: Carbon dioxide (主要); Microwave spectroscopy; Molecular physics; Potential energy; Potential energy surfaces; Quantum chemistry


标识符 (关键字): Basis sets, Bound-state energies, CCSD, Global minima, Isotopologues, Microwave spectrum, Microwave transitions

标题: The potential energy surface and microwave spectra of the Xe-CO$_2$ complex

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Multi-objective channel assignment and gateway deployment optimizer for wireless mesh network

Authors: Zhao, Chuanxin 1 ; Chen, Fulong 1 ; Wang, Ruchuan 2 ; Zhao, Cheng 1 ; Luo, Yonglong 1 1 School of Mathematics and Computer Science, Anhui Normal University, 241000, China zcxonline@126.com ; ylluo@ustc.edu.cn 2 School of Computer Science and Technology, Nanjing University of Posts and Telecommunications, 210003, China

Abstract (English): Gateway deployment and channel assignment are important for the wireless mesh network planning because they influence the network quality of service directly. Traditionally, the two problems are studied separately. In this paper, a comprehensive strategy is proposed to minimize both the link collision and the cost of gateway deployment for wireless mesh network. In addition, the load balance is also considered in the planning stage and characteristics of the aggregation of flow traffic near the gateway in wireless mesh network are reflected by the degree of link collision. For the gateway deployment, it has been proved to be NP-hard. Here a novel multi-objective particle swarm algorithm is proposed to optimize both channel assignment and gateway deployment. The route of nodes is built through creating a tree algorithm after the channel are assigned and gateway are selected. Thus, the two problems are decoupled. The channel assignment and gateway deployment are then obtained in polynomial time for wireless mesh network planning. Comparing with the existing algorithms based on balanced channel repartition, the simulation results show that our proposed algorithm can reduce network collision effectively and improve network performance significantly, while reducing the path length and obtaining load balance of the gateways.

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Minimizing upper bound of ruin probability under discrete risk model with Markov chain interest rate

作者: Lin, Xu 1; Dongjin, Zhu 1; Yanru, Zhou 1

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摘要 (English): This article focuses on minimal upper bound of ruin probability for a discrete time risk model with Markov chain interest rate and stochastic investment return. The interest rate of bond market is assumed to be a stationary Markov chain, and the return process of a stock market can be negative. This article presents two kinds of methods for minimizing the upper bound of ruin probability. One method relies on recursive equations for finite time ruin probabilities and inductive approach, the other one depends on martingale approach. Numerical examples show that the martingale approach is better than the inductive one.

摘要语言: English

主题: Markov processes; Chains; Commerce; Financial markets; Investments; Probability; Risk assessment; Stochastic models; Stochastic systems

分类: 602.1: Mechanical Drives; 911.2: Industrial Economics; 922.1: Probability Theory; 961: Systems Science


标题: Minimizing upper bound of ruin probability under discrete risk model with Markov chain interest rate

通讯作者: Lin, Xu School of Mathematics and Computer Science, Anhui Normal University, 241000, China.

语言: 英文

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Copper oxide nanofilm on 3D copper foam as a novel electrode material for supercapacitors

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摘要 (English): CuO nanofilm arrays on copper foam are synthesized through a simple hydrothermal method. The unique nanostructure features endow them excellent electrochemical performance. It should be pointed out that the charge–discharge voltage of these integrated electrodes was improved by testing in LiPF$_6$/EC:DEC electrolyte solution, which greatly increases the power densities and energy density. For example, the energy densities are 23.3, 20.6, 16.5, 11.8 and 9.7 W h kg$^{-1}$ at different power densities of 0.4, 0.7, 1.6, 2.9 and 6.8 kW kg$^{-1}$ in NaOH solution and 190.6, 125.5, 95.5, 26.7 and 15.1 W h kg$^{-1}$ at different power densities of 1.43, 3.42, 26.2, 64 and 90 kW kg$^{-1}$ in LiPF$_6$/EC:DEC electrolyte solution. Hence, the integrated electrode can be potentially used in some novel electrochemical supercapacitors and other electronic devices.

主题: Electrochemical electrodes (主要); Capacitors; Copper; Electric discharges; Electrodes; Electrolytes; Electrolytic capacitors

标识符 (关键字): Discharge voltages, Electrochemical performance, Electrochemical supercapacitor, Electrode material, Electrolyte solutions, Electronic device, Hydrothermal methods, Integrated electrodes
Electrodeposition of Pt-Fe(III) nanoclusters on graphene modified glassy carbon electrode for sensitive detection of nitrite

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摘要 (English): A novel electrochemical sensor for the detection of nitrite was fabricated by co-deposition of Pt nanoparticles and Fe(III) on reduced graphene oxide (RGO) modified glassy carbon electrode (GCE). Field emission scanning electron microscope (FE-SEM), transmission electron microscopy (TEM), and electrochemical techniques were used to characterize the structure of these nanocomposites. Electrochemical results showed that the Pt-Fe(III)/RGO/GCE exhibited remarkable electrocatalytic activity toward the oxidation of nitrite in phosphate buffer solution (pH 4.0). Under the optimum conditions, the linear range for the detection of nitrite was $4.0 \times 10^{-6}$ to $2.5 \times 10^{-4}$ M and a low detection limit of $6.0 \times 10^{-7}$ M. The proposed method was successfully applied in the detection of nitrite in salt samples.

主题: Electrochemical sensors (主要); Carbon; Electrochemical electrodes; Electrodes; Glass; Glass membrane electrodes; Glassy carbon; Graphene; Nanoclusters; Platinum; Scanning electron microscopy; Transmission electron microscopy

分类: 547.1: Precious Metals; 704.1: Electric Components; 741.1: Light and Optics; 741.3: Optical Devices and Systems; 761: Nanotechnology; 801: Chemistry; 801.4.1: Electrochemistry; 804: Chemical Products Generally; 812.3: Glass; 933: Solid State Physics; 951: Materials Science

标识符 (关键字): Electrocatalytic activity, Electrochemical techniques, Field emission scanning electron microscopes, Modified glassy carbon electrode, Nitrite, Phosphate buffer solutions, Reduced graphene oxides (RGO), Sensitive detection, Electrochemical sensor, Fe(III), Pt

标题: Electrodeposition of Pt-Fe(III) nanoclusters on graphene modified glassy carbon electrode for sensitive detection of nitrite

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语言: 英文

摘要语言: English

文档类型: Article

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Near-infrared light-triggered drug release nanogels for combined photothermal-chemotherapy of cancer

Near-infrared (NIR) light-triggered drug release systems are promising for drug delivery applications in view of the advantages of NIR light, which include high tissue penetration and low damage. In this report, we developed nanogels (NGs) by supramolecular self-assembly from adamantane (AD)-conjugated copolymer, poly[poly(ethylene glycol)monomethyl ether methacrylate]-co-poly(N-(2-hydroxypropyl)methacrylamide)-co-poly(N-adamantan-1-yl-2-methacrylamide) (PPEGMA-co-PHPMA-co-
PADMA), and β-cyclodextrin (β-CD)-functionalized poly(amidoamine) (PAMAM) dendrimer based on the host-guest interaction of the AD and β-CD moieties, and they were used to encapsulate indocyanine green (ICG) and doxorubicin (DOX) for combined photothermal-chemotherapy. NGs simultaneously loading ICG and DOX (DINGs) showed significant photothermal effects and stimuli-triggered drug release under NIR laser irradiation by the photothermal-induced relaxation or dissociation of the NGs. In vitro cytotoxicity evaluation of DINGs under NIR irradiation demonstrated the synergistic effects of hyperthermia, photothermal-triggered drug release, and chemotherapy. In vivo investigation revealed their high accumulation in tumor tissue and significant tumor growth suppression under NIR irradiation. These NIR light-triggered drug release NGs represent efficient and promising anticancer drug vectors for the combined photothermal-chemotherapy of cancer to maximize therapeutic efficacy and minimize side effects.
Discovery of a dual-targeting organometallic ruthenium complex with high activity inducing early stage apoptosis of cancer cells

Authors: Du, Jun 1; Zhang, Erlong 2; Zhao, Yao 3; Zheng, Wei 3; Zhang, Yang 3; Lin, Yu 3; Wang, Zhaoying 3; Luo, Qun 3; Wu, Kui 3; Wang, Fuyi 3 1 College of Chemistry and Materials Science, Key Laboratory of Functional Molecular Solids, Ministry of Education, Anhui Laboratory of Molecular-Based Materials, Anhui Normal University, 241000, China 2 College of Chemistry and Materials Science, Key Laboratory of Functional Molecular Solids, Ministry of Education, Anhui Laboratory of Molecular-Based Materials, Anhui Normal University, 241000, China, Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Analytical Chemistry for Living Biosystems, Beijing Centre for Mass Spectrometry, Institute of Chemistry, Chinese Academy of Sciences, 100190, China 3 Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Analytical Chemistry for Living Biosystems, Beijing Centre for Mass Spectrometry, Institute of Chemistry, Chinese Academy of Sciences, 100190, China

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Publication information: Metallomics 7.12 (Dec 1, 2015): 1573-1583.

ProQuest document link

Abstract (English): Ruthenium based complexes are promising antitumour candidates due to their lower toxicity and better water-solubility compared to the platinum antitumour complexes. An epidermal growth factor receptor (EGFR) has been found to be overexpressed in a large set of tumour cells. In this work, a series of organoruthenium complexes containing EGFR-inhibiting 4-anilinoquinazoline pharmacophores were synthesised and characterised. These complexes exhibited excellent inhibitory activity against EGFR and high affinity to interact with DNA via minor groove binding, featuring dual-targeting properties. In vitro screening demonstrated that the as-prepared ruthenium complexes are anti-proliferating towards a series of cancer cell lines, in particular the non-small-cell lung cancer cell line A549. Fluorescence-activated cell sorting analysis and fluorescence microscopy revealed that the most active complex 3 induced much more early-stage cell apoptosis than its cytotoxic arene ruthenium analogue and the EGFR-inhibiting 4-anilinoquinazolines, verifying the synergetic effect of the two mono-functional pharmacophores.

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Discovery of a dual-targeting organometallic ruthenium complex with high activity inducing early stage apoptosis of cancer cells

通讯作者: Zhao, Yao Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Analytical Chemistry for Living Biosystems, Beijing Centre for Mass Spectrometry, Institute of Chemistry, Chinese Academy of Sciences, 100190, China.
Fast synthesis and electrochemical performance of hollow NiCo$_2$O$_4$ flowerlike microstructures

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摘要 (English): In the present work, a two-step route was designed for fast synthesis of hollow NiCo$_2$O$_4$ flowerlike microstructures. A flowerlike precursor containing Ni and Co was firstly prepared via a fast microwave-assisted hydrothermal route. Then, hollow NiCo$_2$O$_4$ flowerlike microstructures were successfully obtained through pyrolyzing the above precursor. Experiments showed that the pyrolysis temperature could strongly affect the performance of the final product. The product prepared at 280 °C exhibited a bigger BET surface area and higher specific capacitance than that prepared at 400 °C. The as-prepared NiCo$_2$O$_4$ microstructures were characterized by X-ray powder diffraction (XRD), field emission scanning electron microscopy (FESEM), (high resolution) transmission electron microscopy (HRTEM/TEM) and energy dispersive X-ray spectrometry (EDS).

主题: High resolution transmission electron microscopy (主要); Electron microscopy; Field emission microscopes; Microstructure; Scanning electron microscopy; Transmission electron microscopy; X ray powder diffraction

分类: 741.1: Light and Optics; 741.3: Optical Devices and Systems; 933: Solid State Physics; 933.1.1: Crystal Lattice; 951: Materials Science

标识符 (关键字): BET surface area, Electrochemical performance, Energy dispersive x-ray spectrometries (EDS), Field emission scanning electron microscopy, High resolution, Microwave-assisted hydrothermal, Pyrolysis temperature, Specific capacitance

标题: Fast synthesis and electrochemical performance of hollow NiCo$_2$O$_4$ flowerlike microstructures

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语言: 英文

摘要语言: English

文档类型: Article

出版物名称: RSC Advances
ZnO nanoplates assembled by rod-like nanoparticles: simple reflux synthesis, influential factors and shape evolution towards nanorings

ZnO nanoplates assembled by rod-like nanoparticles have been successfully prepared by a simple reflux route without the assistance of a structure-directing agent or template. The as-synthesized products were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), (high resolution) transmission electron microscopy (HRTEM/TEM), selected area electron diffraction (SAED), UV-vis diffuse reflectance spectroscopy (DRS) and photoluminescence spectroscopy (PL). Some factors influencing the morphology of the ZnO nanostructures were investigated, including the type of polyol and Zn$^{2+}$ ion source,
the amounts of zinc nitrate hexahydrate and hexamine, and the reaction temperature. It was found that the
volume ratio of diethylene glycol and water in the system played a crucial role in the formation of ZnO
nanoplates. The time-dependent shape evolution experiments revealed that under the present experimental
conditions, the formation of the ZnO nanostructures underwent a transition from nanoparticles to nanoplates,
and finally to nanorings. Experiments showed that the as-obtained ZnO nanostructures presented good visible-
light photocatalytic activity and a wide range of PL properties.
Facile Fabrication of Bi$_{12}$O$_{17}$Br$_2$/Bi$_{24}$O$_{31}$Br$_{10}$ Type II Heterostructures with High Visible Photocatalytic Activity

Author: Peng, Yin 1 ; Yu, Pian-Pian 1 ; Chen, Qing-Guo 1 ; Zhou, Hai-Yan 1 ; Xu, An-Wu 2 1 Key Laboratory of Functional Molecular Solids, Ministry of Education, Anhui Normal University, 241000, China 2 Hefei National Laboratory for Physical Sciences at Microscale, Department of Chemistry, University of Science and Technology of China, 230026, China anwuxu@ustc.edu.cn


Abstract (English): One-dimensional (1D) Bi$_{12}$O$_{17}$Br$_2$/Bi$_{24}$O$_{31}$Br$_{10}$ type II heterostructures were synthesized by calcining BiOBr/Bi(OHC$_2$O$_4$)$_2$·2H$_2$O heterostructures in air at 400 °C. The photocatalytic activity of the as-prepared products was evaluated by the degradation of phenol and Rhodamin B (RhB) under visible light irradiation. The Bi$_{12}$O$_{17}$Br$_2$/Bi$_{24}$O$_{31}$Br$_{10}$ hierarchical heterostructures show enhanced visible light catalytic activity with the increase of the loaded/Bi$_{24}$O$_{31}$Br$_{10}$ content, which results from the efficient separation of photogenerated charge carriers due to the staggered band potentials of the two materials. Radical scavenger experiments confirm that photogenerated holes (h+) are the main active species for oxidizing RhB molecules during the photocatalytic processes.

Theme: Catalyst activity (主要); Biodegradation; Light; Photocatalysis; Photodegradation

Category: 741.1: Light and Optics; 801.2: Biochemistry; 803: Chemical Agents and Basic Industrial Chemicals; 804: Chemical Products Generally

Identifier (Keywords): Degradation of phenols, Photocatalytic activities, Photocatalytic process, Photogenerated charge carriers, Photogenerated holes, Radical scavengers, Visible-light irradiation, Visible-photocatalytic activities
Enantioselective addition of ArTi(O\text{Pr})_3 to aldehydes catalyzed by a titanium complex of an N-sulfonylated amino alcohol
Asymmetric additions of $\text{ArTi(O}^\text{iPr})_3$ to aldehydes catalyzed by a titanium catalyst of N-sulfonylated amino alcohols were reported, and results showed that the chiral N-sulfonylated amino alcohol with two stereogenic centers could catalyze the asymmetric addition of $\text{ArTi(O}^\text{iPr})_3$ to aldehydes to afford desired secondary alcohols in good yields with good to excellent enantioselectivities of up to 95% ee.
Site occupancy of Ce³⁺ in β-Ca₂SiO₄: A combined experimental and ab initio study

Authors: Liu, Yuewei 1; Fang, Qin 2; Ning, Lixin 2; Huang, Yucheng 2; Huang, Shizhong 2; Liang, Hongbin 1

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ProQuest document link

Abstract (English): Low-temperature photoluminescence properties of the β-Ca₂(1-x)CeₓNaₓSiO₄ (x = 0.0005) phosphor synthesized by a solid-state reaction method are investigated with excitation energies in the vacuum ultraviolet (VUV) to ultraviolet (UV) range. Two distinct types of emission and excitation spectra are observed, which are attributed to 4f-5d transitions of two different sets of Ce³⁺ centers. On the basis of density functional theory (DFT) calculations within the supercell model and wave function-based CASSCF/CASPT2 embedded cluster calculations, the two sets of Ce³⁺ centers are ascribed to the Ce³⁺ located on the seven-coordinated Ca1 and eight-coordinated Ca2 sites, respectively. Furthermore, from the observed relative spectral intensities, DFT total energy calculations, and comparison of experimental and calculated 4f → 5d transition energies, it is concluded that the occupation of Ce³⁺ on the Ca2 site is more energetically favorable than the occupation on the Ca1 site. Finally, the redshift of the lowest 4f → 5d transition of Ce³⁺ on the Ca2 site relative to that on the Ca1 site is discussed in terms of the changes of the 5d centroid energy and crystal-field splitting with the local coordination structure.

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Topics: Calculations (主要); Calcium; Crystal structure; Density functional theory; Excited states; Photoluminescence; Praseodymium compounds; Solid state reactions; Temperature; Wave functions

Identifiers (关键词): Ab initio calculations, Crystal-field splitting, Embedded cluster calculations, Local coordination structures, Low temperature photoluminescence, Site occupancy, Solid state reaction method, Total energy calculation, Ce3+ ion, β-Ca2SiO4
MgBr$_2$-promoted enantioselective arylation of ArTi(OiPr)$_3$ to ketones catalyzed by a titanium(IV) catalyst of N,N'-sulfonylated (1R,2R)-cyclohexane-1,2-diamine

作者: Shu, Chao-Chi; Zhou, Shuangliu; Gau, Han-Mou
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MgBr₂-promoted asymmetric addition of ArTi(O'iPr)₃ to ketones catalyzed by a titanium catalyst of N,N'-sulfonylated (1R,2R)-cyclohexane-1,2-diamines is reported, and results showed that the chiral N,N'-sulfonylated cyclohexane-1,2-diamines with electron-withdrawing groups could effectively catalyze asymmetric addition of ArTi(O'iPr)₃ to ketones to afford desired tertiary alcohols in good yields with good to excellent enantioselectivities of up to 95% ee.
A two-coordinate cobalt(II) imido complex with NHC ligation: Synthesis, structure, and reactivity

作者: Du, Jingzhen 1 ; Wang, Linbo 2 ; Xie, Meihua 3 ; Deng, Liang 1 1 State Key Laboratory of Organometallic Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, 345 Lingling Road, 200032, China deng@sioc.ac.cn 2 State Key Laboratory of Organometallic Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, 345 Lingling Road, 200032, China, Anhui Key Laboratory of Molecular Based Materials, College of Chemistry and Materials Science, Anhui Normal University, 241000, China 3 Anhui Key Laboratory of Molecular Based Materials, College of Chemistry and Materials Science, Anhui Normal University, 241000, China


摘要 (English): The synthesis, structural characterization, and reactivity of the first two-coordinate cobalt complex featuring a metal-element multiple bond [(IPr)Co(NDmp)] (4; IPr=1,3-bis(2′,6′-diisopropylphenyl)imidazole-2-ylidene; Dmp=2,6-dimesitylphenyl) is reported. Complex 4 was prepared from the reaction of [(IPr)Co(η2-vtms)]2 (vtms=vinyltrimethylsilane) with DmpN3. An X-ray diffraction study revealed its linear C-Co-N core and a short Co-N distance (1.691(6) Å). Spectroscopic characterization and calculation studies indicated the high-spin nature of 4 and the multiple-bond character of the Co-N bond. Complex 4 effected group-transfer reactions to CO and ethylene to form isocyanide and imine, respectively. It also facilitated E-H (E=C, Si) σ-bond activation of terminal alkyne and hydrosilanes to produce the corresponding Co(II) alkynyl and hydride complexes as 1,2-addition products. Dipp=2,6-diisopropylphenyl.
[G₃T]₅/Tb³⁺ based DNA biosensor with target DNA-triggered autocatalytic multi-cycle-amplification and magnetic nanoparticles assisted-background-lowered
Due to terbium's unique photophysical properties, nucleic-acid-sensitized terbium (DNA/Tb$^{3+}$) bioluminescent system becomes a potential candidate for the fabrication of DNA biosensors. However, the low sensitivity of DNA/Tb$^{3+}$ bioluminescent system limits its development. In this paper, a strategy combining autocatalytic multi-cycle-amplification (including exonuclease III (exo III)-aided and Zn$^{2+}$-requiring DNAzyme-assisted target recycling amplifications) and magnetic nanoparticles assisted-background-lowering to improve the sensitivity of DNA/Tb$^{3+}$ bioluminescent system is presented for sensitive detection of target DNA (tDNA).

The DNA/Tb$^{3+}$ bioluminescent system was investigated by ultraviolet-visible (UV-vis) absorption and luminescence spectra. The possible conjugation mechanism and mode of DNA with Tb$^{3+}$ were discussed. The autocatalytic multi-cycle-amplification effect was investigated by the comparison of the luminescence. The carboxylation-functionalized Fe$_3$O$_4$ magnetic nanoparticles (MNPs) were characterized and its role in background lowering was proved. As a result, with the designed protocol, the detection limit for the tDNA detection reached a low level to aM, which is especially exciting for the DNA/Tb$^{3+}$ bioluminescent system. In the process, due to the separation effect of MNPs, the assay solution was purified to avoid the nonspecific luminescence of DNA/Tb$^{3+}$, not only lowering the background signal greatly (about five times lower than that without the use of MNPs but also improving the reproducibility and stability. We hope that our attempt in this field will not only extend the application of DNA/Tb$^{3+}$ luminescent system in biosensing areas but also open the road to adaptation of the protocols to other related analytes.
Random weighting empirical distribution function and its applications to goodness-of-fit testing

作者: He, Daojiang 1 ; Xu, Kai 1 ; Xu, Xingzhong 2 1 Department of Statistics, Anhui Normal University, 241000, China djheahnu@163.com 2 School of Mathematics, Beijing Institute of Technology, 100081, China

出版物信息: Communications in Statistics: Simulation and Computation 44.6 (Jan 1, 2015): 1441-1452.

