Record 1 of 52

**Author(s):** Wang, ZC (Wang, Zhan Chang); Lin, YM (Lin, Yi Ming); Feng, DQ (Feng, Dan Qin); Ke, CH (Ke, Cai Huan); Lin, P (Lin, Peng); Yan, CL (Yan, Chong Ling); De Chen, J (De Chen, Jun)

**Title:** A New Atisane-Type Diterpene from the Bark of the Mangrove Plant Excoecaria Agallocha

**Source:** MOLECULES, 14 (1): 414-422 JAN 2009

**Language:** English

**Abstract:** A new atisane-type diterpene, ent-16 alpha-hydroxy-atisane-3,4-lactone (4) and three known diterpenes, ent-16 alpha-hydroxy-atisane-3-one (1), ent-atisane-3 beta, 16 alpha-diol (2), ent-3,4-seco-16 alpha-hydroxyatis-4(19)-en -3-oic acid (3) were isolated from the bark of the mangrove plant Excoecaria agallocha. Their structures and relative stereochemistry were elucidated by means of extensive NMR and MS analysis. Compound 3 exhibited significant anti-microfouling activity against the adherence of Pseudomonas pseudoalcaligenes, with an EC50 value of 0.54 +/- 0.01 ppm.

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**Times Cited:** 0

**ISSN:** 1420-3049

**DOI:** 10.3390/molecules14010414

**Subject Category:** Chemistry, Organic

**ISI Document Delivery No.:** 399HO

Record 2 of 52

**Author(s):** Wang, D (Wang, Dan); Huang, JL (Huang, Jialiang); Lan, WY (Lan, Weiyao); Li, XQ (Li, Xiaoqiang)

**Title:** Neural network-based robust adaptive control of nonlinear systems with unmodeled dynamics

**Source:** MATHEMATICS AND COMPUTERS IN SIMULATION, 79 (5): 1745-1753 JAN 2009

**Language:** English

**Abstract:** A neural network-based robust adaptive control design scheme is developed for a class of nonlinear systems represented by input-output models with an unknown nonlinear function and unmodeled dynamics. By on-line approximating the unknown nonlinear functions and unmodeled dynamics by radial basis function (RBF) networks, the proposed approach does not require the unknown parameters to satisfy the linear dependence condition. It is proved that with the proposed control law, the closed-loop system is stable and the tracking error converges to zero in the presence of unmodeled dynamics and unknown nonlinearity. A simulation example is presented to demonstrate the method. (C) 2008 IMACS. Published by Elsevier B.V. All rights reserved.

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**Times Cited:** 0

**ISSN:** 0378-4754

**DOI:** 10.1016/j.matcom.2008.09.002

**Subject Category:** Computer Science, Interdisciplinary Applications; Computer Science, Software Engineering; Mathematics, Applied

**ISI Document Delivery No.:** 399MV

Record 3 of 52

**Author(s):** Zhao, YR (Zhao, Yingru); Chen, JC (Chen, Jincan)

**Title:** Modeling and optimization of a typical fuel cell-heat engine hybrid system and its parametric design criteria

**Source:** JOURNAL OF POWER SOURCES, 186 (1): 96-103 JAN 1 2009

**Times Cited:** 0

**ISSN:** 0378-7758

**DOI:** 10.1016/j.jpower sources.2008.07.021

**Subject Category:** Energy, Aerospace Engineering; Energy, General; Engineering, Mechanical

**ISI Document Delivery No.:** 399MU
Abstract: A theoretical modeling approach is presented, which describes the behavior of a typical fuel cell-heat engine hybrid system in steady-state operating condition based on an existing solid oxide fuel cell model, to provide useful fundamental design characteristics as well as potential critical problems. The different sources of irreversible losses, such as the electrochemical reaction, electric resistances, finite-rate heat transfer between the fuel cell and the heat engine, and heat-leak from the fuel cell to the environment are specified and investigated. Energy and entropy analyses are used to indicate the multi-irreversible losses and to assess the work potentials of the hybrid system. Expressions for the power output and efficiency of the hybrid system are derived and the performance characteristics of the system are presented and discussed in detail. The effects of the design parameters and operating conditions on the system performance are studied numerically. It is found that there exist certain optimum criteria for some important parameters. The results obtained here may provide a theoretical basis for both the optimal design and operation of real fuel cell-heat engine hybrid systems. This new approach can be easily extended to other fuel cell hybrid systems to develop irreversible models suitable for the investigation and optimization of similar energy conversion settings and electrochemistry systems. (c) 2008 Elsevier B.V. All rights reserved.

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Record 4 of 52
Author(s): Zhao, Y (Zhao, Yi); Liang, WZ (Liang, WanZhen)
Title: Non-Condon nature of fluctuating bridges on nonadiabatic electron transfer: Analytical interpretation
Language: English
Abstract: Rigorous expressions for the calculation of nonadiabatic electron transfer rates are presented in closed forms for donor-acceptor systems incorporated fluctuating bridges and their non-Condon electronic couplings. In high temperature limit, they show a similar property to the Marcus formula. However, the Marcus parabolic with respect to the driving force is shifted for the exponential coupling while it becomes an overlap of several Gaussian functions for the linear coupling. Furthermore, the effective couplings are exponentially and linearly dependent on temperature and the squared frequencies of bridge modes for the exponential and linear couplings, respectively.


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Record 5 of 52
Author(s): Chen, XJ (Chen, Xiaojing); Lei, XX (Lei, Xinxiang)
Title: Application of a Hybrid Variable Selection Method for Determination of Carbohydrate Content in Soy Milk Powder Using Visible and Near Infrared Spectroscopy
Language: English
Abstract: Visible and near-infrared (Vis-NIR) spectroscopy was investigated to fast determine the carbohydrate content in soy milk powder. A hybrid variable selection method was proposed. In this method, a simulate annealing (SA) algorithm was first operated to search the optimal band (OB) in the wavelet packet transform (WPT) tree. The OB with 47 variables was further selected by SA (WTP-OB-SA). Finally, the number of variables was reduced from 47 to 20. The best partial least-squares prediction with a high residual predictive deviation (RPD) value of 12.2242 was obtained using these 20 variables with the
correlation coefficient (and root-mean-square error of prediction (RMSEP) being 0.9967 and 0.1669, respectively. The results indicated that Vis-NIR spectroscopy could efficiently determine the carbohydrate content in soy milk powder. The WPT-OB-SA selection method eliminated redundant variables and improved the prediction ability.


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ISSN: 0021-8561

DOI: 10.1021/jf8025887

Subject Category: Agriculture, Multidisciplinary; Chemistry, Applied; Food Science & Technology

ISI Document Delivery No.: 397LU

Record 6 of 52

Author(s): Li, J (Li, Jun); Liang, Y (Liang, Ying); Liao, Q (Liao, Qiang); Zhu, X (Zhu, Xun); Tian, X (Tian, Xin)

Title: Comparison of the electrocatalytic performance of PtRu nanoparticles supported on multi-walled carbon nanotubes with different lengths and diameters


Language: English

Abstract: To investigate the electrocatalytic performance of PtRu nanoparticles supported on multi-walled carbon nanotubes (MWCNTs) with different lengths and diameters, X-ray diffraction, transmission electron microscopy, X-ray photoelectron spectroscopy, and cyclic voltammetry experiments were conducted. It is demonstrated that the length and diameter of MWCNTs play an important role in the electrocatalytic performance of PtRu catalysts. The co-existence of amorphous carbon impurities on the MWCNT10-2 support lowered the accessible surface area of the PtRu nanoparticles, hampered the dispersion of the PtRu nanoparticles, and induced the formation of a low degree of PtRu alloy, thus lowered the electrocatalytic performance of the PtRu/MWCNT10-2 catalyst for methanol oxidation. The highest mass-specific activity of PtRu/MWCNT3050-2 results from a highly accessible PtRu surface and a good dispersion of PtRu particles. Our experimental results also demonstrate that the tube length of MWCNT samples has little effect of the Surface area specific activity of the PtRu/MWCNT catalyst, whereas the PtRu nanoparticles supported on the MWCNT samples with large tube diameter tends to exhibit a higher surface area specific activity for methanol oxidation reaction. This result is suggested to be the combined effects of a high degree of PtRu alloying and the high electronic conductivity of these MWCNT samples. (C) 2008 Elsevier Ltd. All rights reserved.