摘要 (English): In this article, a randomized estimator of the empirical distribution function (EDF) called random weighting empirical distribution function (RWEDF) is introduced, one special case of which is just equivalent to the Bayesian bootstrap. The consistency of the RWEDF is established under certain conditions. By substituting
this new EDF for the classical EDF, we obtain new versions of some EDF test statistics for goodness-of-fit. The simulation results show that the new tests are more powerful than the corresponding tests based on the classical EDF under some cases.

**Title:** Random weighting empirical distribution function and its applications to goodness-of-fit testing

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**Language:** English

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**Creation Date:** 2014-12-20

**Document Status:** New

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Detection of heparin based on the conformational switch of DNA

作者: Jiang, Hong 1 ; Wang, Guangfeng 1 ; Zhang, Xiaojun 1 1 Anhui Normal University, China

出版物信息: Analytical Methods 7.18 (Jan 1, 2015): 7852-7857.

摘要 (English): We report a simple, fast, sensitive and label-free fluorescent assay for sensing heparin based on the electrostatic attraction between heparin and coralyne. Under optimal conditions, the sensor exhibits high sensitivity, and needs just 10 min to complete the detection process. Additionally, the proposed sensor is simple to operate and low cost with no chemical labeling or modification of DNA required. Finally, the constructed sensor can be applied in Tris-HCl buffers and also complicated human serum samples.

链接: [Check for full text via 360 Link](#)

主题: Polysaccharides (主要); Chemical modification

分类: 802.2: Chemical Reactions; 804.1: Organic Compounds

标识符 (关键字): Chemical labeling, Conformational switches, Detection process, Electrostatic attractions, Fluorescent assays, High sensitivity, Human serum, Optimal conditions

标题: Detection of heparin based on the conformational switch of DNA

语言: 英文

摘要语言: English

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DOI: [http://dx.doi.org/10.1039/c5ay01613d](http://dx.doi.org/10.1039/c5ay01613d)
Hypterball batch key update method based on members' behavior

作者: Liu, Shuying 1 ; Xu, Yong 1 ; Yang, Fan 1 1 Department of Mathematics and Computer Science, Anhui Normal University


摘要 (English):  The core issue of secure multicast is the safe management of the group key. Through the analyzing of the multicast rekeying method of hypterball, and combining the batch key update and member’s behavior, the hypterball multicast key management method based on members' behavior is proposed in this paper. The scheme breaks through the traditional method of LKH, and it not only makes full use of independence and cooperation between members, but also considers the members’ behavior, and then improves the communication’s efficiency. Simulation experiment results show that when members join in or leave the group, especially when the probability of the members’ change is largely different, this scheme will greatly reduce the cost of key update and improve the efficiency of the key update, and at the same time the forward security and backward security are ensured.

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主题: Multicasting (主要); Probability


标识符 (关键字): Batching rekey, Forward security, Hypterball, Key updates, Multicast key management, Re-keying, Safe managements, Secure multicasts, Members’ behavior, Multicast secure
The magnetic properties of the spin-1 Heisenberg antiferromagnetic chain with single-ion anisotropy
The magnetic properties of the spin-1 Heisenberg antiferromagnetic chain with exchange anisotropy and single-ion anisotropy are studied by the double-time Green's function method. The determinative equations for the critical temperature, the magnetization, and the zero-field susceptibility are derived analytically. The effects of the anisotropies on the magnetic properties are presented.
Synthesis and photophysics of BF$_2$-rigidified partially closed chain bromotetrapyrroles: Near infrared emitters and photosensitizers

**Authors:** Dai, En 1; Pang, Weidong 1; Zhang, Xian-Fu 2; Yang, Xudong 2; Jiang, Ting 1; Zhang, Ping 1; Yu, Changjiang 1; Hao, Erhong 1; Wei, Yun 1; Mu, Xiaolong 1; Jiao, Lijuan 1

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**Publication:** Chemistry - An Asian Journal 10.6 (Jun 1, 2015): 1327-1334.

**Abstract (English):** We report the synthesis, crystallographic, optical, and triplet and singlet oxygen generation properties of a series of BF$_2$-rigidified partially closed chain bromotetrapyrroles as near infrared emitters and photosensitizers. These novel dyes were efficiently synthesized from a nucleophilic substitution reaction between pyrroles and the 3,5-bromo-substituents on the tetra- and hexabromoBODIPYs and absorb in the near-infrared region (681-754 nm) with high molar extinction coefficients. Their fluorescent emission (708-818 nm) and singlet oxygen generation properties are significantly affected by alkyl substitutions on the two uncoordinated pyrrole units of these dyes and the polarity of solvents. Among them, dyes 4-ca and 4-da show good singlet oxygen generation efficiency and good NIR fluorescence emission (fluorescence quantum yields of 0.14-0.43 in different solvents studied). Don’t be so rigid: A novel type of NIR BF$_2$-rigidified open-chain bromotetrapyrrole dyes has been developed, which show variable singlet oxygen generation properties depending on the alkyl substitutions on the two uncoordinated pyrrole units of these dyes.

**Links:** Check for full text via 360 Link; Order Full Text from Infotrieve?
Horseradish peroxidase immobilization on carbon nanodots/CoFe layered double hydroxides: Direct electrochemistry and hydrogen peroxide sensing

作者: Wang, Yinling ; Wang, Zhangcui ; Rui, Yeping ; Li, Maoguo 1 1 Key Laboratory of Chemo-Biosensing, Anhui Province, College of Chemistry and Materials Science, Anhui Normal University, 241000, China wyinl@mail.ustc.edu.cn ; limaoguo@mail.ahnu.edu.cn

出版物信息: Biosensors and Bioelectronics 64.1 (Feb 15, 2015): 57-62.

摘要 (English): Carbon nanodots and CoFe layered double hydroxide composites (C-Dots/LDHs) were prepared via simply mixing C-Dots and CoFe-LDHs. The as-prepared composites were used for the immobilization of horseradish peroxidase (HRP) on the glass carbon (GC) electrode. The electrochemical behavior of the HRP/C-Dots/LDHs/GC electrode and its application as a $\text{H}_2\text{O}_2$ biosensor were investigated. The results indicated that HRP immobilized by C-Dots/LDHs retained the activity of enzyme and displayed quasi-reversible redox behavior and fast electron transfer with an electron transfer rate constant $k_s$ of 8.46 s$^{-1}$. Under optimum experimental conditions, the HRP/C-Dots/LDHs/GC electrode displayed good electrocatalytic reduction activity and excellent analytic performance toward $\text{H}_2\text{O}_2$. The $\text{H}_2\text{O}_2$ biosensor showed a linear range of 0.1-23.1μM ($R^2=0.9942$) with a calculated detection limit of 0.04μM (S/N=3). In addition, the biosensor exhibited high sensitivity, good selectivity, acceptable reproducibility and stability. The superior properties of this biosensor are attributed to the synergistic effect of HRP, C-Dots and CoFe-LDHs, which has been proved by investigating their electrochemical response to $\text{H}_2\text{O}_2$. Thus the C-Dots and LDHs composites provide a promising platform for the immobilization of redox enzymes and construction of sensitive biosensors.

主题: Electrocatalysis (主要); Hydrogen peroxide

分类: 802.2: Chemical Reactions; 804.2: Inorganic Compounds

标识符 (关键字): Carbon nanodots, Direct electrochemistry, Horse-radish peroxidase, Hydrogen peroxide sensing, Layered double hydroxides, CoFe layered double hydroxides, Horseradish peroxidase

标题: Horseradish peroxidase immobilization on carbon nanodots/CoFe layered double hydroxides: Direct electrochemistry and hydrogen peroxide sensing

通讯作者: Wang, Yinling Key Laboratory of Chemo-Biosensing, Anhui Province, College of Chemistry and Materials Science, Anhui Normal University, 241000, China.
Ethylenediamine-assisted preparation of carbon nanofiber supported nickel oxide electrocatalysts for sensitive and durable detection of insulin

**Abstract (English):** A uniform nickel oxide (NiO) nanoparticle decorated on carbon nanofibers (CNFs) hybrid with the assistance of ethylenediamine (EDA) following a simple on-spot pyrolysis route has been fabricated for insulin electrocatalytic oxidation. The fabricated hybrid displayed superior catalytic performance due to the synergetic effects between NiO nanoparticles and CNFs. Excellent analytical features, including high sensitivity (1.55 μA μM⁻¹), short response time (<3 s), low detection limit (12.1 nM) and satisfactory linear dynamic range (20-1020 nM) were achieved. Moreover, this EDA-CNFS-NiO hybrid showed good stability and antifouling
property in a 0.1 M NaOH electrolyte toward insulin after successive potential cycling, which is highly required for a promising insulin electrocatalyst.
Simple hydrothermal synthesis and photocatalytic performance of coral-like BaTiO$_3$ nanostructures

Authors: Ni, Yonghong 1; Zheng, Hangsong 1; Xiang, Nannan 1; Yuan, Kefeng 1; Hong, Jianming 2  
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2 Centers of Modern Analysis, Nanjing University, 210093, China  

Publication Information: RSC Advances 5.10 (Jan 1, 2015): 7245-7252.  

Abstract (English): Coral-like BaTiO$_3$ nanostructures were successfully synthesized via a simple hydrothermal route at 150°C for 15 h employing BaCl$_2$, tetrabutyl titanate [(C$_{4}$H$_{9}$O)$_{4}$Ti] and NaOH as reactants without the assistance of any surfactant or template. The phase of the as-obtained BaTiO$_3$ was characterized by X-ray powder diffraction (XRD). Energy dispersive spectrometry (EDS), scanning electron microscopy (SEM) and (high-resolution) transmission electron microscopy (TEM/HRTEM) were employed for the composition and morphology analyses of the final product. Some factors influencing the formation of the coral-like BaTiO$_3$ nanostructures were investigated, including the amount of NaOH, the barium ion source, and the reaction temperature and time. Experiments showed that the as-prepared coral-like BaTiO$_3$ nanostructures presented good photocatalytic activity for the degradation of methyl orange (MO) dye under the irradiation of artificial sunlight. It was found that the photocatalytic activity of the coral-like BaTiO$_3$ nanostructures could be affected by the pH value of the system.
Preparation of porous flower-like SnO$_2$ micro/nano structures and their enhanced gas sensing property

作者: Ren, Haibo 1 ; Zhao, Wei 2 ; Wang, Liyou 1 ; Ryu, Si Ok 3 ; Gu, Cuiping 1 1 College of Chemistry and Materials Science, Center for Nano Science and Technology, Anhui Normal University, 241000, China cpgu2008@mail.ahnu.edu.cn 2 School of Materials Science and Engineering, Yeungnam University, 712749, South Korea soryu@ynu.ac.kr
Porous flower-like tin oxide (SnO\textsubscript{2}) structures were obtained using a hydrothermal method combined with a subsequent calcination and acid-washing process. The morphologies and crystal structures of the products were characterized by field emission scanning electron microscopy, transmission electron microscopy, energy dispersive spectroscopy, X-ray diffraction, X-ray photoelectron spectroscopy, and Brunauer-Emmett-Teller N\textsubscript{2} adsorption-desorption analyses. The process of inducing porosity begins with a flower-like nickel tin sulfur precursor. Thermal decomposition of this flower-like nickel tin sulfur precursor leads to an intimate mixture of porous flower-like NiO/SnO\textsubscript{2} hybrids. Porous SnO\textsubscript{2} flowers were obtained after removing the cubic phase NiO by an acid-washing process. Furthermore, the gas sensing properties of the as-prepared porous SnO\textsubscript{2} flowers to VOCs, such as ethanol, formaldehyde, benzene, toluene, and acetone, were investigated. The porous SnO\textsubscript{2} flowers showed a good response and reversibility to some organic vapors, such as ethanol and formaldehyde. The sensing responses to 100 ppm ethanol and formaldehyde were 42.4 and 24.8, respectively. The sensors also exhibited a good response to benzene, toluene, methanol, and 2-propanol. The relationship between the gas-sensing properties and the microstructure of the as-prepared flower-like SnO\textsubscript{2} structures was also examined.
Detection of human leptin in serum using chemiluminescence immunosensor: Signal amplification by hemin/G-quadruplex DNAzymes and protein carriers by Fe$_3$O$_4$/polydopamine/Au nanocomposites

**Authors:** He, Yuezhen 1; Sun, Jian 1; Wang, Xiaoxun 1; Wang, Lun 1
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**Publication Information:** Sensors and Actuators, B: Chemical 221 (Jul 27, 2015): 792-798.

**Abstract (English):** A sandwich chemiluminescence (CL) immunosensor for sensitive detection of human leptin was developed with a multiple signal amplification strategy from catalytic hemin/G-quadruplex DNAzymes and functional superparamagnetic nanocomposites. To construct this sensing platform, core-shell structural Fe$_3$O$_4$/polydopamine (PD)/Au superparamagnetic nanocomposites were synthesized by an in situ method with PD as a substrate adhesive. These nanocomposites were further characterized by scanning electron microscopy, transmission electronic microscopy, energy-dispersive spectroscopy, Fourier transform infrared spectrum and a vibrating sample magnetometer at room temperature. In this immunosensor, the monoclonal anti-human leptin antibody (capture antibody) was bound to the Fe$_3$O$_4$/PD/Au nanocomposites. Human leptin, biotinylated detection antibodies and streptavidin-DNAzymes were successively combined the above-mentioned nanocomposites to form sandwich-type immunocomplex through specific interactions. The magnetic particles loaded with the immunocomplex were separated by an external magnet, and the DNAzymes in the immunocomplex greatly enhanced the CL emission of the luminol-H$_2$O$_2$ system. The immunosensor exhibited a
high sensitivity, a good specificity, and a wide linear range for human leptin detection from $1.0 \text{ pg mL}^{-1}$ to $8.0 \times 10^{2} \text{ pg mL}^{-1}$ with a low detection limit of $0.3 \text{ pg mL}^{-1}$. This sensor is one of the most sensitive methods for leptin detection due to the highly efficient catalysis of the DNAzymes and analyte enrichment on magnetic capture.
Identification and characterization of a novel citrate synthase from Streptomyces diastaticus No. 7 strain M1033

作者: Ge, Yadong ; Cao, Zhengyu ; Song, Ping ; Zhu, Guoping 1 Institute of Molecular Biology and Biotechnology, Key Laboratory of the Biotic Environment and Ecological Safety in Anhui Province, Anhui Normal University, China gpz1996@yahoo.com


摘要 (English): Citrate synthase (CS) is a key enzyme of the tricarboxylic acid cycle and is widely distributed among prokaryotes and eukaryotes. Here, we report for the first time, the cloning, expression, and characterization of a novel CS from Streptomyces diastaticus No. 7 strain M1033 (SdCS). Gel filtration chromatography and matrix-assisted laser-desorption ionization-time-of-flight mass spectrometry (MALDI-TOF-MS) analyses indicate that SdCS forms homodimers with a molecular mass of approximately 100.0 kDa. The predicted amino acid sequence of SdCS is highly similar to those of bacterial homodimeric type I CSs. The pH and temperature optima for SdCS activity were 8.0 and 35 °C, respectively. The half-life (t_{1/2}) of SdCS was 10 Min at 50 °C and was increased to 210 Min in the presence of oxaloacetate. The kinetic parameters of SdCS (k_{cat} = 262.8 and 230.7 s^{-1}; K_m = 58.4 and 11.2 μM for acetyl-CoA and oxaloacetate, respectively) were comparable to those of dimeric CSs isolated from Gram-positive bacteria and eukaryotes. Moreover, SdCS activity was inhibited by ATP and ADP and stimulated by AMP. These findings provide a foundation for further investigations on the three-dimensional structure and mechanism of catalysis of SdCS.

链接: Check for full text via 360 Link, Order Full Text from Infotrieve

主题: Mass spectrometry (主要); Amino acids; Bacteria; Characterization; Chromatography; Desorption; Gel permeation chromatography; Inductively coupled plasma; Ionization; Polyacrylates; Research aircraft

标识符 (关键字): Citrate synthase, Gel-filtration chromatography, MALDI TOF MS, Streptomyces diastaticus, Western blots, enzymatic characterization, gel filtration chromatography, matrix-assisted laser-desorption ionization-time-of-flight mass spectrometry (MALDI-TOF-MS), Western blot

标题: Identification and characterization of a novel citrate synthase from Streptomyces diastaticus No. 7 strain M1033

通讯作者: Zhu, Guoping Institute of Molecular Biology and Biotechnology, Key Laboratory of the Biotic Environment and Ecological Safety in Anhui Province, Anhui Normal University, China.
Aluminum alkyl complexes supported by bidentate N,N ligands: Synthesis, structure, and catalytic activity for guanylation of amines

Authors: Wei, Yun; Wang, Shaowu; Zhou, Shuangliu; Feng, Zhijun; Guo, Liping; Zhu, Xiancui; Mu, Xiaolong; Yao, Fangshi

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The reactions of AlMe₃ or AlEt₃ with 2-pyridyl- or indolyl-substituted imines were studied, leading to the formation of different organoaluminum complexes. While the reactions of the iminopyridine Cy[N=CMe-2-(C₅H₄N)]₂ (L₁) derived from 1-(pyridin-2-yl)ethanone and trans-1,2-cyclohexanediamine with AlEt₃ gave the aluminum complex Cy[NC(Me)(Et)-2-(C₅H₄N)AlEt₂]₂ (1), in which the two ketimine groups of the ligand were transformed into the amido functionality through the addition of two ethyl groups, the reaction of L₁ with AlMe₃ afforded the aluminum complex Cy[NC(=CH₂)-2-(C₅H₄N)AlMe₂]₂ (2) via a sp³ C-H activation with elimination of two methane molecules. The reactions of indolyl-2-aldimines (2-(RN=CH)C₈H₅NH (R = t-Bu (L₂H), C₆H₅ (L₃H), 2,6-Me₂C₆H₃ (L₄H))) with AlMe₃ or AlEt₃ afforded only the deprotonated indolyl aluminum complexes [2-(RN=CH)C₈H₅N]AlMe₂ (R = t-Bu (3), C₆H₅ (4), 2,6-Me₂C₆H₃ (5)) and [2-(2,6-Me₂C₆H₃N=CH)C₈H₅N]AlEt₂ (6), respectively. The structures of complexes 2-6 were characterized by spectral methods and X-ray crystallographic analyses. These aluminum complexes showed a high catalytic activity in the addition of amines to carbodiimides to form guanidines. The mechanism of the catalytic process was studied by control experiments and ¹H NMR monitoring. Together with the isolation of the complex [2-(2,6-Me₂C₆H₃N=CH)C₈H₅N]Cy[N=C(4-MeC₆H₃N)(NHCy)]AlMe (7), a probable mechanism for the guanylation reaction was proposed.
Ordered spinel LiMn$_2$O$_4$ as cathode for high performance aqueous energy storage

作者: Tao, Haisheng 1 ; Zhang, Xuemei 2 ; Du, Lisha 2 ; Zhang, Shuqiong 2 ; Cheng, Yingying 2 ; Tong, Xiang 2 ; Dong, Ran 3

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摘要 (English): Well-ordered nano-LiMn$_2$O$_4$ is successfully prepared. The preparation follows two steps: synthesis of oval MnCO$_3$ by hydrothermal reaction and preparation of LiMn$_2$O$_4$ through sol-gel route. The as-prepared LiMn$_2$O$_4$ preserves cubic spinel morphology and consists of uniform particles with a diameter of ~200 nm. It exhibits an excellent electrochemical performance in aqueous electrolytes. A cell with the LiMn$_2$O$_4$ cathode and active carbon anode is fabricated. The initial discharge capacity of the cell is 119 mAh/g and it retains 88% even at the current density of 10000 mA/g. The coulombic efficiency maintains nearly 100% over 700 cycles at the current density of 5000 mA/g. Moreover, the cell could be fully charged with total time of ~2 min. The superior rate capability and excellent cycling stability show that the LiMn$_2$O$_4$ is a promising cathode.
Ordered spinel LiMn$_2$O$_4$ as cathode for high performance aqueous energy storage

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Gravitational inspired spectral clustering with constraint

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**Abstract (English):** Spectral clustering with pairwise constraints (i.e. mustlink and cannotlink) has been a hot topic in the machine learning community in recent years. Its performances are significantly influenced by utilizing the constraints. To make full use of the constraints' effect, pairwise constraints are integrated into an affinity matrix based on the gravitational method. In the data set as input, each point has mass property, and interacts with each other according to the universal law of gravitation. A Gravitational inspired constrained spectral clustering (GCSC) algorithm is proposed in this paper. Our algorithm is evaluated on multiple benchmark classification datasets. Compared with the existing approaches, experimental results demonstrate the effectiveness of our presented algorithm.

**Themes:** Clustering algorithms (主要); Algorithms; Artificial intelligence; Classification (of information); Gravitation; Learning systems

**Categories:** 716.1: Information and Communication Theory; 721: Computer Circuits and Logic Elements; 723: Computer Software, Data Handling and Applications; 723.4: Artificial Intelligence; 921: Applied Mathematics; 931.5: Gravitation and Relativity

**Identifiers (Keywords):** Affinity matrix, Benchmark classification, Constrained spectral clustering, Gravitation models, Machine learning communities, Mass properties, Pairwise constraints, Spectral clustering, Gravitation model, Pairwise constraint

**Language:** English
The design of double electrostatic-lens optics for resonance enhanced multiphoton ionization and photoelectron imaging experiments

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摘要 (English): Compared to single ion/electron-optics for velocity-map imaging, a double-focusing lens assembly designed not only allows for mapping velocity imaging of photoelectrons but also allows for investigating the vibrational structure of the intermediate states of neutral species in resonance enhanced
multiphoton ionization (REMPI) spectra. In this presentation, in order to record REMPI and photoelectron spectra separately, we have constructed a compact photoelectron velocity-map imaging (VMI) apparatus combined with an opposite linear Wiley-McIaren time-of-flight mass spectrometer (TOFMS). A mass resolution \((m/\Delta m)\) of \(~1300\) for TOFMS and electron energy resolution \((\Delta E/E)\) of \(2.4\%\) for VMI have been achieved upon three-photon ionization of Xe atom at 258.00 nm laser wavelength. As a benchmark, in combination of one-color \((1 + 1)\) REMPI and photoelectron imaging of benzene via \(6^1\) and \(6^1\) vibronic levels in the \(S_1\) state, the vibrational structures of the cation and photoelectron angular anisotropy are unraveled. In addition, two-color \((1 + 1')\) REMPI and photoelectron imaging of aniline was used to complete the accurate measurement of ionization potential \((62.271 \pm 3\) cm\(^{-1}\)). The results suggest that the apparatus is a powerful tool for studying photoionization dynamics in the photoelectron imaging using vibrational-state selected excitation to the intermediate states of neutrals based on REMPI technique.