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ISSN: 0013-4686

DOI: 10.1016/j.electacta.2008.09.005

Subject Category: Electrochemistry

ISI Document Delivery No.: 399PD

Record 7 of 52

Author(s): Zhang, QG (Zhang, Qiu Gen); Liu, QL (Liu, Qing Lin); Chen, Y (Chen, Yu); Wu, JY (Wu, Jian Yang); Zhu, AM (Zhu, Ai Mei)

Title: Microstructure dependent diffusion of water-ethanol in swollen poly(vinyl alcohol): A molecular dynamics simulation study

Source: CHEMICAL ENGINEERING SCIENCE, 64 (2): 334-340 JAN 16 2009

Language: English

Abstract: Molecular dynamics (MD) simulation was used to study the swelling properties of poly(vinyl alcohol) (PVA) in ethanol solutions containing 15, 30 and 45 wt% water. The characteristics of the swollen PVA, intrinsic relation between the microstructure of the swollen PVA and the diffusion of water and ethanol in the PVA matrix were analyzed. It was found that the free volume of the swollen PVA reduced with reductions in the degree of crystallinity was accompanied by an increase in the mobility of PVA chains. Water located mostly in the hydrophilic region of the hydroxyl groups of PVA chains; and hydrogen bonding formed between water and PVA. It was also noted water clusters form in the swollen PVA, whose size increased with increasing degree of swelling, whereas ethanol molecules disperse almost individually in the PVA matrix. The diffusion
coefficients of water and ethanol in the swollen PVA are predicted to increase linearly with increasing swelling. (C) 2008 Elsevier Ltd. All rights reserved.

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**Times Cited:** 0

**ISSN:** 0009-2509

**DOI:** 10.1016/j.ces.2008.10.028

**Subject Category:** Engineering, Chemical

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**Author(s):** Xu, QJ (Xu Qun-Jie); Li, CX (Li Chun-Xiang); Zhou, GD (Zhou Guo-Ding); Zhu, LJ (Zhu Lue-Jun); Lin, CJ (Lin Chang-Jian)

**Title:** Copper Corrosion Inhibition and Adsorption Behavior of 3-Amino-1,2,4-triazole

**Source:** ACTA PHYSICO-CHIMICA SINICA, 25 (1): 86-90 JAN 2009

**Language:** Chinese

**Abstract:** Corrosion inhibition of copper in 3% NaCl Solution by 3-amino-1,2,4-triazole (ATA) was studied in relation to the concentration of the inhibitor using electrochemical (ac impedance and dc polarization) and surface enhanced Raman spectroscopy (SERS) techniques. The results indicated that ATA was a good corrosion inhibitor for copper in a 3% NaCl solution. The inhibition efficiency was 97.65% at an ATA concentration of 20 mg.L-1. Polarization curves showed that ATA behaved as a type of cathodical inhibitor in 3% NaCl solution. Adsorption of ATA followed Langmuir’s adsorption isotherm and the adsorption mechanism was typical of chemisorption. SERS revealed that inhibition of copper corrosion was due to adsorption of ATA molecules on the surface of copper. SERS also confirmed that the adsorbed ATA molecules formed a complex with Cu+ which prevented the formation of copper chloride complexes, CuCl2-

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**Times Cited:** 0

**ISSN:** 1000-6818

**Subject Category:** Chemistry, Physical

**ISI Document Delivery No.:** 397TN

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**Author(s):** Chen, XJ (Chen Xiao-jing); Wu, D (Wu Di); He, Y (He Yong); Liu, S (Liu Shou)

**Title:** Study on Application of Multi-Spectral Image Texture to Discriminating Rice Categories Based on Wavelet Packet and Support Vector Machine

**Source:** SPECTROSCOPY AND SPECTRAL ANALYSIS, 29 (1): 222-225 JAN 2009

**Language:** Chinese

**Abstract:** Based on multi-spectral digital image texture feature, a new rapid and nondestructive method for discriminating rice categories was put forward. The new method combined the advantages of wavelet packet and support vector machine (SVM). In the present study, the images which are 1 036 pixels in vertical direction by 1 384 pixels in horizontal direction with 24-bit depth were captured using a red (R) waveband, near infrared (NIR) waveband and green (G) waveband multi-spectral digital imager. The three wavebands of image (red, green and NIR) can be composed into one image which contains more information than images captured by ordinary digital cameras, and the NIR image can catch more information than visible spectrum. NIR waveband images were decomposed to 16 subbands using three wavelet packet multi-resolution. Because the main feature of texture information is concentrated on the middle frequency, the 8 subbands of middle frequency were selected to calculate entropy, and the entropy of three wavebands of original image was calculated at the same time. Eighty images (twenty for each category) were used for calibration set and eighty images (twenty for each category) were used as the prediction set. Then the rice categories were classified by SVM. The classification rate of rice categories was only 93.75% using the entropy of original image, but reached 100% by wavelet packet decomposition. The overall results show that the technique combining wavelet packet and support vector machine can be efficiently utilized for texture recognition of multi-spectra, and is an effective and simple technique
for discriminating the rice categories. This study also provides a foundation for rice grading and other rice industry processing such as quality diction and milling degree.

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Record 10 of 52

Author(s): Zhu, HL (Zhu, Huili); Chen, XP (Chen, Xiaping); Cai, JF (Cai, Jiafa); Wu, ZY (Wu, Zhengyun)

Title: 4H-SiC ultraviolet avalanche photodetectors with low breakdown voltage and high gain


Language: English

Abstract: The separate absorption and multiplication (SAM) 4H-SiC ultraviolet (UV) avalanche photodetectors (APDs) have been designed, fabricated and characterized. A gain higher than 1.8 x 10(4) was achieved at 90% breakdown voltage of similar to 55 V. At 0 V, the peak absolute responsivity was estimated to be larger than 0.078 A/W at 270 nm, corresponding to a peak external quantum efficiency of over 35.8%. The long-wavelength cutoff was about 380 nm. In addition, the UV-to-visible rejection ratio of around three orders of magnitude was extracted from the spectra response. When the reverse bias was larger than 35 V, the spectral responsivity enhanced distinctly. At the reverse bias of 42 V, the peak responsivity increased to 0.203 A/W at 270 nm, corresponding to a maximum external quantum efficiency of similar to 93%, which showed a distinct avalanche behavior. Furthermore, the ideality factor around 1.65 and the spectral detectivity about 3.1 X 10(13) cm Hz(1/2) W-1 were estimated. in conclusion, the 4H-SiC APD have excellent performance for UV detection. (C) 2008 Elsevier Ltd. All rights reserved.

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Times Cited: 0

ISSN: 0038-1101


Subject Category: Engineering, Electrical & Electronic; Physics, Applied; Physics, Condensed Matter

ISI Document Delivery No.: 395VS

Record 11 of 52

Author(s): Wen, YH (Wen, Yuhua); Fang, H (Fang, Hui); Zhu, ZZ (Zhu, Zizhong); Sun, SG (Sun, Shigang)

Title: Molecular dynamics investigation of shape effects on thermal characteristics of platinum nanoparticles

Source: PHYSICS LETTERS A, 373 (2): 272-276 JAN 5 2009

Language: English

Abstract: Using molecular dynamics simulations with the quantum corrected Sutton-Chen type many-body potential, we investigate the thermal characteristics and Structural evolution of Pt nanoparticles with spherical and polyhedral shapes under the heating process. The main focus of this work is the shape effects on the thermal characteristics of Pt nanoparticles. The simulation results show that all types of nanoparticles present the same overall melting temperature ill spite of their different shapes. These nanoparticles can hold their initial shapes and structures at low temperature. However, polyhedral nanoparticles undergo a remarkable shape transformation before their overall melting. The critical temperature of shape transformation depends oil their shapes and associated Miller index of the surface. Our study indicates that octahedron-truncated nanoparticle displays a better thermal stability than other polyhedral nanoparticles. Crown Copyright (C) 2008 Published by Elsevier B.V. All rights reserved.

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Times Cited: 0
Record 12 of 52

Author(s): Zheng, J (Zheng, Jun); Jiang, ZY (Jiang, Zhi-Yuan); Kuang, Q (Kuang, Qin); Xie, ZX (Xie, Zhao-Xiong); Huang, RB (Huang, Rong-Bin); Zheng, LS (Zheng, Lan-Sun)

Title: Shape-controlled fabrication of porous ZnO architectures and their photocatalytic properties

Source: JOURNAL OF SOLID STATE CHEMISTRY, 182 (1): 115-121 JAN 2009

Language: English

Abstract: In this paper, we report a simple two-step approach to prepare porous octahedron- and rod-shaped ZnO architectures. The morphology of Porous ZnO particles can be conveniently tuned by controlling morphologies of the ZnC(2)O4·2H(2)O precursor. SEM and TEM characterization results indicate that these porous ZnO architectures are built up by numerous ZnO primary nanoparticles with random attachment. Based on thermogravimetry analysis, we believe that the release of water vapor, CO, and CO2 leads to the formation of high-density pores in shape-controlled particles during the calcination process. Further experimental results indicate that as-prepared porous ZnO particles exhibit good photocatalytic activity due to large surface area. (C) 2008 Elsevier Inc. All rights reserved.