链接: Check for full text via 360 Link, Order Full Text from Infotrieve?

主题: Photoionization (主要); Atom lasers; Electron energy levels; Electrostatic lenses; Excited states; Ionization; Ionization potential; Mass spectrometers; Photoelectron spectroscopy; Photoelectrons; Photons


标识符 (关键字): Accurate measurement, Photoelectron imaging, Photoelectron spectrum, Photoionization dynamics, Resonance-enhanced multiphoton ionization, Time-of-flight mass spectrometers, Velocity map imaging, Vibrational structures

标题: The design of double electrostatic-lens optics for resonance enhanced multiphoton ionization and photoelectron imaging experiments

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摘要语言: English

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Six Zn(ii) and Cd(ii) coordination polymers assembled from a similar binuclear building unit: Tunable structures and luminescence properties

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摘要 (English): Six Zn(ii) and Cd(ii) coordination polymers were constructed by treating a 2-substituted 8-hydroxyquinolinate ligand containing a pyridyl group with zinc or cadmium salts, and characterized by a variety of techniques. Interestingly, based on a similar binuclear Zn(ii) or Cd(ii) building unit, the supramolecular structures of the six coordination polymers (1-6) exhibit an unprecedented structural diversification due to the different choices of metal salts. 1 and 2 represent a novel 2D framework containing 1D infinite right- and left-handed helical chains. 4 and 5 are 2D coordination frameworks based on binuclear Cd(ii) building units. For 3 and 6, the ligands can bridge binuclear building units forming a 1D infinite chain. Interestingly, the adjacent CdO2 planes of the 1D chain in 6 are in parallel with each other, while the dihedral angle between the two ZnO2 planes in 3 is 83.43°. Photoluminescence properties revealed that the six coordination polymers exhibit redshifted emission maximum compared with the free ligand HL, which can be ascribed to an increased conformational rigidity and the fabrication of coplanar binuclear building units M2L2 in 1-6. Coordination polymers 1-6 also display distinct fluorescence lifetimes and quantum yields because of their different metal centers and supramolecular structures. This journal is

链接: Check for full text via 360 Link, Order Full Text from Infotrieve?

主题: Polymers (主要); Buildings; Cadmium; Chains; Dihedral angle; Ligands; Luminescence; Salts; Supramolecular chemistry; Zinc; Zinc compounds
Hierarchical ZnO@MnO$_2$@PPy ternary core-shell nanorod arrays: An efficient integration of active materials for energy storage

 authors: Ma, Wenqin 1; Shi, Qiangqiang 1; Nan, Honghong 1; Hu, Qingqing 1; Zheng, Xiaoting 1; Geng, Baoyou 1; Zhang, Xiaojun 1

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摘要 (English): In this paper, ZnO@MnO$_2$@PPy ternary core-shell nanorod arrays (NRAs) were fabricated through the layer-by-layer process. In this process, the incorporation of polypyrrole, a highly conductive material, on the surface of a binary ZnO@MnO$_2$ core-shell structured composite is adopted to optimize the charge transfer process to further improve the electrochemical performance. Because of enhanced electron transfer capability, charge transfer resistances of the ZnO@MnO$_2$@PPy ternary core-shell nanorod arrays are reduced and the electrochemical performances are improved. The electrochemistry tests show that these self-supported electrodes are able to deliver ultrahigh specific capacitance (1281 F g$^{-1}$ at a current density of 2.5 A g$^{-1}$), together with a considerable areal capacitance (1.793 F cm$^{-2}$ at a current density of 3.5 mA cm$^{-2}$). Furthermore, a capacitance retention of 90% after 5000 charge-discharge cycles at 5 A g$^{-1}$ is obtained, indicating the excellent cycling stability of the ZnO@MnO$_2$@PPy ternary core-shell electrode. The superior electrochemical capacity demonstrates the potential of ZnO@MnO$_2$@PPy ternary core-shell NRAs to further improve the performance in supercapacitor electrodes.

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主题: Electrochemical electrodes (主要); Capacitance; Charge transfer; Conductive materials; Electric discharges; Electrochemistry; Electrodes; Electrolytic capacitors; Electron transport properties; Manganese oxide; Nanorods; Polypyrroles; Shells (structures); Zinc oxide


标识符 (关键字): Capacitance retention, Charge transfer process, Charge transfer resistance, Charge-discharge cycle, Electrochemical capacities, Electrochemical performance, Electrochemistry tests, Supercapacitor electrodes

标题: Hierarchical ZnO@MnO$_2$@PPy ternary core-shell nanorod arrays: An efficient integration of active materials for energy storage

通讯作者: Zhang, Xiaojun Key Laboratory for Functional Molecular Solids of the Education Ministry of China, College of Chemistry and Materials Science, Anhui Normal University, 241000, China.
An optical FRET inhibition sensor for serum ferritin based on Mn²⁺-doped NaYF₄:Yb,Tm NIR luminescence up-conversion nanoparticles

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A new serum ferritin (SF) biosensor based on fluorescence resonance energy transfer (FRET) from Mn\(^{2+}\)-doped NaYF\(_4\):Yb,Tm up-converting rare-earth nanophosphors (UCNPs, donor) to gold nanorods (GNRs, acceptor) was developed in the near-infrared (NIR) region. The as-prepared Mn\(^{2+}\)-doped NaYF\(_4\):Yb,Tm UCNPs exhibited a strong emission at 807 nm in the NIR region and were modified with poly-(acrylic acid) (PAA) before conjugating with anti-SF (Ab\(_1\)). The negatively charged donor (Ab\(_1\)-UCNPs) and the positively charged acceptor (GNRs) were mixed in close proximity due to electrostatic interactions, which quenched the fluorescence emission of the Mn\(^{2+}\)-doped NaYF\(_4\):Yb,Tm UCNPs. However, added SF combines with the anti-SF because the binding affinity between SF and Ab\(_1\) is stronger than the electrostatic interactions. Thus, the acceptor separated from the donor, and the fluorescence was restored. Under optimal conditions, the restored fluorescence exhibited a linear relationship with SF concentrations ranging from 0.23 to 16.88 ng/mL and a limit of detection as low as 0.12 ng/mL. The proposed method was also used to monitor SF in human serum samples.
Synthesis of nitrogen-doped graphene-Ag$_2$CO$_3$ composites with enhanced photocatalytic efficiency

作者: Dong, Chao 1; Jiang, Bin-Bin 2; Wu, Kong-Lin 1; Hu, Yu 1; Xia, Shan-Hui 1; Wei, Xian-Wen 1
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摘要 (English): A series of nitrogen-doped graphene-Ag$_2$CO$_3$ (NG-Ag$_2$CO$_3$) composites with different weight addition ratios of NG as a visible-light-induced photocatalyst were fabricated through a facile precipitation method. It was found that NG-Ag$_2$CO$_3$ composite with a proper addition amount of NG exhibited higher photocatalytic activity and improved anti-photocorrosion than Ag$_2$CO$_3$ toward degradation of rhodamine B (RhB) in water under visible light irradiation. The rodlike Ag$_2$CO$_3$ sub-microcrystals with 4.5 wt% NG content exhibited the highest photodegradation efficiency of RhB (92% in 60 min), which was about 1.2 times of pure Ag$_2$CO$_3$ sub-microcrystals (76% in 60 min). The improved photocatalytic performance could be ascribed to the enhanced visible light absorption efficiency and more effective separation of photo-generated electron-hole pairs.

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Synthesis of nitrogen-doped graphene-\(\text{Ag}_2\text{CO}_3\) composites with enhanced photocatalytic efficiency

通讯作者: Wei, Xian-Wen Key Laboratory of Functional Molecular Solids, Ministry of Education, Anhui Normal University, 241000, China.
Identification of a new microcystin-degrading bacterium isolated from Lake Chaohu, China

Abstract A microcystin-LR (MC-LR)-degrading bacterium was isolated from Lake Chaohu, a eutrophic freshwater lake containing toxic cyanobacterial blooms. Based on the analysis of 16S rDNA gene sequence and physiobiochemical characteristics, the isolated strain, most likely belongs to the genus Bacillus with the highest sequence similarity value with Bacillus nanhaiencis strain K-W39 (JQ799091.1), was named B. nanhaiencis strain JZ-2013. The strain JZ-2013 could grow on mineral salt medium supplied with MC-LR as sole carbon and nitrogen sources. The optimal temperature and pH for strain JZ-2013 growth and MC-LR biodegradation were 30°C and 8.0, respectively. The MC-LR with the initial concentration of 15 mg/L could be consumed 80 % by strain JZ-2013 within 9 days. The existence of exogenous carbon and nitrogen sources could significantly increase the removal efficiency of MC-LR. The strain JZ-2013 can efficiently removed MC-LR of low concentration in real water sample.

主题: Toxic materials (主要); Bacteria; Bacteriology; Biodegradation; Carbon; Identification (control systems); Lakes; Microbiology; Nitrogen; Nitrogen removal; pH effects

标识符 (关键字): Carbon and nitrogen, Initial concentration, Microcystin-degrading bacterium, Microcystin-LR, Mineral salt mediums, Removal efficiencies, Sequence similarity, Toxic cyanobacterial blooms, Bacillus nanhaiencis, Identification

标题: Identification of a new microcystin-degrading bacterium isolated from Lake Chaohu, China

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Temperature Dependence of Thermal Expansion for Geophysical Minerals

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摘要 (English): A simple and straightforward method for evaluating and predicting the volume and volumetric thermal expansivity for geophysical minerals at high temperatures is developed in this paper based on the approximations that the product of the thermal expansion coefficient and the isothermal bulk modulus as well as the isothermal bulk modulus are both linearly dependent with temperature. The tests on four geophysical minerals (MgO, CaO, (Formula presented.), and (Formula presented.) lend strong support to the validity of this method. The analyses and comparisons presented here demonstrate that this method is far better than similar models given by earlier workers.

主题: Thermal expansion (主要); Elastic moduli; Geophysics; Isotherms; Minerals; Temperature distribution

分类: 421: Strength of Building Materials; Mechanical Properties; 481.3: Geophysics; 482.2: Minerals; 641.1: Thermodynamics; 951: Materials Science
Comprehensive study of equations of state for isothermal compression of α-Fe

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When applying the Rydberg-Vinet equation of state (R-V EOS) or the 3rd order Birch-Murnaghan equation of state (B-M EOS) directly to the analysis of the experimental isothermal compression data of a solid in the high-pressure phase, the three zero-pressure parameters of the equation have actually no physical meaning and there is no way to judge what values are the "best" for them. The modified Rydberg-Vinet equation of state (mR-V EOS) with an arbitrary nonzero pressure reference point is suggested and its derivation is presented at length. The mR-V EOS is physically equivalent to the R-V EOS completely for both are derived strictly from the same potential function. The advantages of the mR-V EOS over the R-V EOS and B-M EOS for describing the pressure-volume relation of a solid in the high-pressure phase are that the two free parameters in it represent the elastic properties of the real state of the solid under study and the reliability of the values obtained by the fitting may be checked with the measured ones; moreover, the fitting accuracy of the mR-V EOS, though with fewer free parameters, is not less than the other ones. The test on ε-Fe in the isothermal compression up to pressure 330 GPa has lent strong support to the validity of the mR-V EOS.
Analysis of the relations for temperature dependence of elastic constants of solids

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出版物信息: High Temperatures - High Pressures 44.2 (Jan 1, 2015): 117-123.

Abstract (English): The relations, that have been developed based on three different assumptions of the isothermal Anderson-Gruneisen parameter and the method of generalization as suggested by Tallon [J. Phys. Chem. Solids 41, (1980) 837], for temperature dependence of elastic constants of solids are analysed in the paper. It is concluded that, as far as the goodness of fit is concerned, these relations are identical and further theoretical and experimental studies on the reasonableness of these assumptions are still necessary.

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主题: Temperature distribution (主要); Elastic constants

分类: 641.1: Thermodynamics; 931.2: Physical Properties of Gases, Liquids and Solids

标识符 (关键字): Anderson-Gruneisen parameters, Goodness of fit, Ionic solids, Temperature dependence, The anderson-gruneisen parameter

标题: Analysis of the relations for temperature dependence of elastic constants of solids

通讯作者: Fang, Zheng-Hua Department of Physics, Anhui Normal University, 241000, China.

语言: 英文

摘要语言: English
Kaleidoscope of supersolid phases of interacting hard-core bosons on the dice lattice

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摘要 (English): The stability of supersolid (SS) state in lattice boson model is highly dependent on lattice topology and particle-particle interaction. We investigate hard-core bosons on dice lattice where the bosons interact via nearest-neighbor (NN) repulsion either on whole lattice or on sublattices, by using large-scale quantum Monte Carlo simulations which are based on a continuous-time worm algorithm. In the case with NN repulsion on the whole lattice, we confirm the particle density modulation which arises from the asymmetry between sublattices — honeycomb and triangular sublattices — of dice lattice. We then place emphasis on the
case with NN repulsion on the sublattices, and demonstrate spontaneously broken translational symmetries on
different sublattices which lead to various crystalline orders. By evaluating the coexistence of crystalline order
and superfluidity, we identify a variety of SS phases and establish a rich phase diagram. The microscopic
pictures of these SS phases are figured out. Further, we demonstrate paradigmatic examples of first-order solid-
to-SS and SS-to-SS quantum phase transitions.

主题: Bosons (主要); Continuous time systems; Crystalline materials; Intelligent systems; Monte Carlo methods;
Phase diagrams; Phase transitions; Quantum theory; Topology

分类: 531: Metallurgy and Metallography; 531.2: Metallography; 701: Electricity and Magnetism; 723.4: Artificial
Intelligence; 921: Applied Mathematics; 921.4: Combinatorial Mathematics, Includes Graph Theory, Set Theory;
922.2: Mathematical Statistics; 931.3: Atomic and Molecular Physics; 931.4: Quantum Theory; 961: Systems
Science

标识符 (关键字): Crystalline order, Nearest neighbors, Particle densities, Particle-particle interactions, Quantum
Monte Carlo simulations, Quantum phase transitions, Solid State and Materials, Translational symmetry

标题: Kaleidoscope of supersolid phases of interacting hard-core bosons on the dice lattice

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语言: 英文
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Measurement of aerosol optical properties using a chernin multipass cell

作者: Zhang, Qilei 1 ; Xu, Xuezhe 2 ; Zhao, Weixiong 2 ; Cui, Zhifeng 1 ; Zhang, Weijun 2 1 School of Physics and Electronic Information, Anhui Normal University, 241000, China zhangqilei08@126.com 2 Anhui Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, 230031, China wjzhang@aiofm.ac.cn

出版物信息: Guangxue Xuebao/Acta Optica Sinica 35.9 (Jan 1, 2015).

摘要 (English):  Using the Chernin multipass cell for measurement of aerosol extinction coefficient is reported. Within 38.4 m absorption optical path can realize detection sensitivity to 18 Mm\(^{-1}\) (5 s integrating time, and 30 times average). Combining a laboratory aerosol generation system, the extinction coefficients of 250 nm diameter monodispersed ammonium sulfate aerosol are measured under different particle concentrations. Three cross sections of 1.410×10\(^{-9}\), 3.727×10\(^{-10}\), 2.948×10\(^{-10}\) cm\(^2\) for ammonium sulfate aerosols at 300, 532, 532 nm is obtained, respectively. Error analysis carried out on the experimental results shows that this system can be used in the quantitative study of aerosol optical properties.

主题: Optical properties (主要); Aerosols; Spectroscopy

分类: 741.1: Light and Optics

标识符 (关键字): Aerosol extinction coefficient, Aerosol generation, Aerosol optical property, Ammonium sulfate aerosols, Detection sensitivity, Extinction coefficients, Particle concentrations, Quantitative study, Aerosol, Chernin cell

标题: Measurement of aerosol optical properties using a chernin multipass cell

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语言: 英文

摘要语言: English

文档类型: Article

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Analysis on the effect of a balanced diet on the body mass control and their body tissues for athletes

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ProQuest 文档链接

摘要 (English): This paper aims to analyze the effect of a balanced diet on the body mass control and their body tissues for athletes. In this paper, one healthy female gymnastics athlete was voluntarily included as the study object that had a clear idea of the whole research schema and supervision index. Her body composition before weight control was as follows: 51.6 kg in body mass, 37.1 kg in muscle weight, and 11.8kg in fat, 22.9% in body fat percentage, and 29.1 kg in total water content. This athlete enjoyed a little higher body fat and the first goal for weight loss was less fat. This paper applied a combined method of slow weight control with diet control and more exercises so as to reduce and control her body mass. Besides, the changes of body tissues were also constantly monitored. Within 12 weeks of the weight control schema implementation, she lost 5.4 kg
in body mass, including 5.0 kg fat, 0.2 kg muscle and the decline in body mass percentage from 22.9% to 14.8%. In terms of her functional status, in the initial stage of weight control, she often felt a sense of fatigue and hunger. But she still persisted in exercises for this was under her toleration limits. Three or five days later, those feelings began to reduce or even disappear. One week later, she restored her vitality and kept a good feeling about herself with an accurate technical execution. Besides, this athlete was treated with blood routine examination at fixed time during this study. The blood routine was 134g/L before weight control and it was found a rise to 146g/L since week 3 and then it maintained between 146 and 149 g/L. This gave the hint that she acquired some improvement in her body functions during the process of weight control. In conclusion, athletes should apply the combination of diet control and more exercises in reducing and controlling the body mass. Weight control is supposed to be predominated by a slow negative energy balance. Besides, a scientific arrangement of diet and nutrition supplement is also necessary during the process of weight control.
A four-dimensional potential energy surface for the Ar-D$_2$O van der Waals complex: Bending normal coordinate dependence

作者: Wang, Shenhao 1 ; He, Shanshan 1 ; Dai, Liangchen 1 ; Feng, Eryin 1 ; Huang, Wuying 1 1 Department of Physics, Anhui Normal University, 241000, China fengbf@mail.ahnu.edu.cn

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摘要 (English): In this paper, we report a four-dimensional potential energy surface (PES) of the Ar-D$_2$O complex. The ab initio calculations are carried out by the coupled-cluster singles and doubles level with noniterative inclusion of connected triples [CCSD(T)] method with a large basis set supplemented with bond functions. The PES includes explicit dependence on the $v_2$ bending normal coordinate of Q$_2$ the D$_2$O molecule. Two vibrationally averaged PESs with D$_2$O molecule in its ground and first $v_2$ excited vibrational states are generated by integrating over the Q$_2$ normal coordinate. Based on these two PESs, the bound state energies are determined and used in the infrared spectra prediction. The theoretical frequencies for 104 infrared transitions of $\Pi_1'_{11}$($v_2 = 1$)$\rightarrow$$\Sigma_0''_{00}, \Sigma_1'_{11}$($v_2 = 1$)$\rightarrow$$\Sigma_0''_{00}, \Pi_1'_{01}$($v_2 = 1$)$\rightarrow$$\Sigma_0''_{01}$, and $\Pi_1'_{01}$($v_2 = 1$)$\rightarrow$$\Sigma_1'_{01}$ of Ar-D$_2$O complex are in good agreement with the available experimental values.

主题: Potential energy (主要); Calculations; Molecular physics; Molecules; Numerical methods; Potential energy surfaces; Quantum chemistry; Van der Waals forces


标识符 (关键字): Ab initio calculations, Bound-state energies, Coupled-cluster singles and doubles, Excited vibrational state, Experimental values, Explicit dependences, Infrared transition, Van der Waals complex

链接: Check for full text via 360 Link, Order Full Text from Infotrieve?
Analysis of the Interrelationship Between Melting and Fracturing of Alkali Halides

Authors: Zou, Yong 1; Huang, Hulin 2; Cui, Guang Lei 3
1 College of Energy and Power Engineering, Nanjing University of Aeronautics and Astronautics, 210016, China, School of Mathematics and Physics, Anhui University of Technology, 243032, China 2 College of Energy and Power Engineering, Nanjing University of Aeronautics and Astronautics, 210016, China hlhuang@nuaa.edu.cn 3 Department of Physics, Anhui Normal University, 241000, China


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On the basis of the lattice potential energy with two forms proposed by Born–Mie and Born–Mayer, respectively, the critical interionic separations \( R_{c} \) where the lattice is fractured due to tensile force have been evaluated for alkali metal halides. The theoretical results are analyzed together with the interionic separations \( R_{m} \) determined by the melting temperature and the help of the isobaric equation of state. A new and simple interrelationship between \( R_{c} \) and \( R_{m} \) is obtained, and the crystal melting behavior can be accordingly predicted for NaCl-structure ionic crystals.

**Title:** Analysis of the Interrelationship Between Melting and Fracturing of Alkali Halides

**Authors:** Huang, Hulin

**Journal:** International Journal of Thermophysics

**DOI:** http://dx.doi.org/10.1007/s10765-015-1896-1
Palladium-catalyzed Hiyama coupling reaction of arylsulfonyl hydrazides under oxygen

**Authors:** Miao, Hui; Wang, Fenhua; Zhou, Shuangliu; Zhang, Guangchao; Li, Yang

**Institution:** Key Laboratory of Functional Molecular Solids, College of Chemistry and Materials Science, Anhui Normal University, 241000, China

**Email:** shuangliu_zhou@126.com

**Publication Details:** Organic and Biomolecular Chemistry 13.16 (Apr 28, 2015): 4647-4651.

**Abstract (English):** Palladium-catalyzed Hiyama cross-coupling reactions of various arylsulfonyl hydrazides with a wide variety of aryl silanes have been achieved in good to excellent yields under simple conditions. The newly developed catalytic system does not require the use of expensive silver- or copper-based stoichiometric oxidants and can be accelerated by the addition of TBAT under an atmosphere of oxygen. The reported Hiyama-type coupling reactions are tolerant to common functional groups, making these transformations attractive alternatives to the traditional cross-coupling approaches.