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Times Cited: 0

ISSN: 0375-9601

DOI: 10.1016/j.physleta.2008.11.017

Subject Category: Physics, Multidisciplinary

ISI Document Delivery No.: 396TK

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Record 13 of 52

Author(s): Yang, SY (Yang Sheng-Yan); Zhang, N (Zhang Na); Wu, ZY (Wu Zhen-Yi)

Title: Synthesis and Property of Novel Solar Energy of C60Pt(dpdp)


Language: Chinese

Abstract: The fullerene complex C60Pt (dpdp) was prepared by reacting C-60 with dpdp in nitrogen atmosphere. The synthesized fullerene complex was characterized by means of Mass Spectrometry (MS), Elemental Analysis, FT-IR, UV-Vis and XPS. Besides these, the photoelectric properties and redox property of this complex were also studied. The results show that the greatest value of photovoltaic potential is 371mV in the benzoquinone/hydroquinone redox couple, and the value of photovoltaic effects reach the maximum when the thickness of complex film is 1 μm. Based on the merits mentioned above, the complex has excellent photoelectric properties, therefore it has potential application in solar cells.

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ISSN: 0022-4596

DOI: 10.1016/j.jssc.2008.10.009

Subject Category: Chemistry, Inorganic & Nuclear; Chemistry, Physical

ISI Document Delivery No.: 395TK

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Record 14 of 52

Author(s): Dai, ZH (Dai, Zhonghua); Chen, ZZ (Chen, Zuozhou); Ye, H (Ye, Hua); Zhou, LH (Zhou, Longhai); Cao, LX (Cao, Lixue); Wang, YQ (Wang, Yiquan); Peng, SH (Peng, Sihua); Chen, LB (Chen, Liangbiao)

Title: Characterization of microRNAs in cephalochordates reveals a correlation between microRNA repertoire homology and morphological similarity in chordate evolution

Abstract: Cephalochordates, urochordates, and vertebrates comprise the three extant groups of chordates. Although higher morphological and developmental similarity exists between cephalochordates and vertebrates, molecular phylogeny studies have instead suggested that the morphologically simplified urochordates are the closest relatives to vertebrates. MicroRNAs (miRNAs) are regarded as the major factors driving the increase of morphological complexity in early vertebrate evolution, and are extensively characterized in vertebrates and in a few species of urochordates. However, the comprehensive set of miRNAs in the basal chordates, namely the cephalochordates, remains undetermined. Through extensive sequencing of a small RNA library and genomic homology searches, we characterized 100 miRNAs from the cephalochordate amphioxus, Branchiostoma japonicum, and B. florideae. Analysis of the evolutionary history of the cephalochordate miRNAs showed that cephalochordates possess 54 miRNA families homologous to those of vertebrates, which is threefold higher than those shared between urochordates and vertebrates. The miRNA contents demonstrated a clear correlation between the extent of miRNA overlapping and morphological similarity among the three chordate groups, providing a strong evidence of miRNAs being the major genetic factors driving morphological complexity in early chordate evolution.


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Record 16 of 52

Author(s): Chen, Z (Chen Zhong); Lin, MJ (Lin MeiJin); Chen, X (Chen Xi); Cai, SH (Cai ShuHui)

Title: Advances in high-resolution nuclear magnetic resonance methods in inhomogeneous magnetic fields using intermolecular multiple quantum coherences


Language: English

Abstract: The reaction pathways for selective oxidation of propane to acrolein over Ce0.1Ag0.3Mo0.5P0.3Ox Catalyst were investigated by three methods, (i) steady-state reaction test of the individual oxidation of propane and the probe molecule of possible reaction intermediates, (ii) temperature-programmed surface reaction (TPSR) study of propane oxidation in presence of gas phase O-2 or not, and (ii) in situ Raman spectroscopy investigation of propane oxidation and propylene oxidation on the catalyst. Based on the obtained results, three possible reaction pathways for selective oxidation of propane to acrolein on the catalysts are proposed. The major reaction pathway is that propylene (pi-allyl species) is produced from the activation of the methylene C-H bond of propane and further oxidizes to acrolein through or-allyl species. However, the presence of gas phase O-2 favors the formation of acrolein in propane oxidation on the catalyst. (C) 2008 Elsevier B.V. All rights reserved.


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Record 15 of 52

Author(s): Zhang, X (Zhang, Xin); Wan, HL (Wan, Huilin); Weng, WZ (Weng, Weizheng)

Title: Reaction pathways for selective oxidation of propane to acrolein over Ce-Ag-Mo-P-O catalysts


Language: English

Abstract: The reaction pathways for selective oxidation of propane to acrolein on Ce0.1Ag0.3Mo0.5P0.3Ox Catalyst were investigated by three methods, (i) steady-state reaction test of the individual oxidation of propane and the probe molecule of possible reaction intermediates, (ii) temperature-programmed surface reaction (TPSR) study of propane oxidation in presence of gas phase O-2 or not, and (ii) in situ Raman spectroscopy investigation of propane oxidation and propylene oxidation on the catalyst. Based on the obtained results, three possible reaction pathways for selective oxidation of propane to acrolein on the catalysts are proposed. The major reaction pathway is that propylene (pi-allyl species) is produced from the activation of the methylene C-H bond of propane and further oxidizes to acrolein through or-allyl species. However, the presence of gas phase O-2 favors the formation of acrolein in propane oxidation on the catalyst. (C) 2008 Elsevier B.V. All rights reserved.
Abstract: Strong and extremely homogeneous static magnetic field is usually required for high-resolution nuclear magnetic resonance (NMR). However, in the cases of in vivo and so on, the magnetic field inhomogeneity owing to magnetic susceptibility variation in samples is unavoidable and hard to eliminate by conventional methods such as shimming. Recently, intermolecular multiple quantum coherences (iMQCs) have been employed to eliminate inhomogeneous broadening and obtain high-resolution NMR spectra, especially for in vivo samples. Compared to other high-resolution NMR methods, iMQC method exhibits its unique feature and advantage. It simultaneously holds information of chemical shifts, multiplet structures, coupling constants, and relative peak areas. All the information is often used to analyze and characterize molecular structures in conventional one-dimensional NMR spectroscopy. In this work, recent technical developments including our results in this field are summarized; the high-resolution mechanism is analyzed and comparison with other methods based on interactions between spins is made; comments on the current situation and outlook on the research directions are also made.

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Times Cited: 0

ISSN: 1672-1799

DOI: 10.1007/s11433-009-0001-9

Subject Category: Physics, Multidisciplinary

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ISSN: 0026-3672

DOI: 10.1007/s00604-008-0038-x

Subject Category: Chemistry, Analytical

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Record 19 of 52

Author(s): Chen, YZ (Chen, Yuanzhi); Luo, XH (Luo, Xiaohua); Yue, GH (Yue, Guang-Hui); Luo, XT (Luo, Xuetao); Peng, DL (Peng, Dong-Liang)

Title: Synthesis of iron-nickel nanoparticles via a nonaqueous organometallic route


Language: English

Abstract: Fe-Ni nanoparticles have been synthesized via a nonaqueous solution-phase approach using thermal decomposition of Ni(II) acetylacetonate and Fe(III) acetylacetonate in oleylamine without further reducing agents. The analyses of powder X-ray diffraction and transmission electron microscopy show that the as-synthesized Fe-Ni nanoparticles possess a face-centered cubic (fcc) crystalline structure and exhibit a polydispersed characteristic. The particle morphology and size distribution can be further controlled by introducing surfactants in the reaction system, and the final chemical composition also can be tuned to some extent by varying the initial molar ratios of metal precursors. Room temperature magnetic measurements reveal a ferromagnetic characteristic for the as-synthesized nanoparticles. An increased saturation magnetization has been observed with increasing Fe contents. (C) 2008 Elsevier B.V. All rights reserved.

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DOI: 10.1016/j.matchemphys.2008.07.118

Subject Category: Materials Science, Multidisciplinary

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Record 20 of 52

Author(s): Merlitz, H (Merlitz, Holger); He, GL (He, Gui-Li); Sommer, JU (Sommer, Jens-Uwe); Wu, CX (Wu, Chen-Xu)

Title: Reversibly Switchable Polymer Brushes with Hydrophobic/Hydrophilic Behavior: A Langevin Dynamics Study


Language: English

Abstract: Binary polymer brushes with hydrophobic/hydrophilic behavior are forming a two-layer system with a collapsed hydrophobic and a swollen hydrophilic phase. The process of switching upon Sudden change of he solvent quality is analyzed in detail for Various solvent selectivities, chain lengths, and grafting densities. This process is highly reversible since after a microphase separation the chains are moving collectively inside their phase domains so that the interactions between chains of different species are diminished. The thickness of the collapsed layer does not scale linearly with the chain length N, an unexpected result which is discussed in the paper. The switching relaxation times display a scaling of N-2 like Rouse relaxation and not of N-3 like vertical relaxation times in equilibrium.