**Keywords:** Catalytic system, Copper-based, Coupling reaction, Cross-couplings, Hiyama coupling, Hiyama cross-coupling reaction, Palladium-catalyzed, Stoichiometric oxidant

**Title:** Palladium-catalyzed Hiyama coupling reaction of arylsulfonyl hydrazides under oxygen

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**Language:** English

**Abstract Language:** English

**Document Type:** Article

**Publication Name:** Organic and Biomolecular Chemistry

**Volume:** 13

**Issue:** 16
Superior performance asymmetric supercapacitors based on ZnCo$_2$O$_4$@MnO$_2$ core-shell electrode

作者: Ma, Wenqin 1 ; Nan, Honghong 1 ; Gu, Zhengxiang 1 ; Geng, Baoyou 1 ; Zhang, Xiaojun 1 1 College of Chemistry and Materials Science, Center for Nano Science and Technology, Anhui Normal University, 241000, China xjzhang@mail.ahnu.edu.cn


摘要 (English): In this study, a hierarchical ZnCo$_2$O$_4$@MnO$_2$ core-shell nanotube arrays electrode was developed by a facile two-step method. The electrode exhibits high specific capacitance of 1981 F g$^{-1}$ (2.38 F cm$^{-2}$) at a current density of 5 A g$^{-1}$ and excellent cycling stability (5000 cycles). Furthermore, a low-cost, high-performance asymmetric supercapacitor (ASC) with ZnCo$_2$O$_4$@MnO$_2$ core-shell nanotube arrays on Ni foam (as positive electrode) and 3D porous α-Fe$_2$O$_3$ on Fe foil (as negative electrode) was successfully designed. The as-designed ASC device with an extended operating voltage window of 1.3 V achieved a specific capacitance of 161 F g$^{-1}$ at 2.5 mA cm$^{-2}$ with a maximum energy density of 37.8 W h kg$^{-1}$ and excellent stability with a capacitance retention of 91% after 5000 cycles. Furthermore, after being charged for dozens of seconds, the ZnCo$_2$O$_4$@MnO$_2$//α-Fe$_2$O$_3$-ASC can easily light up a LED. These fascinating performances indicate that the present ZnCo$_2$O$_4$@MnO$_2$ core-shell nanotube arrays with remarkable electrochemical properties could be
considered as potential electrode materials for next generation supercapacitors in high energy density storage systems.

**主题**: Electrochemical electrodes (主要); Capacitance; Capacitors; Electrodes; Electrolytic capacitors; Light emitting diodes; Manganese oxide; Nanotubes; Shells (structures); Yarn

**分类**: 408.2: Structural Members and Shapes; 701.1: Electricity, Basic Concepts and Phenomena; 704.1: Electric Components; 741.1: Light and Optics; 761: Nanotechnology; 804: Chemical Products Generally; 819.4: Fiber Products

**标识符 (关键字)**: Asymmetric supercapacitor, Capacitance retention, Electrode material, High energy densities, High specific capacitances, Negative electrode, Positive electrodes, Specific capacitance

**标题**: Superior performance asymmetric supercapacitors based on ZnCo$_2$O$_4$@MnO$_2$ core-shell electrode

**通讯作者**: Zhang, Xiaojun College of Chemistry and Materials Science, Center for Nano Science and Technology, Anhui Normal University, 241000, China.

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**摘要语言**: English

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**收录号**: 20151000594911
Photoinduced electron transfer between 2-methylanthraquinone and triethylamine in an ionic liquid: Time-resolved EPR and transient absorption spectroscopy study

Author: Zhu, Guanglai 1; Wang, Yu 1; Fu, Haiying 2; Xu, Xinsheng 1; Cui, Zhifeng 1; Ji, Xuehan 1; Wu, Guozhong 2 1 Institute of Atomic and Molecular Physics, Anhui Normal University, 241000, China zhglai@mail.ahnu.edu.cn 2 Shanghai Institute of Applied Physics, Chinese Academy of Sciences, 201800, China wuguozhong@sinap.ac.cn


Abstract (English): Photoinduced electron transfer between 2-methylanthraquinone (MeAQ) and triethylamine (TEA) in a room-temperature ionic liquid, 1-butyl-3-methylimidazolium hexafluorophosphate ([bmim][PF$_6$]), was investigated by comparing the time-resolved electron paramagnetic resonance (TR-EPR) spectroscopy and the transient absorption spectroscopy. The results of TR-EPR spectroscopy, in which MeAQ was 8 mmol L$^{-1}$ and TEA was 150 mmol L$^{-1}$, indicated that the transient radical would exist longer time in [bmim][PF$_6$] than in acetonitrile. At the delay time of 8 μs after laser excitation, the TR-EPR signal transformed from an emissive peak into an absorptive peak when the experiment was performed in [bmim][PF$_6$]. The results of the transient absorption spectroscopy, in which MeAQ was 0.1 mmol L$^{-1}$ and TEA was 2.2 mmol L$^{-1}$, showed that the efficiency and the rate of the photoinduced electron transfer reaction in [bmim][PF$_6$] were obviously lower than that in acetonitrile. It was concluded that various factors, such as concentration, viscosity and local structural transformation of the solution, have an influence on the process of photoinduced electron transfer in [bmim][PF$_6$].
A multimedia traffic classification method based on improved Hidden Markov Model

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This paper proposes an improved Hidden Markov Model (HMM) based multimedia traffic classification method. This method preserves the classical HMM model structure, and improves the performance of multimedia traffic classification by changing the emitting probability value with the position information of packet size. Theoretical analysis indicates that the new model can reduce the computational complexity of the classical HMM model. Simulation results show that the proposed method can improve the classification performance compared with the existing HMM based classification method.
Optical design of micro DLP projection based on novel light pipe

作者: Wang, Cheng 1 ; Hao, Wenliang 1 ; Tian, Liwei 1 ; Wang, Ruofei 2 ; Zhu, Xiangbing 1 1 Department of Physics, Anhui Normal University, 241000, China cheng0808066@163.com ; asd05tx@126.com 2 Chery New Energy Automotive Technology Co. Ltd, 241000, China


摘要 (English): Traditional DLP technologies can not collect and utilize the light which is reflected by the micromirrors of DMD in the "OFF" state. Aiming at this defect, one design scheme of the micro DLP projection system based on a novel light pipe was presented. This system included LEDs, light pipe, color wheel, the collimation system and projection lens. A bending light pipe was added on the base of the tapered light pipe, and a compound parabolic concentrator (CPC) was used in the input end to collect the extra light reflected by the DMD. First, the related parameters of each part were analyzed and calculated according to the nonimaging optics theory. Second, the collimation system and projection lens were optimized by ZEMAX software. Finally, the model was built and simulated in TracePro software. The simulation results show that: with the number of micromirrors in the "OFF" state growing, the improving light efficiency ability of collecting light pipe first increases then decreases. Comparing with having no collecting light pipe, the light efficiency is increased by 5.33%; light pipe improves the most light efficiency, 5.91%, when half of the micromirrors are in the "OFF" state.

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主题: Light emitting diodes (主要); Collector efficiency; Efficiency; Fiber optics; Light; Optical design

分类: 702.3: Solar Cells; 741.1: Light and Optics; 741.1.2: Fiber Optics; 913.1: Production Engineering

标识符 (关键字): Collimation system, Compound parabolic concentrator, Design scheme, DMD, Light efficiency, Non-imaging optics, Projection lens, Tapered light pipe, LED, Light pipe

标题: Optical design of micro DLP projection based on novel light pipe
Formation of a metal-organic framework with high gas uptakes based upon amino-decorated polyhedral cages

Authors: Yun, Ruirui 1; Cui, Ranran 1; Qian, Fujun 1; Cao, Xiaoyan 1; Luo, Shizhong 1; Zheng, Baishu 2 1 Key Laboratory of Functional Molecular Solids, College of Chemistry and Materials Science, Anhui Normal University, 241000, China; yunruirui@gmail.com 2 School of Chemistry and Chemical Engineering, Hunan University of Science and Technology, 411201, China

Publication Information: RSC Advances 5.4 (Jan 1, 2015): 2374-2377.
A new three-dimensional metal-organic framework 1 was solvothermally synthesized by 1,2,4-triazole and 2-aminoterephthalic acid, and structurally characterized. 1 features a three-dimensional structure with one-dimensional pores along the c axis of 6 × 6 Å². Activated 1 exhibits an H₂ uptake capacity at 77 K. Importantly, it shows excellent enthalpy of CO₂ (35 kJ mol⁻¹) and methane (24 kJ mol⁻¹), compared to previous porous materials.

Yun, Ruirui Key Laboratory of Functional Molecular Solids, College of Chemistry and Materials Science, Anhui Normal University, 241000, China.

DOI: http://dx.doi.org/10.1039/c4ra14607g
URL: http://pubs.rsc.org/en/journals/journalissues
Ultrathin porous nickel-cobalt hydroxide nanosheets for high-performance supercapacitor electrodes

作者: Zheng, Xiaoting 1; Gu, Zhengxiang 1; Hu, Qingqing 1; Geng, Baoyou 1; Zhang, Xiaojun 1 1 Key Laboratory for Functional Molecular Solids of the Education Ministry of China, Center for Nano Science and Technology, Anhui Normal University, 241000, China  

摘要 (English): In this work, ultrathin porous nickel-cobalt layered double hydroxide (Ni-Co LDH) hybrid nanosheets on metal nickel sheets are synthesized via a facile hydrothermal method without any adscititious surfactant. The fabricated Ni-Co LDH hybrid nanosheet-based electrodes for supercapacitors in aqueous electrolyte exhibit a significantly enhanced specific capacitance (2184 F g⁻¹ at 1 A g⁻¹) and energy density (91.76 W h kg⁻¹ at 825.84 W kg⁻¹) due to the pronounced synergistic effect between Ni²⁺ and Co²⁺. Meanwhile, the Ni-Co LDH hybrid nanosheets as electrode materials have excellent long-life cycling stability, retaining 88.5% of the initial capacitance after 2000 cycles. Thereby, the Ni-Co nanocomposites are promising electrode materials for high-energy-density long-life cycling supercapacitors.

主题: Electrolytic capacitors (主要); Capacitance; Capacitors; Cobalt; Cobalt compounds; Electrodes; Hybrid materials; Nanosheets; Nickel


标识符 (关键字): Aqueous electrolyte, Electrode material, High energy densities, Hydrothermal methods, Layered double hydroxides, Specific capacitance, Supercapacitor electrodes, Synergistic effect

通讯作者: Zhang, Xiaojun Key Laboratory for Functional Molecular Solids of the Education Ministry of China, Center for Nano Science and Technology, Anhui Normal University, 241000, China.

语言: 英文
Gold-platinum bimetallic nanotubes templated from tellurium nanowires as efficient electrocatalysts for methanol oxidation reaction

作者: Lu, Chenchen 1 ; Kong, Wei 1 ; Zhang, Huying 1 ; Song, Bo 1 ; Wang, Zhenghua 1 1 Key Laboratory of Functional Molecular Solids, Ministry of Education, College of Chemistry and Materials Science, Anhui Normal University, 241000, China zhwang@mail.ahnu.edu.cn


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In this paper, gold-platinum (Au-Pt) bimetallic nanotubes with different Au/Pt ratio are successfully synthesized through a simple wet-chemical reduction route in which tellurium (Te) nanowires serve as both sacrificial template and reducing agent. The hollow nanostructure of Au-Pt nanotubes is formed due to Kirkendall effect. The as-prepared Au-Pt nanotubes can be applied as catalyst for methanol oxidation reaction, and the results indicate that the Au-Pt nanotubes with an Au/Pt ratio of 1:1 show the best electrochemical catalytic performances. Furthermore, the catalytic activity of the Au-Pt nanotubes is also better than Pt nanotubes and commercial Pt/C catalyst.

Gold-platinum bimetallic nanotubes templated from tellurium nanowires as efficient electrocatalysts for methanol oxidation reaction

Wang, Zhenghua

Key Laboratory of Functional Molecular Solids, Ministry of Education, College of Chemistry and Materials Science, Anhui Normal University, 241000, China.

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Synthesis and characterization of gold complexes with pyridine-based SNS ligands and as homogeneous catalysts for reduction of 4-nitrophenol

Authors: Jia, Wei-Guo 1; Dai, Yuan-Chen 1; Zhang, Hai-Ning 1; Lu, Xiaoqin 1; Sheng, En-Hong 1 1 Key Laboratory of Functional Molecular Solids, Ministry of Education, Anhui Normal University, 241000, China

Abstract (English): Three gold complexes with pyridine-based SNS type ligands, 2,6-bis(1-methylimidazole-2-thione)pyridine (Bmtp), 2,6-bis(1-ethylimidazole-2-thione)pyridine (Betp) and 2,6-bis(1-isopropylimidazole-2-thione)pyridine (Bptp) have been synthesized and characterized. Reactions of HAuCl₄·H₂O with three pyridine-based SNS ligands result in the formation of the complexes [(L)AuCl₂Cl] (L = Bmtp (1); L = Betp (2) and L = Bptp (3)). All compounds are investigated by elemental analysis, NMR, MS and UV-Vis as well as IR spectral analysis. The molecular structure of 3 has been confirmed by X-ray crystallography. Moreover, all gold complexes are efficient homogeneous catalysts and catalyze the reduction of 4-nitrophenol (4-NP) to 4-nitroaniline (4-AP) in the presence of NaBH₄ reducing agent in water. And complex 3 exhibits an exceptionally high turn over frequency (TOF) of 1.20 min⁻¹ for the reduction of 4-NP. This journal is

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Highly sensitive surface enhanced Raman scattering substrates based on Ag decorated Si nanocone arrays and their application in trace dimethyl phthalate detection
Abstract (English): Wafer-scale three-dimensional (3D) surface enhancement Raman scattering (SERS) substrates were prepared using the plasma etching and ion sputtering methods that are completely compatible with well-established silicon device technologies. The substrates are highly sensitive with excellent uniformity and reproducibility, exhibiting an enhancement factor up to 1012 with a very low relative standard deviation (RSD) around 5%. These are attributed mainly to the uniform-distributed, multiple-type high-density hot spots originating from the structural characteristics of Ag nanoparticles (NPs) decorated Si nanocone (NC) arrays. We demonstrate that the trace dimethyl phthalate (DMP) at a concentration of 10^{-7}M can be well detected using this SERS substrate, showing that the AgNPs-decorated SiNC arrays can serve as efficient SERS substrates for phthalate acid esters (PAEs) detection with high sensitivity.
A highly sensitive and direct competitive enzyme-linked immunosorbent assay for the detection of di-(2-ethylhexyl) phthalate (DEHP) in infant supplies

Authors: Zhang, Mingcui 1; Hong, Wentong 1; Wu, Xiaoyu 1; Zhang, Yue 1; Li, Fengzhu 1; Zhao, Su-Qing 2 1
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Abstract (English): A sensitive and specific direct competitive enzyme-linked immunosorbent assay (dc-ELISA) was studied in this paper for the detection of di-(2-ethylhexyl) phthalate (DEHP) based on an antigen-coating format. The DEHP-specific polyclonal antibody was raised in rabbits and used to construct the dc-ELISA for the measurement of DEHP. The conjugates of the antibody with horseradish peroxidase (HRP) were used as the detection probe. Under optimal conditions, the assay had a detection limit (LOD) of about 0.0042 ng mL\(^{-1}\), with an apparent linear range of \(10^{-3}-10^{3}\) ng mL\(^{-1}\) \((R^2 = 0.998)\). The cross-reactivity with six other structurally related phthalate esters was below 1%. The recoveries of DEHP ranged from 80.8% to 119.2% indicating that the method was successfully applied for the determination of DEHP in infant supplies.
Adsorption and removal of sulfonic dyes from aqueous solution onto a coordination polymeric xerogel with amino groups

作者: Cheng, Yong 1; Feng, Qichun 1; Ren, Xiaoyan 1; Yin, Ming 1; Zhou, Yinghua 1; Xue, Ziling 2

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2 Department of Chemistry, The University of Tennessee, 37996-1600, United States


摘要 (English): A coordination polymeric xerogel based on copper acetate and 2-amino-5-mercpto-1,3,4-thiadiazole was prepared and characterized by SEM, EDX and FTIR, respectively. It exhibits favorable adsorption behavior for sulfonic dyes such as Thymol blue, Acid fuchsin and Methyl orange. The effects of various experimental parameters including initial dye concentrations, exposure time, temperature, pH and ion strength were investigated. Adsorption kinetics, isotherms and adsorption mechanism were also analyzed. The desorption profile revealed that a significant portion (>80%) of sulfonic dyes could be desorbed by using sodium chloride aqueous solution as eluting agent.

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主题: Adsorption (主要); Azo dyes; Desorption; pH effects; Polymers; Solutions; Stripping (dyes); Xerogels

分类: 801: Chemistry; 801.1: Chemistry, General; 802.3: Chemical Operations; 803: Chemical Agents and Basic Industrial Chemicals; 804: Chemical Products Generally; 815.1: Polymeric Materials

标识符 (关键字): Adsorption behavior, Adsorption kinetics, Adsorption mechanism, Copper acetates, Desorption profiles, Experimental parameters, Exposure-time, Initial dye concentration, Coordination Polymeric Xerogel, Sulfonic dye

标题: Adsorption and removal of sulfonic dyes from aqueous solution onto a coordination polymeric xerogel with amino groups

通讯作者: Cheng, Yong Laboratory of Functional Molecular Solids, Ministry of Education, College of Chemical and Materials Science, Anhui Normal University, 241000, China.

语言: 英文

摘要语言: English

文档类型: Article

出版物名称: Colloids and Surfaces A: Physicochemical and Engineering Aspects

卷: 485
Structural evolution of Ge-rich Si$_{1-x}$Ge$_x$ films deposited by jet-ICPCVD

**Authors:** Wang, Yu 1; Yang, Meng 1; Wang, Gang 1; Wei, Xiaoxu 2; Wang, Junzhuan 2; Li, Yun 2; Zou, Zewen 3; Zheng, Youdou 2; Shi, Yi 2 1 Key Laboratory of Advanced Photonic and Electronic Materials, School of Electronic Science and Engineering, Nanjing University, 210093, China 2 Key Laboratory of Advanced Photonic and Electronic Materials, School of Electronic Science and Engineering, Nanjing University, 210093, China, Collaborative Innovation Center of Advanced Micro-structures, Nanjing University, 210093, China 3 College of Physics and Electronics Information, Anhui Normal University, 241000, China

**Publication Information:** AIP Advances 5.11 (Nov 1, 2015).

**Abstract (English):** Amorphous Ge-rich Si$_{1-x}$Ge$_x$ films with local Ge-clustering were deposited by dual-source jet-type inductively coupled plasma chemical-vapor deposition (jet-ICPCVD). The structural evolution of the deposited films annealed at various temperatures (Ta) is investigated. Experimental results indicate that the crystallization occurs to form Ge and Si clusters as Ta = 500 °C. With raising Ta up to 900 °C, Ge clusters percolate together and Si diffuses and redistributes to form a Ge/SiGe core/shell structure, and some Ge atoms
partially diffuse to the surface as a result of segregation. The present work will be helpful in understanding the structural evolution process of a hybrid SiGe films and beneficial for further optimizing the microstructure and properties.

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主题: Crystal atomic structure (主要); Amorphous films; Amorphous silicon; Chemical vapor deposition; Germanium; Inductively coupled plasma; Plasma CVD; Silicon; Surface segregation

分类: 549.3: Others, incl. Bismuth, Boron, Cadmium, Cobalt, Mercury, Niobium, Selenium, Silicon, Tellurium; 802.2: Chemical Reactions; 813.1: Coating Techniques; 931.3: Atomic and Molecular Physics; 932.3: Plasma Physics; 933.2: Amorphous Solids

标识符 (关键字): Core/shell structure, Deposited films, Dual source, Inductively coupled plasma chemical vapor deposition, Microstructure and properties, Si clusters, Si-Ge films, Structural evolution

标题: Structural evolution of Ge-rich Si\textsubscript{1-x}Ge\textsubscript{x} films deposited by jet-ICPCVD

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摘要语言: English

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更新: 2015-11-22
Flexible superior electrode architectures based on three-dimensional porous spinous α-Fe₂O₃ with a high performance as a supercapacitor

Authors: Nan, Honghong 1 ; Yu, Liutao 1 ; Ma, Wenqin 1 ; Geng, Baoyou 1 ; Zhang, Xiaojun 1 1 Key Laboratory for Functional Molecular Solids of the Education Ministry of China, College of Chemistry and Materials Science, Anhui Normal University, 241000, China xjzhang@mail.ahnu.edu.cn


Abstract (English): Flexible supercapacitors have recently attracted increasing attention as they show unique promising advantages, such as flexibility and shape diversity, and they are light-weight and so on. Herein, we designed a series of 3D porous spinous iron oxide materials synthesized on a thin iron plate through a facile method under mild conditions. The unique nanostructural features endow them with excellent electrochemical performance. The electrochemical properties of the integrated electrodes as active electrode materials for supercapacitors have been investigated using different electrochemical techniques including cyclic voltammetry, and galvanostatic charge-discharge in Na₂SO₄ and LiPF₆/EC:DEC electrolyte solutions. These integrated electrodes showed high specific capacitance (as high as 524.6 F g⁻¹ at the current density of 1 A g⁻¹) in 1.0 M Na₂SO₄ (see Table S1). Moreover, the integrated electrodes also show high power densities and high energy densities in a LiPF₆/EC:DEC electrolyte solution; for example, the energy densities were 319.3, 252.5, 152.1, 74.13 and 38.6 W h kg⁻¹ at different power densities of 8.81, 21.59, 56.65, 92.09 and 152.64 kW kg⁻¹, respectively. Additionally, the flexible superior electrode exhibited excellent stability with capacitance retention of 92.9% after 5000 cycles. Therefore, such flexible integrated devices might be used in smart and portable electronics.

Theme: Electrochemical electrodes (主要); Capacitance; Capacitors; Cyclic voltammetry; Electric discharges; Electrodes; Electrolytes; Electrolytic capacitors; Flexible electronics; Lithium compounds; Sodium

Category: 549.1: Alkali Metals; 701.1: Electricity, Basic Concepts and Phenomena; 702: Electric Batteries and Fuel Cells; 704.1: Electric Components; 715: Electronic Equipment, General Purpose and Industrial; 803: Chemical Agents and Basic Industrial Chemicals; 804: Chemical Products Generally; 942.2: Electric Variables Measurements

Keywords: Active electrode materials, Electrochemical performance, Electrochemical techniques, Electrode architecture, Electrolyte solutions, Galvanostatic charge discharges, High energy densities, High specific capacitances

Title: Flexible superior electrode architectures based on three-dimensional porous spinous α-Fe₂O₃ with a high performance as a supercapacitor

Corresponding Author: Zhang, Xiaojun Key Laboratory for Functional Molecular Solids of the Education Ministry of China, College of Chemistry and Materials Science, Anhui Normal University, 241000, China.