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ISSN: 0024-9297

DOI: 10.1021/ma8019877
Record 21 of 52

Author(s): Song, XY (Song, Xinyu); Li, SL (Li, Senlin); Li, A (Li, An)
Title: ANALYSIS OF A STAGE-STRUCTURED PREDATOR-PREY SYSTEM WITH IMPULSIVE PERTURBATIONS AND TIME DELAYS
Language: English
Abstract: In this paper, a stage-structured predator-prey system with impulsive perturbations and time delays is presented to investigate the ecological problem of how a pest population and natural enemy population can coexist. Sufficient conditions are obtained using a discrete dynamical system determined by a stroboscopic map, which guarantee that a 'predator-extinction' periodic solution is globally attractive. When the impulsive period is longer than some time threshold or the impulsive harvesting rate is below a control threshold, the system is permanent. Our results provide some reasonable suggestions for pest management.
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Times Cited: 0
ISSN: 0304-9914
Subject Category: Mathematics, Applied; Mathematics
ISI Document Delivery No.: 391UY

Record 22 of 52

Author(s): Pan, YM (Pan, Ying-ming); Zhao, SY (Zhao, Su-yan); Ji, WH (Ji, Wen-hua); Zhan, ZP (Zhan, Zhuang-ping)
Title: One-Pot Synthesis of Substituted Furans Using Cu(OTf)(2)-Catalyzed Propargylation/Cycloisomerization Tandem Reaction
Language: English
Abstract: A convenient one-pot propargylation/cycloisomerization tandem process has been developed for the synthesis of substituted furans derivatives from 1,3-dicarbonyl compounds and enoxysilanes with propargylic alcohols or acetates using copper(II) triflate as a bifunctional catalyst. This method provides a flexible and rapid route to substituted furans.
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ISSN: 1520-4766
DOI: 10.1021/cc8001316
Subject Category: Chemistry, Applied; Chemistry, Medicinal; Chemistry, Multidisciplinary
ISI Document Delivery No.: 391UY

Record 23 of 52

Author(s): Xue, H (Xue, Hao); Xiong, ZX (Xiong, Zhaoxian)
Title: The structure and dielectric tunable properties of < 0 0 1 > preferred oriented BST ceramics prepared by templated grain growth method
Source: JOURNAL OF ALLOYS AND COMPOUNDS, 467 (1-2): 338-341 JAN 7 2009
Language: English
Abstract: In this work, textured barium strontium titanate ceramics with a high degree of < 0 0 1 > preferred orientation were prepared by templated grain growth technique. The structure and dielectric tunable properties of < 0 0 1 > textured BST ceramic were investigated. A high degree of fiber texture was achieved using < 0 0 1 > oriented SrTiO3 as template particles in fine-grained BST matrix. The dielectric tunability of < 0 0 1 > textured BST ceramic were significantly increased compared to random oriented ceramic. Furthermore the P-E curve of < 0 0 1 > textured BST ceramic presented a more visible hysteresis loop. Combined with origin of the tunability, these effects could be interpreted on the base of both hardening mechanism of soft mode and polar nano-region mechanism. (C) 2007 Elsevier B.V. All rights reserved.
Controlling Morphologies and Tuning the Related Properties of Nano/Microstructured ZnO Crystallites

In this paper, we successfully synthesized three kinds of typical ZnO micro/nanocrystallites including flakes, columns, and pyramids by means of different facile wet chemical routes. The growth environment plays a crucial role in the morphologies of these ZnO micro/nanocrystallites. At the same time, we find that physical/chemical properties of these ZnO samples are dependent on their exposed surface, and the order of gas sensing and photocatalytic efficiency of the ZnO crystal planes is (0001) > {10 (1) over bar0} > {10 (1) over bar1} and (000 (1) over bar). On the basis of structural analyses of various exposed surfaces and related X-ray photoelectron spectroscopy, we deeply discussed the effect of definite surface structures on their gas sensing and photocatalytic properties.