Language: English
Vibrational resonance and nonlinear vibrational resonance in square-lattice neural system

Vibrational resonance and nonlinear vibrational resonance in square-lattice neural system

作者: Sun, Run-Zhi 1 ; Wang, Zhi-Zhong 1 ; Wang, Mao-Sheng 1 ; Zhang, Ji-Qian 1 1 College of Physics and Electronic Information, Anhui Normal University, 241000, China maosheng@ustc.edu
出版物信息: Wuli Xuebao/Acta Physica Sinica 64.11 (Jan 1, 2015).

摘要 (English): Response characteristics of FitzHugh-Nagumo neurons to low frequency signal have been investigated by numerical simulation. Neurons are arranged on a square-lattice and are subjected to two
frequency signals. Results show that, vibrational resonance of the membrane potential can be induced by varying the amplitude of the high-frequency signal, when the control parameter is selected in the excitable region. In addition, the responses of neurons to higher harmonics of low-frequency signal have been studied, and nonlinear vibrational resonances are also found. With the increase of frequency in the low-frequency signal, the response of the system to low-frequency signal can resonate. Thus, the double resonance can occur by changing the frequency in low-frequency signal and the amplitude in high-frequency signal. Moreover, effects of electrical synapses and chemical synapses on vibrational resonance and nonlinear vibrational resonance of the neurons have also been studied. Effect of the number of neurons, which are subjected to two frequency signals in the square-lattice, on the response characteristic of the system is also studied. It is found that the response characteristic of the electrical coupling neurons is quite different from that of chemical coupling neurons.

主题: Resonance (主要); Crystal lattices; Neural networks; Neurons

分类: 461.1: Biomedical Engineering; 461.9: Biology; 701: Electricity and Magnetism; 933.1.1: Crystal Lattice

标识符 (关键字): Electrical synapsis, Fitzhugh Nagumo neurons, High frequency signals, Low-frequency signals, Membrane potentials, Response characteristic, Two frequency signals, Vibrational resonance, FitzHugh-Nagumo neuron, Nonlinear vibrational resonance

标题: Vibrational resonance and nonlinear vibrational resonance in square-lattice neural system

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语言: 英文

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Optical trapping Rayleigh dielectric particles with focused partially coherent dark hollow beams

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摘要 (English): The focusing properties of coherent and partially coherent dark hollow beams (DHBs) through a paraxial ABCD optical system are theoretically investigated. It is found that the evolution behavior of the intensity distribution of focused partially coherent DHBs is closely related to their spatial coherence. The radiation forces (RFs) of focused coherent and partially coherent DHBs acting on a Rayleigh dielectric particle are also theoretically investigated. Numerical results show that the coherent and partially coherent DHBs can be focused into a tight focal spot, which can be used to stably trap a Rayleigh dielectric particle with high refractive index at the focus point. The influences of different beam parameters, including the spatial coherence, beam waist width, beam order, and hollow parameter of partially coherent DHBs, on the RFs and the trap stiffness are analyzed in detail. Finally, the stability conditions for effective trapping particles are also discussed.

主题: Dielectric properties (主要); Optical systems; Refractive index; Stiffness

标识符 (关键字): ABCD optical systems, Dark hollow beam, Focusing properties, High refractive index, Intensity distribution, Radiation forces, Rayleigh dielectrics, Trap stiffness, partially coherent dark hollow beam, radiation force

标题: Optical trapping Rayleigh dielectric particles with focused partially coherent dark hollow beams

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语言: 英文

摘要语言: English
CO$_2$ capture on h-BN sheet with high selectivity controlled by external electric field

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Developing highly efficient sorbent materials for CO$_2$ separation and capture from gas mixture is most important for reducing impact of CO$_2$ on the environment. On the basis of density functional theory calculations with dispersion correction, we show that hexagonal boron nitride sheet (h-BN), when under an external electric field, can become an effective sorbent for CO$_2$ capture. In the absent of the electric field, CO$_2$ molecules are physisorbed on the h-BN sheet. Under the external electric field, the adsorption of CO$_2$ molecules on h-BN monolayer can be strongly strengthened. Compared to CO$_2$, the adsorption of H$_2$, N$_2$, CH$_4$, CO, or H$_2$O on h-BN sheet is notably weaker, indicating that the capture of CO$_2$ on h-BN sheet under the electric field is highly preferred over other gas molecules. The calculated ratio of adsorption rate constant of CO$_2$ to other gas molecule can be as high as $10^5$. Moreover, the capture of CO$_2$ molecule on h-BN sheet is reversible; that is, the adsorbed CO$_2$ can be released by shutting down the applied electric field. This study suggests potential application of h-BN sheet not only for CO$_2$ capture but also as a gas-storage material with high selectivity. The degree of selectivity can be controlled by an applied external electric field.
First-Principles Study on Structural, Electronic, and Spectroscopic Properties of $\gamma$-Ca$_2$SiO$_4$:Ce$^{3+}$ Phosphors

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Abstract (English): In the present work, geometric structures, electronic properties, and 4f → 5d transitions of $\gamma$-Ca$_2$SiO$_4$:Ce$^{3+}$ phosphors have been investigated by using first-principles calculations. Four categories of typical substitutions (i.e., the doping of the Ce$^{3+}$ without the neighboring dopants/defects and with the neighboring V$_{O}^{-}$, Al$^{3+}$, and V$_{Ca}^{2+}$) are taken into account to simulate local environments of the Ce$^{3+}$ located at two crystallographically different calcium sites in the $\gamma$-Ca$_2$SiO$_4$. Density functional theory (DFT) geometry
Optimization calculations are first performed on the constructed supercells to obtain the information about the local structures and preferred sites for the Ce\(^{3+}\). On the basis of the optimized crystal structures, the electronic properties of γ-Ca\(_2\)SiO\(_4\);Ce\(^{3+}\) phosphors are calculated with the Heyd-Scuseria-Ernzerhof screened hybrid functional, and the energies and relative oscillator strengths of the 4f → 5d transitions of the Ce\(^{3+}\) are derived from the ab initio embedded cluster calculations at the CASSCF/CASPT2/RASSI-SO level. A satisfactory agreement with the available experimental results is thus achieved. Moreover, the relationships between the dopants/defects and the electronic as well as spectroscopic properties of γ-Ca\(_2\)SiO\(_4\);Ce\(^{3+}\) phosphors have been explored. Such information is vital, not least for the design of Ce\(^{3+}\)-based phosphors for the white light-emitting diodes (w-LEDs) with excellent performance. (Graph Presented).
Directly carbonized lotus seedpod shells as high-stable electrode material for supercapacitors

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摘要 (English): In this work, we demonstrate a simple and effective activation-free carbonization method to prepare porous carbon from lotus seedpod shell—a kind of natural biomass. It reveals that the carbonization temperature plays a crucial role in the determination of surface areas and capacitive performances of as-obtained porous carbon samples. The pore size and specific surface area of the samples were measured to be in the ranges of 2.0–2.2 nm and 261.7–563.4 m² g⁻¹, respectively. The carbon sample obtained at a carbonization temperature of 600 °C (carbon-600) exhibits the maximum Barrett–Emmett–Teller (BET) surface area of 563.4 m² g⁻¹ and the highest specific capacitance of 165 F g⁻¹ at a current density of 0.5 A g⁻¹. More importantly, the carbon-600 sample reveals unexceptionable capacitance retention of 95.3 % after 10,000 charge–discharge cycles, clearly indicating its excellent cycling stability. This work gives a simple and efficient approach for producing cost-effective porous carbons with high performance for supercapacitors.

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主题: Carbon (主要); Capacitance; Capacitors; Carbonization; Convergence of numerical methods; Cost effectiveness; Electrolytic capacitors; Pore size; Porous materials

Directly carbonized lotus seedpod shells as high-stable electrode material for supercapacitors

Wang, Zhenghua
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Abstract

Microbial biomass carbon is continuously rich in terrestrial biomass. In this work, direct carbonization of lotus seedpod shells without any additive agent was used to prepare carbon materials, which were the electrode materials for supercapacitors. The carbon samples were tested at different carbonization conditions, and the optimized carbonization temperature was determined to be 750℃. The stability for the cyclic voltammetry of the optimized carbon sample was tested at 25℃. The specific capacitances of materials were tested by cyclic voltammetry at a voltage window of -0.7 to 0.7 V. The carbonization process was investigated to understand the influence of the carbonization temperature on its capacitance performance. In addition, the influences of the electrodes materials on the capacitance retention were also studied. The result shows the carbon materials directly carbonized from lotus seedpod shells are suitable for supercapacitors.
Carbon dots based turn-on fluorescent probes for oxytetracycline hydrochloride sensing

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出版物信息: RSC Advances 5.26 (Jan 1, 2015): 19853-19858.

摘要 (English): In this paper, we have presented a facile, economic and green one-step hydrothermal synthesis route using tannic acid as carbon source to prepare water-soluble fluorescent carbon dots (CDs). The as-prepared CDs contain distinctive catechol groups on their surfaces, which have a special response toward Fe$^{3+}$ ions. So the fluorescence emission of CDs gradually decreased with increasing Fe$^{3+}$ ions. Such fluorescence responses can be used for well quantifying Fe$^{3+}$ ions in the range of 0-5 μM with the detection limit of 24.4 nM. Most importantly, quenched fluorescence of CDs-Fe$^{3+}$ could be recovered with the addition of oxytetracycline hydrochloride based on a competition mechanism, which provides a turn-on sensing strategy for oxytetracycline hydrochloride assay. The proposed sensing system has been successfully used for the assay of oxytetracycline hydrochloride in milk samples, indicating the practical potential. This journal is

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主题: Fluorescence (主要); Carbon; Hydrothermal synthesis; Ions

分类: 741.1: Light and Optics; 801: Chemistry; 802.2: Chemical Reactions; 804: Chemical Products Generally

标识符 (关键字): Carbon source, Competition mechanism, Detection limits, Fluorescence emission, Fluorescent probes, Oxytetracyclines (OTC), Sensing systems, Watersoluble

标题: Carbon dots based turn-on fluorescent probes for oxytetracycline hydrochloride sensing

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A combined ab initio and Franck-Condon simulation study of the photodetachment spectra of the HCBr⁻ anion

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摘要 (English): Geometry optimization and harmonic vibrational frequency calculations have been performed on the X′\(\sim\)2\(A''\) state of HCBr⁻, and X′\(\sim\)1\(A'\) and a\(\sim\)3\(A''\) states of HCBr. The term energy and electron affinity of HCBr were calculated and extrapolated to the complete basis set limit. The Duschinsky matrix and displacement vector were calculated at the CCSD(T)/aug-cc-pVQZ level. The normal mode mixing effects played a minor role and can be neglected for the HCBr(X′\(\sim\)1\(A'\))→HCBr⁻(X′\(\sim\)2\(A''\)) photodetachment. Spectral simulations involved the HCBr(X′\(\sim\)1\(A'\))-HCBr⁻(X′\(\sim\)2\(A''\)) and HCBr(a\(\sim\)3\(A''\))-HCBr⁻(X′\(\sim\)2\(A''\)) photodetachments were carried out on HCBr⁻ at CCSD(T)/aug-cc-pVQZ level, respectively.

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主题: Negative ions (主要); Calculations; Electron affinity

Note: A simple method to suppress the artificial noise for velocity map imaging spectroscopy

作者: Qin, Zhengbo 1 ; Li, Chunsheng 1 ; Qu, Zehua 1 ; Tang, Zichao 2 1 Department of Physics, Anhui Normal University, 241000, China wave0403@163.com 2 State Key Laboratory of Molecular Reaction Dynamics, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, 116023, China zctang@dicp.ac.cn


摘要 (English): A simple method has been proposed to suppress artificial noise from the counts with respect to the central line (or point) for the reconstructed 3D images with cylindrical symmetry in the velocity-map imaging spectroscopy. A raw 2D projection around the z-axis (usually referred to as central line) for photodetachment, photoionization, or photodissociation experiments is pre-processed via angular tailored method to avoid the signal counts distributed near the central line (or point). Two types of photoelectron velocity-map imaging (O\(^-\) and Au\(^+\) \(\text{NH}_3\)) are demonstrated to give rise to the 3D images with significantly reduced central line noise after pre-processing operation. The major advantages of the pre-operation are the ability of suppression of central-line noise to resolve weak structures or vibrational excitation in atoms or molecules near photon threshold.

主题: Image processing (主要); Photons

分类: 741: Light, Optics and Optical Devices; 741.1: Light and Optics

标识符 (关键字): 2D projections, Artificial noise, Cylindrical symmetry, Photo-detachment, Pre-processing operations, SIMPLE method, Velocity map imaging, Vibrational excitation

标题: Note: A simple method to suppress the artificial noise for velocity map imaging spectroscopy

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摘要语言: English

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The variational iteration method for characteristic problem of strong damping generalized sine-Gordon equation

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摘要 (English): A class of nonlinear strong damping sine-Gordon disturbed evolution differential equation is studied which appears widely in mathematics and mechanics. Firstly, we introduce a traveling wave transformation, and obtain the exact solution of degenerate equation. Then a functional calculating method for variational iteration is constructed, thus an iterative expansion is found. Finally, the approximate traveling wave analytic solutions for the original strong damping generalized sine-Gordon disturbed evolution equation are found. The arbitrary order approximate solutions, and the simple variational iteration method are obtained with higher accuracy. The approximate analytic solution can make up for the imperfection of the simple numerical simulation solution.

主题: sine-Gordon equation (主要); Damping; Differential equations; Iterative methods; Nonlinear equations

分类: 921: Applied Mathematics; 931.1: Mechanics

标识符 (关键字): Approximate analytic solutions, Approximate solution, Degenerate equation, Evolution differential equations, Evolution equations, Strong damping, Traveling wave, Variational iteration method
Solvothermal synthesis of octahedral NiFe$_2$O$_4$ nanocrystals and catalytic properties for the reduction of some aromatic nitrocompounds
In this paper, we report the successful synthesis of octahedral NiFe$_2$O$_4$ nanocrystals with room-temperature ferrimagnetism via a mixed solvothermal process at 170 °C for 15 h, using Fe(NO$_3$)$_3$ and NiCl$_2$ as starting reagents. The phase and morphology of the as-prepared product is characterized by means of powder X-ray diffraction, energy dispersive spectrometry, selected area electron diffraction (SAED), (high resolution) transmission electron microscopy, and scanning electron microscopy. Experiments showed that the as-prepared octahedral NiFe$_2$O$_4$ nanocrystals owned strong catalytic activity for the reduction of some aromatic nitro-compounds such as 4-nitrophenol, 2-nitroaniline, 4-nitroaniline, and 2,4-dinitrophenol. Under the presence of 9 mg NiFe$_2$O$_4$ nanocrystals, the rate constants of the reductive reactions were in turn $3.16 \times 10^{-2}$ min$^{-1}$ for 4-nitrophenol, $4.28 \times 10^{-2}$ min$^{-1}$ for 2-nitroaniline, $6.79 \times 10^{-2}$ min$^{-1}$ for 4-nitroaniline, and $3.26 \times 10^{-2}$ min$^{-1}$ for 2,4-dinitrophenol. Moreover, the present catalyst could be conveniently recycled due to its magnetism. After ten cycles, its catalytic efficiency did not obviously decrease.
Fe/N/C electrocatalysts for oxygen reduction reaction in PEM fuel cells using nitrogen-rich ligand as precursor

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Abstract (English): High temperature pyrolysis can significantly improve the activity and stability of Fe-based catalysts. However, unwanted iron nanoparticles, which are proven inactive to oxygen reduction reaction (ORR), will form under this procedure. Herein, a nitrogen-rich and hindrance multifunctional 6,7-di(pyridin-2-yl)pteridine-2,4-diamine (DPPD) monomer was deliberately designed and synthesized. High content of thermally stable nitrogen in DPPD can increase the degree of coordination with iron and provide a high content of active nitrogen after pyrolysis. Distorted nitrogen-rich ferrous complex polymers were successfully prepared to keep iron ions well separated and prevent them from aggregating during the heat treatment. Carbon-supported Fe-based catalysts with different initial iron loadings from 0.2 to 4.0 wt % were obtained.
Transmission electron microscopy (TEM) revealed that there were no obvious nanocrystals observed, even the initial iron loading was up to 2.0 wt %. The electrochemical performance of the Fe-based catalysts was evaluated via cyclic voltammetry (CV) and linear sweep voltammetry (LSV). The result shows that an Fe-based catalyst with 2.0 wt % initial iron loading is the best ORR catalyst in acid media among all the iron loadings. Typically, in basic media, the catalyst with 2.0 wt % initial iron loading exhibits comparable electrocatalytic activity to commercial Pt/C material via an efficient four-electron-dominant ORR pathway coupled with better methanol tolerance as well as durability. XPS measurements confirmed that the outstanding activity of the catalyst with 2.0 wt % initial iron loading was likely attributed to higher content of pyridinic nitrogen, providing the highest density of active site structures.

主题: Catalyst activity; Carbon; Catalysts; Cyclic voltammetry; Electrocatalysts; Electrocatalytic activity; Electrochemical performance; Fuel cells; Ionization of gases; Iron; Iron compounds; Metal ions; Nitrogen; Proton exchange membrane fuel cells (PEMFC); Reduction; Transmission electron microscopy

分类: 533: Ore Treatment and Metal Refining; 545.1: Iron; 702.2: Fuel Cells; 741.3: Optical Devices and Systems; 802.2: Chemical Reactions; 803: Chemical Agents and Basic Industrial Chemicals; 804: Chemical Products Generally; 942.2: Electric Variables Measurements

标识符 (关键字): Active site structure, Degree of coordination, Electrocatalytic activity, Electrochemical performance, High-temperature pyrolysis, Linear sweep voltammetry, Methanol tolerance, Oxygen reduction reaction

标题: Fe/N/C electrocatalysts for oxygen reduction reaction in PEM fuel cells using nitrogen-rich ligand as precursor

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Flowerlike copper(II)-based coordination polymers particles: Rapid room-temperature fabrication, influencing factors, and transformation toward CuO microstructures with good catalytic activity for the reduction of 4-nitrophenol

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摘要 (English): A facile and environment-friendly approach for synthesis of flowerlike copper-based coordination polymer particles (CPPs) was reported. Copper acetate (CuAc₂) and sodium pyridine-2,3-dicarboxylate (2,3-Na₂PDC) were used as the initial reactants. The flowerlike Cu-PDC microstructures were obtained based on a simple direct precipitation between CuAc₂ and 2,3-Na₂PDC in a mixed solution of water and methanol with the volume ratio of 20:10 at room temperature. The as-obtained products were characterized by X-ray powder diffraction (XRD), scanning electron microscopy (SEM), thermogravimetric analysis (TGA), Fourier transform infrared (FTIR), and elemental analysis. Some factors to affect the morphology and size of the Cu-PDC microstructures were systematically investigated such as the molar ratio of reactants, the volume ratio of water/methanol, acetic groups, and the reaction time. It was found that flowerlike Cu-PDC microstructures could be transformed into flowerlike CuO microstructures by heat-treating in air at 350 °C for 30 min. Experiments showed that the as-obtained flowerlike CuO microstructure exhibited a high catalytic activity for the reduction of 4-nitrophenol in excess NaBH₄ solution.
Enzyme membrane reactor coupled with nanofiltration membrane process for difructose anhydride III from inulin conversion

作者: Hang, Hua 1; Bao, Shibao 1; Zhao, Meng 2; Wang, Bo 1; Zhou, Shoubiao 1; Jiang, Bo 3 1 College of Environmental Science and Engineering, Anhui Normal University, 241000, China 2006hanghua@163.com 2 Glyn O. Phillips Hydrocolloids Research Centre, Hubei University of Technology, HUT, 430068, China 3 State Key Laboratory of Food Science and Technology, Jiangnan University, 214122, China bjiang@jiangnan.edu.cn

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摘要 (English): Difructosan anhydride III (DFA III) is produced by inulin conversion with inulin fructotransferase (IFTase). The objectives of this study were to investigate enzyme membrane reactor (EMR) coupled with nanofiltration (NF) membrane system for the high concentration of DFA III from inulin conversion. The system could make IFTase recycle to reactor in the EMR performance, while the EMR permeate (mainly DFA III) was concentrated and NF permeate (water) could be recycled to reactor for dissolving inulin in the NF performance. The EMR amplification and optimal operational membranes were also explored. The results showed that the system of EMR coupled with NF membrane contained solution volume of 5 L, the molecular weight cut-off (MWCO) for ultrafiltration and nanofiltration membranes of 5 kDa and 150 Da, and DFA III concentration was enhanced to about 400 g/L. The system could provide a steady operation and be persistent for 8 runs. The research can realize material circulation (enzyme and water) and product concentration, which could also provide theoretical basis for the industrial scale-up production.

主题: Nanofiltration membranes; Bioreactors; Coupled circuits; Enzymes; Industrial research; Membranes; Nanofiltration; Polysaccharides; Recycling

分类: 452.3: Industrial Wastes; 713.5: Other Electronic Circuits; 802.1: Chemical Plants and Equipment; 802.3: Chemical Operations; 804.1: Organic Compounds; 901.3: Engineering Research; 951: Materials Science

标识符 (关键字): DFA III concentrated, Difructose anhydride III, Enzyme membrane reactor, Industrial scale up, Material circulation, Membrane system, Molecular weight cutoff, Product concentration, Inulin conversion

语言: 英文

摘要语言: English

文档类型: Article
Electronic properties of Ce$^{3+}$-doped Sr$_3$Al$_2$O$_5$Cl$_2$: A combined spectroscopic and theoretical study

作者: Ning, Lixin 1; Zhou, Cuicui 1; Chen, Wanping 2; Huang, Yucheng 1; Duan, Changkui 3; Dorenbos, Pieter 4; Tao, Ye 5; Liang, Hongbin 2

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摘 要 (English): Photoluminescence properties of Ce-doped Sr$_3$Al$_2$O$_5$Cl$_2$ crystals prepared by a solid-state reaction method are first investigated with excitation energies in the vacuum-ultraviolet (VUV) to ultraviolet (UV)
Six bands are observed in the excitation spectrum of the Ce$^{3+}$ 5d → 4f emission at 15 K. The highest energy band is attributed to the host excitonic absorption, from which the band gap energy of the host is estimated to be around 7.2 eV. The four lowest energy bands are assigned to the 4f$_{1} \rightarrow$ 5d$_{1,4}$ transitions of Ce$^{3+}$ located on the three distinct Sr$^{2+}$ sites in Sr$_{3}$Al$_{2}$O$_{5}$Cl$_{2}$ with almost equal probability, based on a comparison between excitation band maxima energies and 4f → 5d transition energies obtained from wave-function-based CASSCF/CASPT2 calculations with spin-orbit coupling on Ce-centered embedded clusters. The 4f$_{1} \rightarrow$ 5d$_{5}$ transition, not observed in the low-temperature excitation spectrum, is found to be overshadowed by a nearby defect-related excitonic absorption. On the basis of present experimental and calculated results for Ce-doped Sr$_{3}$Al$_{2}$O$_{5}$Cl$_{2}$, the energy-level diagram for the 4f ground states and the lowest 5d states of all trivalent and divalent lanthanide ions on the Sr$^{2+}$ sites of Sr$_{3}$Al$_{2}$O$_{5}$Cl$_{2}$ is constructed and discussed in association with experimental findings.
ZnO nanorod/nickel phthalocyanine hierarchical hetero-nanostructures with superior visible light photocatalytic properties assisted by H$_2$O$_2$

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摘要 (English): Needle-like ZnO nanorod (ZnO-NR)/2,9,16,23-tetra-phenoxy nickel phthalocyanine (TPNiPc) nanofiber hierarchical hetero-nanostructures have been successfully designed and constructed via a two-step hydrothermal approach on zinc foil. The as-prepared ZnO-NR/TPNiPc hierarchical hetero-nanostructure exhibited superior photocatalytic activities in degradation of Rhodamine B assisted by H$_2$O$_2$ under visible light irradiation with excellent efficiency, recyclability and stability. The intermolecular electron transfer in the process of photocatalysis was further confirmed by the enhanced photocurrent. This method offers a simple, economical, and convenient way to obtain a highly efficient visible-light photocatalyst based on ZnO, showing great industrial application potential in eliminating the organic pollutants from wastewater.

主题: Light (主要); Nanorods; Nanostructures; Nitrogen compounds; Organic pollutants; Photocatalysis; Photodegradation; Zinc oxide

分类: 741.1: Light and Optics; 761: Nanotechnology; 804.1: Organic Compounds; 804.2: Inorganic Compounds; 933: Solid State Physics
ZnO nanorod/nickel phthalocyanine hierarchical hetero-nanostructures with superior visible light photocatalytic properties assisted by $\text{H}_2\text{O}_2$

通讯作者: Wang, Xiuhua Key Laboratory of Functional Molecular Solids, Ministry of Education, College of Chemistry and Materials Science, Anhui Normal University, 241000, China.
Understanding the influence of interest rate liberalization on economic structure and monetary policy

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出版物信息: Journal of Advanced Computational Intelligence and Intelligent Informatics 19.4 (Jan 1, 2015): 500-507.

摘要 (English): In this paper, a dynamic stochastic general equilibrium model with price stickiness is constructed to analyze quantitatively the effect of interest rate liberalization on economic structure and monetary policy. Using parameter calibration and Bayes estimation, we analyze the impulse responses and numerical simulation of the external shocks of technology shocks and monetary policy shock. The empirical results find the following conclusion: Firstly, the interest rate liberalization is conducive to economic restructuring as the investment ratio and capital growth is suppressed and the household and government consumption ratio is promoted. Secondly, the interest rate liberalization can lower economic fluctuation, and enhance the defense ability against external shocks such as technological shocks and monetary policy shocks. Moreover, the interest rate liberalization is help to dredge the monetary policy transmission channels as the interest rate shocks on the real economy is gradually increased.

主题: Economics (主要); Stochastic models; Stochastic systems

分类: 922.1: Probability Theory; 961: Systems Science; 971: Social Sciences


标题: Understanding the influence of interest rate liberalization on economic structure and monetary policy

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语言: 英文

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Dynamics of the nematic-isotropic sharp interface for the liquid crystal

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摘要 (English): In this paper, we derive the sharp interface model of the nematic-isotropic phase transition from the Landau-de Gennes theory by using the matched asymptotic expansion method. The model includes the evolution equation of the velocity and director field of the liquid crystal, the sharp interface, and the Young-Laplace jump condition on the interface.

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主题: Phase interfaces (主要); Liquid crystals; Liquids

分类: 931.2: Physical Properties of Gases, Liquids and Solids
In this paper, we present a novel memory access reduction scheme (MARS) for two-dimension fast cosine transform (2-D FCT). It targets programmable DSPs with high memory-access latency. It reduces the number of memory accesses by: 1) reducing the number of weighting factors and 2) combining butterflies in vector-radix 2-D FCT pruning diagram from two stages to one stage with an efficient structure. Hardware platform based on general purpose processor is used to verify the effectiveness of the proposed method for vector-radix 2-D FCT pruning implementation. Experimental results validate the benefits of the proposed method with reduced memory access, less clock cycle and fewer memory space compared with the conventional implementation.
Algebraic approach of software reliability estimation based on architecture analysis

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Abstract (English): An algebraic approach of reliability estimation is proposed, which aims at the diversity of architecture styles in complex software systems. The approach is built on algebraic modeling for software architecture and analyzes the characteristic of component interaction. It provides abstract algebraic paradigms for basic structures. By setting up the mapping relation between the paradigms and the system states, the computational rules of reliability parameters and a process of the overall assessment for system reliability are established. Because of the formal features of the algebraic method applied, the process has significant advantages in dealing with the nested structure and calculating automatically. Finally, in order to illustrate the applicability and effectiveness of the proposed approach, the reliability analysis of an actual software system is presented.

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Subjects: Software reliability (主要); Algebra; Computer software; Reliability; Reliability analysis; Software architecture

Classification: 723: Computer Software, Data Handling and Applications; 921.1: Algebra

Identifier (Keywords): Architecture analysis, Complex software systems, Component interaction, Reliability estimation, Reliability parameters, Software architecture style, Software reliability estimations, System reliability, Complex software system
A test for MANVOA in high-dimension data

作者: Cao, Ming-Xiang 1; Xu, Xing-Zhong 2 1 School of Mathematics and Statistics, Beijing Institute of Technology, 100081, China, School of Mathematics and Computer Science, Anhui Normal University, 241000, China caomingx@163.com 2 School of Mathematics and Statistics, Beijing Institute of Technology, 100081, China xuxz@bit.edu.cn
To test the equality of the mean vectors in MANOVA with high dimensional data, a test was proposed. The test permits arbitrary relationship between the data size and the data dimension. The asymptotic distributions were obtained in the null and non-null hypotheses under mild conditions. Simulation results illustrated that the proposed test is superior to the existing test in some cases.
Ultraviolet photodissociation dynamics of the n-propyl and i-propyl radicals

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Abstract (English): Ultraviolet (UV) photodissociation dynamics of jet-cooled n-propyl (n-C₃H₇) radical via the 3s Rydberg state and i-propyl (i-C₃H₇) radical via the 3p Rydberg states are studied in the photolysis wavelength region of 230-260 nm using high-n Rydberg atom time-of-flight and resonance enhanced multiphoton ionization techniques. The H-atom photofragment yield spectra of the n-propyl and i-propyl radicals are broad and in good agreement with the UV absorption spectra. The H + propene product translational energy distributions, P(Eₜ)',s, of both n-propyl and i-propyl are bimodal, with a slow component peaking around 5-6 kcal/mol and a fast one peaking at ~50 kcal/mol (n-propyl) and ~45 kcal/mol (i-propyl). The fraction of the average translational energy in the total excess energy, ∣⟨fₜ⟩∣, is 0.3 for n-propyl and 0.2 for i-propyl, respectively. The H-atom product angular distributions of the slow components of n-propyl and i-propyl are isotropic, while that of the fast component of n-propyl is anisotropic (with an anisotropy parameter ~0.8) and that of i-propyl is nearly isotropic. Site-selective loss of the β hydrogen atom is confirmed using the partially deuterated CH₃CH₂CD₂ and CH₃CDCH₃ radicals. The bimodal translational energy and angular distributions indicate two dissociation pathways to the H + propene products in the n-propyl and i-propyl radicals: (i) a unimolecular dissociation pathway from the hot ground-state propyl after internal conversion from the 3s and 3p Rydberg states and (ii) a direct, prompt dissociation pathway coupling the Rydberg excited states to a repulsive part of the ground-state surface, presumably via a conical intersection.

Keywords: Dissociation pathways, Photodissociation dynamics, Photolysis wavelength, Resonance-enhanced multiphoton ionization, Translational energy distributions, Ultraviolet photodissociation, Unimolecular
dissociation, UV absorption spectrum

**Title:** Ultraviolet photodissociation dynamics of the n-propyl and i-propyl radicals

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**Continuous dependence property of BSDE with constraints**

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In this paper, we study continuous properties of adapted solutions for backward stochastic differential equations with constraints (CBSDEs in short). Comparing with many existing literatures about this topic, our case is very general in the sense that constraints are formulated by general non-negative real functions. In general case, we proved a continuous property from below and a lower semi-continuous property of the minimal super-solution of CBSDE in its effective domain. Furthermore, in the special convex case, we obtained a continuous property with the help of convex analysis.
Emission of oxygenated volatile organic compounds (OVOCs) during the aerobic decomposition of orange wastes

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Abstract (English): Oxygenated volatile organic compounds (OVOCs) emitted from orange wastes during aerobic decomposition were investigated in a laboratory-controlled incubator for a period of two months. Emission of total OVOCs (TOVOCs) from orange wastes reached 1714mg/drykg (330mg/wetkg). Ethanol, methanol, ethyl acetate, methyl acetate, 2-butanone and acetaldehyde were the most abundant OVOC species with shares of 26.9%, 24.8%, 20.3%, 13.9%, 2.8% and 2.5%, respectively, in the TOVOCs released. The emission fluxes of the above top five OVOCs were quite trivial in the beginning but increased sharply to form one "peak emission window" with maximums at days 1-8 until leveling off after 10days. This type of "peak emission window" was synchronized with the CO$_2$ fluxes and incubation temperature of the orange wastes, indicating that released OVOCs were mainly derived from secondary metabolites of orange substrates through biotic processes rather than abiotic processes or primary volatilization of the inherent pool in oranges. Acetaldehyde instead had emission fluxes decreasing sharply from its initial maximum to nearly zero in about four days, suggesting that it was inherent rather than secondarily formed. For TOVOCs or all OVOC species except 2-butanone and acetone, over 80% of their emissions occurred during the first week, implying that organic wastes might give off a considerable amount of OVOCs during the early disposal period under aerobic conditions.

Subjects: Citrus fruits (主要); Acetaldehyde; Acetone; Gas chromatography; Metabolites; Organic compounds; Volatile organic compounds; Waste disposal; Wastes

Classification: 452.3: Industrial Wastes; 452.4: Industrial Wastes Treatment; 801: Chemistry; 801.2: Biochemistry; 804.1: Organic Compounds; 821.4: Agricultural Products
Emission of oxygenated volatile organic compounds (OVOCs) during the aerobic decomposition of orange wastes

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Nonlinear circular states and their non-classical properties

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出版物信息: Guangxue Xuebao/Acta Optica Sinica 35.1 (Jan 1, 2015).

摘要 (English): In order to study the influence of nonlinearity and superposition on quantum state, by applying theoretical analysis and numerical computation, a new quantum state, namely nonlinear circular state, is studied. The nonclassical properties of the state are analyzed such as average photon number distribution, sub-Poisson distribution and squeezing effect, and its Wigner function is calculated. Through numerical analysis, the results show that with the increase of the Lamb-Dicke parameter and superposition number of quantum states, the average photon number of nonlinear circular state is increased and the sub-Poisson distribution and squeezing effect of the state are both weakened. The nonclassical properties of the state are very sensitive to nonlinear effects which are characterized by the Lamb-Dicke parameter and superposition number of quantum states.

主题: Quantum theory (主要); Multiphoton processes; Photons; Poisson distribution; Quantum optics

分类: 741.1: Light and Optics; 922.1: Probability Theory; 931.3: Atomic and Molecular Physics; 931.4: Quantum Theory

标识符 (关键字): Nonclassical properties, Nonlinear circular states, Nonlinear effect, Numerical computations, Photon numbers, Photon-number distribution, Squeezing effect, Wigner functions, Sub-Poisson distribution, Wigner function

标题: Nonlinear circular states and their non-classical properties

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Label-free detection of pathogenic bacteria via immobilized antimicrobial peptides

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**Publication Information:** Talanta 137 (May 15, 2015): 55-61.

**Abstract:** A novel label-free strategy for the detection of bacteria was developed by using a specific antimicrobial peptide (AMP)-functionalized quartz crystal microbalance (QCM) electrode. This electrode interface was successfully applied to detect pathogenic Escherichia coli O157:H7 based on the specific affinity between the small synthetic antimicrobial peptide and the bacterial cell of pathogenic E. coli O157:H7. The concentrations of pathogenic E. coli O157:H7 were sensitively measured by the frequency response of the QCM with a detection limit of 0.4 cfu μL⁻¹. The detection can be fulfilled within 10 min because it does not require germiculture process. On the other hand, if the specific antimicrobial peptides were immobilized on a gold electrode, this label-free strategy can also be performed by electrochemical impedance spectroscopy (EIS). Compared with QCM technique, the EIS measurement gives a lower sensitivity and needs a longer assay time. The combination of antimicrobial peptides with the real-time responses of QCM, as well as electronic readout monitoring of EIS, may open a new way for the direct detection of bacteria.

**Links:** Check for full text via 360 Link, Order Full Text from Infotrieve?

**Keywords:** Quartz crystal microbalances; Bacteria; Electrochemical electrodes; Electrochemical impedance spectroscopy; Electrodes; Escherichia coli; Frequency response; Microorganisms; Peptides; Polypeptides; Quartz
Label-free detection of pathogenic bacteria via immobilized antimicrobial peptides

Zhao, Guang-Chao College of Environmental Science and Engineering, Anhui Normal University, 241000, China.

Abstract: Antimicrobial peptides, also known as biocidal or bioprotective peptides, are a class of natural antimicrobial compounds produced by many living organisms. They are effective against a wide range of bacteria, fungi, and viruses. In recent years, there has been increasing interest in developing antimicrobial peptides for the detection and quantification of pathogenic bacteria. This article describes the development of a label-free detection method for pathogenic bacteria using immobilized antimicrobial peptides. The method involves the immobilization of antimicrobial peptides on an electrode interface, followed by the monitoring of changes in the electrode signal as the pathogenic bacteria interact with the immobilized peptides. This approach offers several advantages over traditional methods, including increased sensitivity and reduced complexity. The results suggest that the method has potential for use in real-time monitoring of pathogenic bacteria in various environmental and clinical settings.

Keywords: Antimicrobial peptide, Bio recognition, Electrode interface, Escherichia coli O157:H7, Label-free detection, Pathogenic bacterium, Pathogenic E. coli, Pathogenic Escherichia coli, Antimicrobial peptide Pathogenic, Biorecognition, Quartz crystal microbalance

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Optimal Investment and Consumption for an Insurer with High-Watermark Performance Fee

The optimal investment and consumption problem is investigated for an insurance company, which is subject to the payment of high-watermark fee from profit. The objective of insurance company is to maximize the expected cumulated discount utility up to ruin time. The consumption behavior considered in this paper can be viewed as dividend payment of the insurance company. It turns out that the value function of the proposed problem is the viscosity solution to the associated HJB equation. The regularity of the viscosity is discussed and some asymptotic results are provided. With the help of the smooth properties of viscosity solutions, we complete the verification theorem of the optimal control policies and the potential applications of the main result are discussed.
An ab initio potential energy surface and infrared spectra for Kr-N$_2$O in the v$_3$ stretching region of N$_2$O

作者: Wang, Zhongquan 1; Feng, Eryin 2; Zhang, Chunzao 1; Sun, Chunyan 1 1 Department of Physics, Huainan Normal University, 232001, China; wlxit@hnnu.edu.cn 2 Department of Physics, Anhui Normal University, 241000, China


摘要 (English): A three-dimensional ab initio potential energy surface of the Kr-N$_2$O complex was calculated using the CCSD(T) method and avqz-pp + 33221 basis set. The potential includes explicit dependence on the v$_3$ stretching coordinate of the N$_2$O molecule. The potential energy surface is characterized by a near T-shaped minimum. The global minimum locates at R = 6.70a$_0$ and θ = 96.00° with a depth of -270.29 cm$^{-1}$. Using the fitted potential energy surface, we have calculated bound energy levels of the Kr-N$_2$O complexes. The result provides a good representation of the experimental data.

主题: Potential energy (主要); Molecular physics; Potential energy surfaces; Quantum chemistry

分类: 931: Applied Physics Generally

标识符 (关键字): Ab initio potential energy surface, Basis sets, CCSD, Explicit dependences, Global minima, Infrared spectrum, Stretching region

标题: An ab initio potential energy surface and infrared spectra for Kr-N$_2$O in the v$_3$ stretching region of N$_2$O

通讯作者: Wang, Zhongquan Department of Physics, Huainan Normal University, 232001, China.

语言: 英文
Electrochemical glucose biosensor with improved performance based on the use of glucose oxidase and Prussian Blue incorporated into a thin film of self-polymerized dopamine

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We report on the use of self-polymerized dopamine (PDA) in an enzyme-based biosensor with improved performance. This is due to the fact that poly-DA strongly improves the stability of the electrocatalyst Prussian Blue (PB) in neutral and alkaline solution. The polymer also effectively entraps the enzyme glucose oxidase (GOx) while retaining its activity. A glucose biosensor was fabricated by modifying a glassy carbon electrode with a thin film of PB into which GOx was incorporated with the assistance of PDA film. The PB films enable a facile electrochemical reduction, and thus the determination, of enzymatically generated H\textsubscript{2}O\textsubscript{2} at a remarkably low potential of 0.0 V (versus Ag/AgCl). The biosensor responds linearly to glucose in the 200 μM to 3.4 mM concentration range, with a sensitivity of 1.59 nA μM\textsuperscript{-1}, a 46.2 μM detection limit, a response time of 15 s, and with storage stabilities of 3 months at 4-8 °C and of >4 weeks at room temperature. The biosensor is highly selective over many other electroactive species, reproducible, and stable even at weakly alkaline pH values. The stabilized PB films by PDA will widen horizons of its applications both as H\textsubscript{2}O\textsubscript{2} sensor and for elaboration of the oxidase-based biosensors in physiological environment.
Spatial-temporal pattern differentiation and its mechanism analysis of using efficiency for provincial cultivated land in China

作者: Zhang, Rongtian 1; Jiao, Huafu 1 1 The College of Territorial Resources and Tourism, Anhui Normal University, 241003, China; nuzrr@163.com; jiaohuafu@163.com


摘要 (English): Cultivated land is the key resource and environment factor affecting human survival and development. With the progress of industrialization and urbanization in China, cultivated land resource is facing great challenges: cultivated land degradation, ecological environment pollution, lacking of cultivated land reserve, etc. Meanwhile, the growth rate of cultivated land resource investment is greater than the output, and the overall efficiency is relatively low. Especially, in the background of new urbanization, enhancing cultivated land's regional use efficiency is of great importance for the supplement of agricultural products and the rise of farmers' income, and it has significant theoretical and practical values. Taking 31 provinces in China as the research object, the paper built up the evaluation system of cultivated land's provincial use efficiency, and discussed the differentiation and mechanism of spatial-temporal pattern of cultivated land's provincial use efficiency from 1994 to 2012, using improved DEA (data envelopment analysis) method, ESDA (exploratory spatial data analysis), R/S (rescaled range) analysis method and Tobit regression model. The results showed that: DEA optimal ratio of cultivated land's provincial use efficiency was relatively small, and spatial characteristics showed a distribution pattern of the East high and the Mid-west low; the comprehensive efficiency was higher in the eastern coastal, northern coastal and northeastern areas, where a rising trend was presented; technical efficiency change was similar to the comprehensive efficiency, and scale efficiency showed a trend of first upward and then downward; cultivated land's provincial use efficiency had a positive
autocorrelation characteristics, and there existed a spatial cluster feature; on the local, efficiency of provincial cultivated land use could be divided into four types: H-H (high-high) efficiency areas, H-L (high-low) efficiency areas, L-H (low-high) efficiency areas and L-L (low-low) efficiency areas; partial H-H efficiency areas were mainly located in the Beijing-Tianjin area and the Yangtze River Delta, and extended to the Pearl River Delta; L-L efficiency areas formed a stable "L"-shaped pattern which were mainly concentrated in the western China; efficiency of cultivated land use had obvious fractal characteristics and showed a growing trend that the areas with significant growth were located in the eastern coast and northern coast. Economic development and agricultural technology advancement were important factors that influenced the spatial differentiation of cultivated land's provincial use efficiency, and natural condition was the basis factor; farmer's characteristics have a certain impact on the efficiency of spatial-temporal differentiation. Lastly, this paper put forward some suggestions for improving cultivated land's provincial use efficiency to promote the sustainable utilization of cultivated land resource in China: 1) Strengthen the agricultural science and technology, cultivate talents with agricultural technology, improve farmers' farming skills, and constantly promote new technologies; 2) Increase the intensity of cultivated land consolidation, guide the redrawing and circulation of cultivated land, and promote scale operation and comprehensive production capacity of cultivated land; 3) Adjust regional agricultural industrial structure, change the traditional way of extensive use, and promote agricultural modernization development; 4) Build "high efficiency, high compensation" operation mechanism, encourage reasonable utilization of cultivated land resource in different regions, and gradually implement cultivated land use policy from "quantitative" to "efficient". Meanwhile, it should be pointed out that this paper also has somewhat limitations. This paper only chose the experimental data from 1994 to 2012, so the time scale was narrow, and evolution differentiation characteristics of cultivated land's use efficiency was ignored in a longer time scale. Based on two basic dimensions of the input and output, the measured results of cultivated land's use efficiency were objective, but the microscopic index of science and technology investment such as improved crop varieties and field management techniques was also needed to be considered. In addition, the output should focus more on environmental bearing capacity of cultivated land resource. On mechanism analysis, the factors of policy system and farmer willingness to which the cultivated land's regional use efficiency had a positive response were not deeply discussed. Next, based on system (macro) and farmers (micro) perspectives, studying the mechanism of spatial-temporal pattern differentiation of cultivated land's regional use efficiency would be the domain and direction for the deep research.

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主题: Land use (主要); Agricultural products; Agriculture; Cultivation; Data envelopment analysis; Economic and social effects; Economics; Efficiency; Fractals; Modernization; Natural resources; Regression analysis; River pollution; Water analysis


标识符 (关键字): Agricultural modernizations, Agricultural science and technologies, Agricultural technologies, Comprehensive efficiencies, Cultivated lands, Dea methods, Exploratory spatial data analysis, Spatial temporals, Cultivated land, Improved DEA method, Spatial-temporal pattern

标题: Spatial-temporal pattern differentiation and its mechanism analysis of using efficiency for provincial cultivated land in China
The first ab initio potential energy surface and predicted infrared spectra for Xe-N₂O in the ν₃ stretching region of N₂O

作者: Wang, Zhongquan 1 ; Feng, Eryin 2 ; Zhang, Chunzao 1 ; Sun, Chunyan 1 1 Department of Physics, Huainan Normal University, 232001, China wlxit@hnnu.edu.cn 2 Department of Physics, Anhui Normal
The first three-dimensional ab initio potential energy surface of the Xe-N$_2$O complex was calculated using the coupled cluster single and double with noniterative treatment of triple excitations [CCSD(T)] level with a large basis set containing bond functions. The potential includes explicit dependence on the v$_3$ stretching coordinate of the N$_2$O molecule. The potential is characterized by a near T-shaped minimum. The global minimum is located at R = 7.05 a$_0$ and θ = 94.50° with a depth of -302.99 cm$^{-1}$. Dynamical calculations are performed to determine the bound state energies. The theoretical results are all in good agreement with the experimental counterparts.
Mean-field backward stochastic differential equations in general probability spaces

作者: Lu, Wen 1 ; Ren, Yong 2 ; Hu, Lanying 2 1 School of Mathematics and Informational Science, Yantai University, 264005, China llcxw@163.com 2 Department of Mathematics, Anhui Normal University, 241000, China brightry@hotmail.com ; lanyinghu@126.com


摘要 (English): In this paper, we deal with a class of mean-field backward stochastic differential equations in continuous time with an arbitrary filtered probability space. We prove the existence and uniqueness of a solution for those equations with strengthened Lipschitz assumption. A comparison theorem is also established.

主题: Stochastic systems (主要); Continuous time systems; Differential equations

分类: 921: Applied Mathematics; 921.2: Calculus; 961: Systems Science

标识符 (关键字): Backward stochastic differential equations, Comparison theorem, Continuous-time, Existence and uniqueness, Lipschitz, Mean field, Probability spaces, Stieltjes measure, Differential equation, Mean-field backward stochastic

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Optimization method for earthquake emergency material distribution based on possibility degree of interval numbers

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摘要 (English): The optimization of earthquake emergency material distribution (EEMD) is of great importance for the decision-making during the relief work in earthquake. It is significant to study the optimal distribution method for EEMD under material deficiencies. The problem of EEMD is uncertain. It is feasible to describe the decision-making information by interval numbers. The normalizing method of numerical data was introduced.
The algorithm for the possibility degree of interval numbers (PDIN) was presented, also the property. The method of the possibility degree for ranking interval numbers was also analyzed. The matrix of the PDIN was ameliorated. Based on the PDIN, the optimal distribution coefficient was defined. The formula of the optimal distribution coefficient was also derived. The size of disaster area, the extent of disaster, the population density, and the demand of people in the disaster were regarded as four properties of the EEMD plan. On the basis of the PDIN, the optimization model for EEMD was built. The algorithm for the model was also given. The validation of the proposed method was revealed through a case study.

主题: Numerical methods (主要); Behavioral research; Decision making; Disasters; Earthquakes; Geophysics; Optimization; Population statistics

分类: 481.3: Geophysics; 484: Seismology; 912.2: Management; 921.5: Optimization Techniques; 921.6: Numerical Methods; 922.2: Mathematical Statistics; 971: Social Sciences

标识符 (关键字): Interval number, Material distribution, Optimal distributions, Optimization method, Optimization modeling, Population densities, Possibility degree, Possibility degree of intervals, Earthquake emergency

标题: Optimization method for earthquake emergency material distribution based on possibility degree of interval numbers

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摘要语言: English

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Selective detection of Hg$^{2+}$ ions based on reduced graphene oxide sensor device

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**Abstract (English):** A reduced graphene oxide sensor device was fabricated by the self-assembly of graphene oxide onto an interdigitated gold microelectrode followed by electrochemical reduction. The sensor exhibited high sensitivity and selectivity to Hg$^{2+}$ ions. The sensor response ($\Delta I$) increased linearly with increasing concentration in the range, 40 nM to 3240 nM. The sensitivity and detection limit of this method were estimated to be 0.08833 nA nM$^{-1}$ and 7.8 nM, respectively. Compared to Cd$^{2+}$, Pb$^{2+}$, Ba$^{2+}$, Ca$^{2+}$, Cu$^{2+}$, and Ni$^{2+}$ ions, the sensor exhibited high selectivity to Hg$^{2+}$ ions. The adsorption of Hg$^{2+}$ ions on the surface of rGO enhanced its electron-deficiency and increased the conductivity.

**Keywords:** Detection limits, Electrochemical reductions, Electron deficiency, Gold microelectrodes, High selectivity, High sensitivity, Reduced graphene oxides, Selective detection, Hg$^{2+}$ ions, Reduced graphene oxide, Sensor

**Main Topic:** Graphene (主要); Cadmium compounds; Electrolytic reduction; Ions; Lead; Microelectrodes; Self assembly; Sensors

**Classification:** 546.1: Lead and Alloys; 761: Nanotechnology; 801: Chemistry; 804: Chemical Products Generally; 951: Materials Science

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Enzymatic Reaction Modulated Gold Nanorod End-to-End Self-Assembly for Ultrahigh Sensitive Colorimetric Sensing of Cholinesterase and Organophosphate Pesticides in Human Blood

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We present herein the first reported self-assembly modulation of gold nanorods (AuNRs) by enzymatic reaction, which is further employed for colorimetric assays of cholinesterase (ChE) and organophosphate pesticides (OPs) in human blood. ChE catalyzes its substrate (acetylthiocholine) and produces thiocholine and acetate acid. The resulting thiols then react with the tips of the AuNRs by S-Au conjunction and prevent subsequent cysteine-induced AuNR end-to-end (EE) self-assembly. Correspondingly, the AuNR surface plasmon resonance is regulated, which results in a distinctly ratiometric signal output. Under optimal conditions, the linear range is 0.042 to 8.4 μU/mL, and the detection limit is as low as 0.018 μU/mL. As ChE is incubated with OPs, the enzymatic activity is inhibited. So, the cysteine-induced assembly is observed again. On the basis of this principle, OPs can be well determined ranging from 0.12 to 40 pM with a 0.039 pM detection limit. To our knowledge, the present quasi pU/mL level sensitivity for ChE and the quasi femtomolar level sensitivity for OPs are at least 500 and 7000 times lower than those of previous colorimetric methods, respectively. The ultrahigh sensitivity results from (1) the rational choice of anisotropic AuNRs as building blocks and reporters and (2) the specific structure of the enzymatic thiocholine. Because of ultrahigh sensitivity, serum samples are allowed to be extremely diluted in the assay. Accordingly, various nonspecific interactions, even from glutathione/cysteine, are well avoided. So, both ChE and OPs in human blood can be directly assayed without any prepurification, indicating the simplicity and practical promise of the proposed method.
Detecting anomalies from big network traffic data using an adaptive detection approach

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摘要 (English): The unprecedented explosion of real-life big data sets have sparked a lot of research interests in data mining in recent years. Many of these big data sets are generated in network environment and are characterized by a dauntingly large size and high dimensionality which pose great challenges for detecting useful knowledge and patterns, such as network traffic anomalies, from them. In this paper, we study the problem of anomaly detection in big network connection data sets and propose an outlier detection technique, called Adaptive Stream Projected Outlier deTector (A-SPOT), to detect anomalies from large data sets using a novel adaptive subspace analysis approach. A case study of A-SPOT is conducted in this paper by deploying it to the 1999 KDD CUP anomaly detection application. Innovative approaches for training data generation, anomaly classification and false positive reduction are proposed in this paper as well to better tailor A-SPOT to
deal with the case study. Experimental results demonstrate that A-SPOT is effective and efficient in detecting anomalies from network data sets and outperforms existing detection methods.
Chemical and biological insights into uranium-induced apoptosis of rat hepatic cell line

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Abstract (English): Uranium release into the environment is a threat to human health, and the mechanisms of cytotoxicity caused by uranium are not well-understood. To improve our understanding in this respect, we herein evaluated the effects of uranium exposure on normal rat hepatic BRL cells. As revealed by scanning electron microscopy and transmission electron microscope analysis, uranyl nitrate was found to be transformed into uranyl phosphate particles in the medium and taken up by BRL cells in an endocytotic uptake manner, which presumably initiates apoptosis of the cell, although soluble uranyl ion may also be toxic. The apoptosis of BRL cells upon uranium exposure was also confirmed by both the acridine orange and ethidium bromide double staining assay and the Annexin V/propidium iodide double staining assay. Further studies revealed that uranium induced the loss of mitochondrial membrane potential in a dose-dependent manner. Moreover, the uranium-induced apoptosis was found to be associated with the activation of caspase-3, caspase-8 and caspase-9, indicating both a mitochondria-dependent signaling pathway and a death receptor pathway by a crosstalk. This study provides new chemical and biological insights into the mechanism of uranium toxicity toward hepatic cells, which will help seek approaches for biological remediation of uranium.

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Subjects: Uranium (主要); Cell culture; Cell death; Cell membranes; Cells; Cytology; Cytotoxicity; Health risks; Mitochondria; Rats; Scanning electron microscopy; Transmission electron microscopy; Uranium alloys; Uranium compounds

Descriptors (关键字): Caspases, Chemical and biologicals, Death receptor pathways, Dose-dependent manner, Hepatic cells, Mitochondrial membrane potential, Signaling pathways, Transmission electron, Apoptosis, Hepatic cell

Title: Chemical and biological insights into uranium-induced apoptosis of rat hepatic cell line

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Language: 英文
Computational spectroscopy for structure characterization of nanomaterials: a case study of graphene oxide

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Nowadays, first-principles electronic structure calculations can be routinely used to analyze energetics and then to obtain the ground-state structure of a specific material. However, with complicated synthesis routes, nanomaterials are not necessarily always in their thermodynamic ground states. In such situations, computational spectroscopy provides a reliable way for structure characterization. We first briefly introduced the theoretical background of spectrum simulation, focusing on infrared (IR) spectroscopy, Raman spectroscopy, optical absorption, nuclear magnetic resonance (NMR), X-ray photoemission spectroscopy (XPS), and scanning tunneling microscopy/spectroscopy (STM/STS). Then, structure characterization of graphene oxide (GO) was used as an example to demonstrate the power of computational spectroscopy. Comparing experimental spectra with simulated data from different candidate structures, we obtained the information about GO structure. It was unambiguously revealed that experimentally obtained GO samples are in a kinetically constrained metastable state instead of the thermodynamic ground state. Based on computational spectroscopic studies, an updated Lerf model for GO structure was proposed.
Tower bio-vermifilter system for rural wastewater treatment: bench-scale, pilot-scale, and engineering applications

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Abstract (English): This paper presents a systematic study of a novel tower bio-vermifilter system for rural wastewater treatment at three scales: bench-scale, pilot-scale, and engineering applications. First, three types of bioreactors were tested in the bench-scale experiments: earthworm bioreactor, soil filter, and one-stage bio-vermifilter. Experiments with the earthworm bioreactor and soil filter determined the optimum earthworm density and soil layer depth to be 12.5 g/L and 40 cm, respectively. The one-stage bio-vermifilter's poor performance in removing nitrogen and phosphorous led to several improvements in the design of the pilot tower bio-vermifilter system including the addition of one anaerobic biofilter for pretreatment, the use of two stages of bio-vermifilters, and the replacement of gravel with ceramsite in the media. Second, a pilot tower bio-vermifilter system built in Yixing City of Jiangsu province showed a good performance in the removal of chemical oxygen demand, ammonium nitrogen, and phosphorous. However, the system's removal of total nitrogen showed considerable fluctuations, possibly due to the low ratio of carbon to nitrogen in its stage two bio-vermifilter. Finally, four operating tower bio-vermifilter systems in three basins of China were evaluated and compared with two other rural sewage treatment technologies in terms of economic costs and pollutant removal performance.
Comparison results show that the tower bio-vermifilter system is a versatile system that can work effectively under a variety of natural and socioeconomic conditions at a reasonable cost.

主题: Chemical oxygen demand (主要); Bioconversion; Biofilters; Bioreactors; Filtration; Nitrogen; Nitrogen removal; Oxygen; Phosphorus; Pollution; Sewage; Sewage treatment; Soils; Storm sewers; Towers; Wastewater treatment

分类: 402.4: Towers; 452: Sewage and Industrial Wastes Treatment; 454.2: Environmental Impact and Protection; 483.1: Soils and Soil Mechanics; 802: Chemical Apparatus and Plants; Unit Operations; Unit Processes; 804: Chemical Products Generally

标识符 (关键字): Anaerobic biofilters, Bench scale experiments, Engineering applications, Evaluation, Pollutant removal, Pollutant removal performance, Socio-economic conditions, Treatment technologies

标题: Tower bio-vermifilter system for rural wastewater treatment: bench-scale, pilot-scale, and engineering applications

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Dilute or Concentrated Electrolyte Solutions? Insight from Ionic Liquid/Water Electrolytes

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摘要 (English): When room-temperature ionic liquids (IL) are used as an electrolyte, their transport behaviors are still under heavy debate due to their complicated ion-associations. In this article, we conducted molecular dynamics simulations to study the molecular scale ion associations from the very dilute 1-butyl-3-methylimidazolium iodide/water solution to the pure IL. It revealed that ions are localized in a multicoordinated ion cage structure with nanoseconds in concentrated IL solutions. Dynamics analyses indicate that the transport of this solution can be depicted by the Debye-Hückel model only in dilute IL/water electrolyte. The velocity and rotational correlation functions showed that the lifetime of translational and rotational motions are at the level of picoseconds and nanoseconds, respectively, because of the ion cage effect. The lifetime of ion association demonstrated that the recombination of association ions was prevalent in IL solutions. It means that the dipolar or stable contact ion-pairs model may not be suitable for depicting the IL transport.

主题: Ionic liquids (主要); Electrolytes; Ions; Liquids; Molecular dynamics

分类: 801: Chemistry; 801.4: Physical Chemistry; 804: Chemical Products Generally; 931.2: Physical Properties of Gases, Liquids and Solids

标识符 (关键字): Concentrated electrolyte solutions, Correlation function, Ion association, Molecular dynamics simulations, Room temperature ionic liquids, Rotational correlation, Rotational motion, Transport behavior, electrolyte, ion cage, Ionic liquid, molecular dynamics simulation

标题: Dilute or Concentrated Electrolyte Solutions? Insight from Ionic Liquid/Water Electrolytes

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语言: 英文
An efficient top-k query processing with result integrity verification in two-tiered wireless sensor networks

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摘要 (English): In two-tiered wireless sensor networks, storage nodes take charge of both storing the sensing data items and processing the query request issued by the base station. Due to their important role, storage nodes are more attractive to adversaries in a hostile environment. Once a storage node is compromised, attackers may falsify or abandon the data when answering the query issued by the base station, which will make the base station get incorrect or incomplete result. This paper proposes an efficient top-k query processing scheme with result integrity verification named as ETQ-RIV in two-tiered sensor networks. According to the basic idea that sensor nodes submit some encoded message containing the sequence relationship as proof information for verification along with their collected sensing data items, a data binding and collecting protocol and a verifiable query response protocol are proposed and described in detail. Detailed quantitative analysis and evaluation experiments show that ETQ-RIV performs better than the existing work in both communication cost and query result redundancy rate.

主题: Sensor nodes (主要); Base stations; Data handling; Digital storage; Information retrieval; Query processing; Wireless sensor networks

分类: 716.3: Radio Systems and Equipment; 722.1: Data Storage, Equipment and Techniques; 723.2: Data Processing; 903.3: Information Retrieval and Use

标识符 (关键字): Analysis and evaluation, Communication cost, Hostile environments, Integrity verifications, Query response, Top-k query processing, Two-tiered sensor networks, Two-tiered wireless sensor networks

标题: An efficient top-k query processing with result integrity verification in two-tiered wireless sensor networks

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A Multiobjective Genetic Algorithm Based on a Discrete Selection Procedure

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Abstract (English): Multiobjective genetic algorithm (MOGA) is a direct search method for multiobjective optimization problems. It is based on the process of the genetic algorithm; the population-based property of the genetic algorithm is well applied in MOGAs. Comparing with the traditional multiobjective algorithm whose aim is to find a single Pareto solution, the MOGA intends to identify numbers of Pareto solutions. During the process of solving multiobjective optimization problems using genetic algorithm, one needs to consider the elitism and diversity of solutions. But, normally, there are some trade-offs between the elitism and diversity. For some multiobjective problems, elitism and diversity are conflicting with each other. Therefore, solutions obtained by applying MOGAs have to be balanced with respect to elitism and diversity. In this paper, we propose metrics to numerically measure the elitism and diversity of solutions, and the optimum order method is applied to identify these solutions with better elitism and diversity metrics. We test the proposed method by some well-known benchmarks and compare its numerical performance with other MOGAs; the result shows that the proposed method is efficient and robust.
Singular convolution operators on Wiener amalgam spaces

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摘要 (English): The purpose of this paper is to investigate some properties of the Wiener amalgam spaces. As applications, we study the boundedness properties of some singular convolution operators on such spaces. From our results, we will see that, besides modulation spaces, Wiener amalgam spaces are another good substitutions for Lebesgue spaces.

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主题: Convolution (主要); Information systems

分类: 716.1: Information and Communication Theory; 903.2: Information Dissemination

标识符 (关键字): Boundedness properties, Convolution operators, Fourier multipliers, Good substitution, Lebesgue space, Modulation spaces, Wiener amalgam spaces, Fourier multiplier, Singular convolution operator, Wiener amalgam space

标题: Singular convolution operators on Wiener amalgam spaces

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Non autonomous semilinear stochastic evolution equations

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出版物信息: Communications in Statistics - Theory and Methods 44.9 (Jan 1, 2015): 1806-1818.

摘要 (English): In this article, we first give a version with continuous paths for stochastic convolution \( \int_{t_0}^{t} U(t, s)\varphi(s)dW(s) \) driven by a Wiener process \( W \) in a Hilbert space under weaker conditions. Based on the Picard approximation and the factorization method, we prove the existence, uniqueness and regularity of mild solutions for non-autonomous semilinear stochastic evolution equations with more general assumptions on the coefficients. As an application, we obtain the Feller property of the associated semigroup.

主题: Stochastic systems (主要); Convolution; Differential equations; Factorization

分类: 716.1: Information and Communication Theory; 921: Applied Mathematics; 921.2: Calculus; 961: Systems Science

标识符 (关键字): Factorization methods, Feller property, Mild solution, Nonautonomous, Picard approximation, Semi-group, Stochastic evolution equations, Wiener process, Factorization method

标题: Non autonomous semilinear stochastic evolution equations

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A coordination polymeric gelator based on Ag(I) and 2, 7-bis(1-imidazole)fluorene: Synthesis, characterization, gelation and antibacterial properties

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摘要 (English): A coordination polymeric gelator based on Ag(I) and 2, 7-bis(1-imidazole) fluorene was synthesized and characterized by $^1$H NMR, FT-IR, FE-SEM, UV-vis. The gelator forms a gel which exhibits thixotropic behavior and stimuli responsive to $S^2$, $I^-$ and displays antibacterial properties against Bacillus subtilis, Streptococcus aureus and Escherichia coli bacteria.
A coordination polymeric gelator based on Ag(I) and 2, 7-bis(1-imidazole)fluorene: Synthesis, characterization, gelation and antibacterial properties

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A novel manganese dioxide-carbon fiber composite with coaxial cable structure is successfully prepared by a direct redox reaction with KMnO₄ and carbon fiber. The composite is combined by carbon fiber cable tracer and MnO₂ cable jacket and it is investigated by scanning electron microscopy, energy dispersive X-ray spectroscopy and X-ray diffraction. The supercapacitor performance of the composite is tested by cyclic voltammetry, electrochemical impedance spectroscopy and galvanostatic charge-discharge. Its initial capacitance is 196 F g⁻¹ at the current density of 0.6 A g⁻¹. The coulombic efficiency is almost 100% with the capacitance above 131.3 F g⁻¹ during the continuous 10,000 cycles. The results indicate that the composite has high capacitance retention and a superior coulombic efficiency at long cycles. It is a promising candidate for supercapacitor in practical applications.
Existence of positive periodic solutions of competitor-competitor-mutualist Lotka-Volterra systems with infinite delays

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In this paper, the authors primarily explore a delayed competitor-competitor-mutualist Lotka-Volterra model, which is a system of differential equation with infinite integral. The authors first study the existence of positive periodic solutions of the model by using the Krasnoselskii’s fixed point theorem, and then present an example to illustrate the main results.

**Title:** Existence of positive periodic solutions of competitor-competitor-mutualist Lotka-Volterra systems with infinite delays

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Soil geochemistry and digestive solubilization control mercury bioaccumulation in the earthworm *Pheretima guillemi*

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**Abstract (English):** Mercury presents a potential risk to soil organisms, yet our understanding of mercury bioaccumulation in soil dwelling organisms is limited. The influence of soil geochemistry and digestive processes on both methylmercury (MeHg) and total mercury (THg) bioavailability to earthworms (*Pheretima guillemi*) was evaluated in this study. Earthworms were exposed to six mercury-contaminated soils with geochemically contrasting properties for 36 days, and digestive fluid was concurrently collected to solubilize soil-associated mercury. Bioaccumulation factors were 7.5-31.0 and 0.2-0.6 for MeHg and THg, respectively, and MeHg accounted for 17-58% of THg in earthworm. THg and MeHg measured in soils and earthworms were negatively associated with soil total organic carbon (TOC). Earthworm THg and MeHg also increased with increasing soil pH. The proportion of MeHg and THg released into the digestive fluid (digestive solubilizable mercury, DSM) was 8.3-18.1% and 0.4-1.3%, respectively. The greater solubilization of MeHg by digestive fluid than CaCl₂, together with a biokinetic model-based estimate of dietary MeHg uptake, indicated the importance of soil ingestion for MeHg bioaccumulation in earthworms.

**Links:** Check for full text via 360 Link, Order Full Text from Infotrieve?

**Keywords:** Soils (主要); Bioaccumulation; Biochemistry; Carbon; Geochemistry; Mercury (metal); Organic carbon; Soil pollution; Solubility

**Classification:** 453: Water Pollution; 454: Environmental Engineering; 481.2: Geochemistry; 483.1: Soils and Soil Mechanics; 549.3: Others, incl. Bismuth, Boron, Cadmium, Cobalt, Mercury, Niobium, Selenium, Silicon, Tellurium; 801.2: Biochemistry; 801.4: Physical Chemistry; 804: Chemical Products Generally; 804.1: Organic
The Role of Exhausted Coffee Compounds on Metal Ions Sorption

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Abstract (English): In the present work, the role of chemical compounds of one abundant vegetable waste, exhausted coffee, on Cr(VI), Cu(II), and Ni(II) sorption has been investigated. For this purpose, exhausted coffee was subjected to sequential extractions by using dichloromethane (DCM), ethanol (EtOH), water, and NaOH 1%. The raw and treated biomass resulting from the extractions were used for metal ions sorption. Sorption results were discussed taking into consideration polarity and functional groups of raw and treated biomass. In general, the successive removal of extractives led to an insignificant increase in the studied metal ions sorption after DCM, EtOH, and water. The sorption results using free-extractive materials showed that metal sorption can be effectively achieved without this non-structural fraction of the sorbent. Alkaline hydrolysis destroyed in part the structural compounds of the sorbent resulting in an insignificant decrease of chromium removal while a significant increase of copper and nickel sorption was observed. The determination of elemental ratios of exhausted coffee and all treated biomass evidenced the involvement of oxygen functional groups in copper and nickel sorption. FTIR analysis confirmed the involvement of lignin moieties in the chromium sorption by exhausted coffee. As a final remark, this study shows that the sequential extraction opens new expectations to the total valorisation of lignocellulosic-based biomasses. The extractives can be removed and used as a biosource of valuable compounds, and the resulting waste can be used as a sorbent for metal ions keeping the same capacity for metal sorption as the non-extracted biomass.

Subject: Sorption (主要); Alkalinity; Biomass; Chemical compounds; Chemicals removal (water treatment); Chromium; Chromium compounds; Copper; Dichloromethane; Extraction; Metal ions; Metals; Nickel; Positive ions

Classification: 525.1: Energy Resources; 531: Metallurgy and Metallography; 533: Ore Treatment and Metal Refining; 543.1: Chromium and Alloys; 544.1: Copper; 548.1: Nickel; 801: Chemistry; 801.1: Chemistry, General; 802.3: Chemical Operations; 803: Chemical Agents and Basic Industrial Chemicals; 804: Chemical Products Generally; 804.1: Organic Compounds

Keywords: Alkaline hydrolysis, Chromium sorption, Divalent metals, Metal ions sorption, Oxygen functional groups, Polarity, Sequential extraction, Structural compounds

Title: The Role of Exhausted Coffee Compounds on Metal Ions Sorption

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Coulomb Liquid Phases of Bosonic Cluster Mott Insulators on a Pyrochlore Lattice

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Abstract (English): Employing large-scale quantum Monte Carlo simulations, we reveal the full phase diagram of the extended Hubbard model of hard-core bosons on the pyrochlore lattice with partial fillings. When the intersite repulsion is dominant, the system is in a cluster Mott insulator phase with an integer number of bosons localized inside the tetrahedral units of the pyrochlore lattice. We show that the full phase diagram contains three cluster Mott insulator phases with 1/4, 1/2, and 3/4 boson fillings, respectively. We further demonstrate that all three cluster Mott insulators are Coulomb liquid phases and its low-energy property is described by the emergent compact U(1) quantum electrodynamics. In addition to measuring the specific heat and entropy of the cluster Mott insulators, we investigate the correlation function of the emergent electric field and verify it is consistent with the compact U(1) quantum electrodynamics description. Our result sheds light on the magnetic properties of various pyrochlore systems, as well as the charge physics of the cluster magnets.

Title: Coulomb Liquid Phases of Bosonic Cluster Mott Insulators on a Pyrochlore Lattice

Language: English

Subject Terms: High energy physics (主要); Bosons; Crystal lattices; Electric fields; Electrodynamics; Intelligent systems; Monte Carlo methods; Phase diagrams; Quantum electronics; Specific heat

Classification: 531: Metallurgy and Metallography; 641.1: Thermodynamics; 701: Electricity and Magnetism; 701.1: Electricity, Basic Concepts and Phenomena; 723.4: Artificial Intelligence; 744: Lasers; 922.2: Mathematical Statistics; 931.3: Atomic and Molecular Physics; 932.1: High Energy Physics; 933.1.1: Crystal Lattice

Keywords: Correlation function, Extended Hubbard model, Hard-core bosons, Mott insulator phase, Mott-insulator phasis, Pyrochlore lattices, Quantum electrodynamics, Quantum Monte Carlo simulations

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Global structure stability for the wave catching-up phenomenon in a prestressed two-material bar

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Abstract (English): Shock waves in a structure can result in the detachment of an interface and induce microcracks. In a recent study [Huang et al., R. Soc. Lond. Proc. Ser. A Math. Phys. Eng. Sci., 468 (2012), pp. 3882-3901], it was shown that for certain nonlinearly elastic materials it is possible to generate a phenomenon in which a tensile wave can catch the first transmitted compressive wave (so the former can be undermined) in an initially stress-free two-material bar. In this study, we consider the wave catching-up phenomenon in a nonlinearly elastic prestressed two-material bar. We use the same method as that used by Huang et al. in the previously mentioned paper to construct solutions. Our main focus is on proving the global structure stability of the solutions in a prestressed (or initially stress-free) two-material bar. We first reduce the corresponding initial boundary value problem into several typical free boundary problems based on the formulation of Riemann invariants. Then, using a constructive method and carefully treating the complexity arising from multiple reflections of waves at the interface in the two-material bar, we successfully prove the global structure stability of the wave catching-up phenomenon.
GIS-based climate change vulnerability mapping at the urban scale: a case study of Shanghai metropolitan area in China

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摘要 (English): Since the publication of the third assessment report of The Intergovernmental Panel on Climate Change, vulnerability to climate change has become an important research question. Vulnerability assessment on the urban scale has become a major issue. This paper describes a conceptual framework for modelling vulnerability at the urban scale, the Climate Change Vulnerability Assessment model. The model is applied to Shanghai, a typical geographically vulnerable and rapidly-urbanizing case study area. Using Arc-GIS, a vulnerability map was created for understanding the spatial dynamics of climate change vulnerability in Shanghai. An additional process, combined with the weighting coefficients, produced different vulnerable areas. Based on the vulnerability map, we located several high risk areas. The vulnerability of each area was assessed. Identifying the risks in each case and associating them with a specific region can be useful for decision makers.

主题: Climate change (主要); Climate models; Decision making; Geographic information systems; Mapping

分类: 405.3: Surveying; 443: Meteorology; 443.1: Atmospheric Properties; 903.3: Information Retrieval and Use; 912.2: Management; 921: Applied Mathematics

标识符 (关键字): Conceptual frameworks, Intergovernmental panel on climate changes, Research questions, Urbanization, Vulnerability, Vulnerability assessments, Vulnerability mappings, Weighting coefficient, GIS

标题: GIS-based climate change vulnerability mapping at the urban scale: a case study of Shanghai metropolitan area in China

通讯作者: Moses, Michael College of Environmental Design, University of California at Berkeley, United States.

语言: 英文

摘要语言: English

文档类型: Article

出版物名称: International Journal of Environmental Studies

卷: 72

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Remote sensing monitoring of grassland vegetation growth in the Beijing-Tianjin sandstorm source project area from 2000 to 2010

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Abstract (English): Grassland is not only an important landscape of the Beijing-Tianjin sandstorm source control project area, but also a significant object of the Beijing-Tianjin sandstorm source control project. By taking the situation in 2000 as the base of comparison and using the established grassland vegetation growth model, the monitoring and evaluation of grassland vegetation dynamic variation in the project area from 2000 to 2010 was conducted based on MODIS 16 days NDVI data. The conclusions are as follows: (1) The comparative result of
average growth between each year from 2001 to 2010 and the base year was on the good side in general; the grassland growth was good both in the early and later periods of grassland growth peak season than in the first years of the project implementation, indicating that the implementation of the Beijing-Tianjin sandstorm source project has significantly improved the growth conditions of grassland vegetation; (2) With regard to the annual dynamic variation of grassland growth, the area proportions of the grasslands, of which the average grassland growth was on the good side, fluctuated and increased slightly with the time changes in general. The area proportions of the grasslands, of which the average grassland growth was on the bad side, fluctuated and decreased in general. The area proportions of the grasslands with normal growth showed an increasing overall trend; (3) From the regional perceptive on four zones, including the northern arid grassland desertification control zone, Hunshandake sandy land control zone, the farming-pastoral area of desertified land control zone, and the water conservation zone of Yanshan hills and mountains, except that the grassland growth in the farming-pastoral area of desertified land control zone was bad, the average growth of other three zones was good each year from 2001 to 2010 compared with the base year. (4) In respect of space, the regions with big grassland growth variation in the project area were concentrated in the western and eastern sections of the northern arid grassland desertification control zone and the western section of Hunshandake sandy land control zone. The grassland growth variation in the water conservation zone of Yanshan hills and mountains and the farming-pastoral area of desertified land control zone were relatively stable. On one hand, the conclusions of this paper can evaluate the effectiveness of the project control, on the other hand, it can also provide scientific basics to grassland management departments, facilitate the rational utilization of grassland, and preserve the regional ecological balance.
Graphene-Enveloped Poly(N-vinylcarbazole)/Sulfur Composites with Improved Performances for Lithium-Sulfur Batteries by a Simple Vibrating-Emulsification Method

作者: Qu, Guoxing 1; Cheng, Jianli 2; Li, Xiaodong 2; Huang, Ling 2; Ni, Wei 2; Wang, Zhiyu 2; Wang, Bin 2

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摘要 (English): (Figure Presented) We prepared the Poly(N-vinylcarbazole)/sulfur@reduced graphene oxide (PVK/S@RGO) composites via a facile vibrating-emulsification synthesis method, which consist of the composites cores of large sulfur particles integrated into PVK conductive network and the conducting shell of reduced graphene oxide sheets. The PVK in the composites plays multiple roles in different processes. In preparation processes, PVK functions as dispersants to prevent sulfur particles from aggregating into excessively large size. And in the cycling test, PVK could play as additional electroactive binders and barriers to reinforce the electrode stability, accommodate volume change and reduce polysulfides shuttling. The resulting PVK/S@RGO composites containing 71 wt % sulfur exhibit excellent cycling performance and rate properties.
with a high discharge capacity of 843.5 mA h g⁻¹ and a charge capacity retention of 77% (only 0.07% capacity degradation per cycle) from 20th to 400th at 1 C, corresponding to an average Coulombic efficiency of over 94%.

主题: Lithium batteries (主要); Agglomeration; Electric batteries; Electric discharges; Emulsification; Graphene; Lithium compounds; Secondary batteries; Sulfur

分类: 701.1: Electricity, Basic Concepts and Phenomena; 702: Electric Batteries and Fuel Cells; 802.3: Chemical Operations; 804: Chemical Products Generally

标识符 (关键字): Capacity degradation, Discharge capacities, Electrochemical performance, Emulsification methods, Lithium sulfur batteries, N-vinylcarbazole, Reduced graphene oxides, Synthesis method, emulsification ratio, lithium-sulfur battery, poly(N-vinylcarbazole), vibrating-emulsification synthesis method

标题: Graphene-Enveloped Poly(N-vinylcarbazole)/Sulfur Composites with Improved Performances for Lithium-Sulfur Batteries by a Simple Vibrating-Emulsification Method

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语言: 英文

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Coordination of monetary and exchange rate policy in China: Market interest rate approach

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出版物信息：Journal of Advanced Computational Intelligence and Intelligent Informatics 19.3 (Jan 1, 2015): 456-464.

摘要 (English): We propose a unique time-varying identification approach to the market interest rate based on Taylor Rule for coordinating the monetary and exchange rate policies. The significant differences exist between real and market interest rates - 2001 and 2009 are high real interest rates, and 2004-2005 and 2010-2012 low real interest rates - that identify monetary and exchange rate policy conflicts in China. These conflicts derive from the indirect effect of monetary factor through interest rate inertia and expected output gap in 2001; the indirect effect of exchange rate factor through interest rates and inflation inertia in 2004-2005; the direct effects of monetary and the exchange rate factors and the indirect effects through interest rate and inflation inertia, and the expected inflation and output gap since 2009. Our empirical results provide decision support for the monetary and exchange rate policy for reforming Chinese market interest rates.

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主题: Finance (主要); Commerce; Decision support systems

分类: 723: Computer Software, Data Handling and Applications; 911.1: Cost Accounting; 911.2: Industrial Economics

标识符 (关键字): Decision supports, Identification approach, Indirect effects, Inflation inertia, Interest rates, Path identifications, Real interest rates, Taylor rules, Market interest rates approach, Path identification, Taylor Rule

标题: Coordination of monetary and exchange rate policy in China: Market interest rate approach

语言: 英文

摘要语言: English

文档类型: Article

出版物名称: Journal of Advanced Computational Intelligence and Intelligent Informatics
Concentration characteristics and potential sources of polycyclic aromatic hydrocarbons in atmospheric deposition in Shanghai

To study the atmospheric deposition in Shanghai, we have collected deposition samples in August, September and October in 2014. The concentration, spatial distribution and composition of sixteen polycyclic aromatic hydrocarbons (PAHs) were analyzed. Atmospheric deposition fluxes of ∑15PAHs at eight...
sampling sites were also calculated. The potential sources of PAHs were apportioned by positive matrix factorization model (PMF), which could produce a quantitative interpretation. Our results indicated that the total concentrations of PAHs ranged from 0.458 μg/L to 21.013 μg/L in atmospheric deposition. Furthermore, the PAHs concentrations in dissolved phase varied from 0.174 μg/L to 0.625 μg/L, while in particulate phase from 0.275 μg/L to 20.455 μg/L. The atmospheric deposition flux of $\Sigma_{15}$PAHs in sampling sites ranged from 0.24 μg/(m$^2$·d) to 14.74 μg/(m$^2$·d) and the mean deposition flux of $\Sigma_{15}$PAHs was 2.77 μg/(m$^2$·d). According to the apportionment results using PMF model, the first major sources of PAHs were categorized as mobile vehicle exhausts, such as gasoline car exhausts and diesel car exhausts, which constantly contribute 40.23% to the total PAHs pollution. Another four sources (residential cooking, coal combustion, oil spill and volatilization, coking and coal smelting) identified by PMF model, account for 23.73%, 14.75%, 14.35% and 6.92% respectively.
Dissolved organic nitrogen (DON) in seventeen shallow lakes of Eastern China

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摘要 (English): The terrestrial export of dissolved organic nitrogen (DON) is associated with climate, geography and land use, and thus is influenced by geo-climatic variability, human interference, the farmland and woodland in soil, and hydrological connection levels to rivers. A data-set was presented including two catchments covering the major land use types and different hydrological connection levels to rivers within Eastern China: Middle Yangtze (river-isolated lakes) and Huai River (non-river-connected lakes). Total dissolved nitrogen (TDN, including DON and dissolved inorganic nitrogen (DIN)), total organic carbon (TOC) and physical variables (T, DO, pH, OPR, conductivity) were measured in seventeen lakes over summer and winter. In all study lakes, both DON and NH\(_4^+\)-N were the major fractions of TDN, with much lower proportions of NO\(_3^-\)-N and NO\(_2^-\)-N. A variation pattern with higher DON and lower NH\(_4^+\)-N concentrations was observed in non-river-connected lakes, and yet reverse pattern in river-isolated lakes. Higher DON concentrations were recorded with a high extent of farmland in land use, reflecting the influence of human impact on DON loads. These relationships and correlation analysis indicated that DON concentrations were controlled by several factors including temperature, latitude, precipitation, hydrological process and farmland cover in land use. Seasonal variations showed that higher mean surface DON concentration (0.004–0.666 mg/L) was measured in winter, which might be due to resuspension of the organic matter from bottom sediments. The uptake of DON by phytoplankton and bacteria was likely to be the most significant reason for low DON concentrations (0.006–0.335 mg/L) during the summer,
supported by increasing DON concentrations accompanied with disappearing Chla after phytoplankton died. Much higher NO$_3^-$-N concentrations in summer were attributed to nitrogenous fertilizer, high rainfall, and inorganic nitrogen suspending brought by frequent wind wave.
Life cycle assessment of ceramic façade material and its comparative analysis with three other common façade materials

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出版物信息: Journal of Cleaner Production 99 (Jan 1, 2015): 86-93.

摘要 (English): Ceramic panels are an emerging construction material and have become popular in China due to the regenerative character of the material and its conformation with Chinese culture. In this paper, we conducted a life cycle assessment (from "cradle" to "grave") of decorative ceramic façade panel products from a typical ceramic enterprise in South China. Both the sales aspect and material recycling were considered. Using Ebalance software and its Chinese parameters, we assessed seven environmental impacts of the ceramic panels, including depletion of abiotic resources, photochemical oxidant creation, global warming, acidification, eutrophication, ozone depletion and human toxicity. We also compared the environmental performance of ceramic façade panels with three other traditional curtain wall materials - glass, marble and aluminum plate - using data from the literature. The results from a consideration of the life cycle from "cradle" to "gate" showed that ceramic façade panels had better environmental performance than the others, in general, but was worse than glass on the depletion of abiotic resources performance and was worse than glass and aluminum on the human toxicity performance. Finally, we offer some suggestions for optimizing the life cycle process of ceramic façade panels for better environmental performance and some recommendations for better selection of façade materials.

主题: Life cycle (主要); Aluminum; Ceramic materials; Ceramic products; Environmental impact; Environmental management; Eutrophication; Glass; Global warming; Marble; Ozone layer; Toxicity

标识符 (关键字): Ceramic, Comparative analysis, Environmental performance, LCA, Life Cycle Assessment (LCA), Material recycling, Photochemical oxidants, Plastic panels, Aluminum-plastic panel, Façade

标题: Life cycle assessment of ceramic façade material and its comparative analysis with three other common façade materials

通讯作者: Wang, Rusong, State Key Laboratory of Urban and Regional Ecology, Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, Shuangqing Road 18, 100085, China.

语言: 英文
T-PHOT: A new code for PSF-matched, prior-based, multiwavelength extragalactic deconfusion photometry

Authors: Merlin, E. 1; Fontana, A. 1; Ferguson, H.C. 2; Dunlop, J.S. 3; Elbaz, D. 4; Bourne, N. 3; Bruce, V.A. 3; Buitrago, F. 5; Castellano, M. 1; Schreiber, C. 4; Grazian, A. 1; McLure, R.J. 3; Okumura, K. 4; Shu, X. 6; Wang, T. 7; Amorín, R. 1; Boutsia, K. 1; Cappelluti, N. 8; Comastri, A. 8; Derriere, S. 9; Faber, S.M. 10; Santini, P. 11 INAF-Osservatorio Astronomico di Roma, via Frascati 33, 00040, Italy emiliano.merlin@oa-roma.inaf.it 2 Space Telescope Science Institute, 3700 San Martin Drive, 21218, United States 3 SUPA (Scottish Universities Physics Alliance), Institute for Astronomy, University of Edinburgh, EH93HJ, United Kingdom 4 Laboratoire AIM-Paris-Saclay, Université Paris Diderot, CEA-Saclay, pt courrier 131, 91191, France 5 SUPA (Scottish Universities Physics Alliance), Institute for Astronomy, University of Edinburgh, EH93HJ,
Astronomy and Astrophysics 582 (Oct 1, 2015).

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摘要 (English): Context. The advent of deep multiwavelength extragalactic surveys has led to the necessity for advanced and fast methods for photometric analysis. In fact, codes which allow analyses of the same regions of the sky observed at different wavelengths and resolutions are becoming essential to thoroughly exploit current and future data. In this context, a key issue is the confusion (i.e. blending) of sources in low-resolution images.

Aims. We present t-phot, a publicly available software package developed within the astrodeep project. t-phot is aimed at extracting accurate photometry from low-resolution images, where the blending of sources can be a serious problem for the accurate and unbiased measurement of fluxes and colours.

Methods. t-phot can be considered as the next generation to tfit, providing significant improvements over and above it and other similar codes (e.g. convphot). t-phot gathers data from a high-resolution image of a region of the sky, and uses this information (source positions and morphologies) to obtain priors for the photometric analysis of the lower resolution image of the same field. t-phot can handle different types of datasets as input priors, namely i) a list of objects that will be used to obtain cutouts from the real high-resolution image; ii) a set of analytical models (as.fits stamps); iii) a list of unresolved, point-like sources, useful for example for far-infrared (FIR) wavelength domains.

Results. By means of simulations and analysis of real datasets, we show that t-phot yields accurate estimations of fluxes within the intrinsic uncertainties of the method, when systematic errors are taken into account (which can be done thanks to a flagging code given in the output). t-phot is many times faster than similar codes like tfit and convphot (up to hundreds, depending on the problem and the method adopted), whilst at the same time being more robust and more versatile. This makes it an excellent choice for the analysis of large datasets. When used with the same parameter sets as for tfit it yields almost identical results (although in a much shorter time); in addition we show how the use of different settings and methods significantly enhances the performance. Conclusions. t-phot proves to be a state-of-the-art tool for multiwavelength optical to far-infrared image photometry. Given its versatility and robustness, t-phot can be considered the preferred choice for combined photometric analysis of current and forthcoming extragalactic imaging surveys.

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主题: Photometry (主要); Codes (symbols); Infrared imaging; Surveys; Systematic errors; Uncertainty analysis

分类: 723.2: Data Processing; 746: Imaging Techniques; 922.1: Probability Theory; 941.4: Optical Variables Measurements

标识符 (关键字): Accurate estimation, Galaxies: photometry, High resolution image, Low resolution images, Lower resolution, State of the art, Techniques: photometric, Wavelength domains

标题: T-PHOT: A new code for PSF-matched, prior-based, multiwavelength extragalactic deconfusion photometry