Performance of Several Density Functional Theory Methods on Describing Hydrogen-Bond Interactions

We have investigated eleven density functionals, including LDA, PBE, mPWPW91, TPSS, B3LYP, X3LYP, PBEO, O3LYP, B97-1, MPW1K, and TPSSh, for their performances on describing hydrogen bond (HB) interactions. The emphasis has been laid not only on their abilities to calculate the intermolecular hydrogen bonding energies but also on their performances in predicting the relative energies of intermolecular H-bonded complexes and the conformer stabilities due to intramolecular hydrogen bondings. As compared to the best theoretical values, we found that although PBE and PBEO gave the best estimation of HB strengths, they might fail to predict the correct order of relative HB energies, which might lead to a wrong prediction of the global minimum for different conformers. TPSS and TPSSh did not always improve over PBE and PBEO. B3LYP was found to underestimate the intermolecular HB strengths but was among the best performers in calculating the relative HB energies. We showed here that X3LYP and B97-1 were able to give good values for both absolute HB strengths and relative HB energies, making these functionals good candidates for HB description.
Record 26 of 52

Author(s): Meng, J (Meng, Jun); Wang, FP (Wang, Fengping); Wang, F (Wang, Feng); Zheng, YP (Zheng, Yanping); Peng, XT (Peng, Xiaotong); Zhou, HY (Zhou, Huaiyang); Xiao, X (Xiao, Xiang)

Title: An uncultivated crenarchaeota contains functional bacteriochlorophyll a synthase


Language: English

Abstract: A fosmid clone 37F10 containing an archaeal 16S rRNA gene was screened out from a metagenomic library of Pearl River sediment, southern China. Sequence analysis of the 35 kb inserted fragment of 37F10 found that it contains a single 16S rRNA gene belonging to Miscellaneous Crenarchaeotal Group (MCG) and 36 open reading frames (ORFs). One ORF (orf11) encodes putative bacteriochlorophyll a synthase (bchG) gene. Bacteriochlorophyll a synthase gene has never been reported in a member of the domain Archaea, in accordance with the fact that no (bacterio)-chlorophyll has ever been detected in any cultivated archaea. The putative archaeal bchG (named as ar-bchG) was cloned and heterologously expressed in Escherichia coli. The protein was found to be capable of synthesizing bacteriochlorophyll a by esterification of bacteriochlorophylide a with phytyl diphosphate or geranylgeranyl diphosphate. Furthermore, phylogenetic analysis clearly indicates that the ar-bchG diverges before the bacterial bchGs. Our results for the first time demonstrate that a key and functional enzyme for bacteriochlorophyll a biosynthesis does exist in Archaea.


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ISSN: 1751-7362

DOI: 10.1038/ismej.2008.85

Record 27 of 52

Author(s): Xu, T (Xu, Tao); Zhou, X (Zhou, Xi); Jiang, ZY (Jiang, Zhiyuan); Kuang, Q (Kuang, Qin); Xie, ZX (Xie, Zhaoxiong); Zheng, LS (Zheng, Lansun)

Title: Syntheses of Nano/Submicrostructured Metal Oxides with All Polar Surfaces Exposed via a Molten Salt Route


Language: English

Abstract: In this paper, a general method for the preparation of metal oxides with all polar surfaces exposed is presented. The syntheses of the products were carried out with simply performing reactions in a molten salt system, in which cations and anions tend to have strong electrostatic interactions with positive or negative charged polar planes so as to lower the surface energy and slow down the growth rate of polar planes, resulting in the formation of exposed polar surfaces. With this strategy, wurtzite structured ZnO, rocksalt structured MgO, spinel structured Co3O4, and ternary element compound ZnFe2O4 of spinel structure were successfully synthesized with all polar surfaces exposed, which demonstrated a universality of our proposed strategy.

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Times Cited: 0

ISSN: 1528-7483

DOI: 10.1021/cg8002096

Subject Category: Chemistry, Multidisciplinary; Crystallography; Materials Science, Multidisciplinary

ISI Document Delivery No.: 392IW

Record 28 of 52
The surface properties of biomaterials determine the interactions between biomedical devices and the surrounding biological environment. The surface modification of biomaterials is extensively recognized as a key strategy in the design of the next generation of bone implants and tissue engineering. In this study, the highly ordered octacalcium phosphate (OCP) coating and OCP/protein coating with hierarchically porous structure in nano-micro scale were constructed on titanium substrate by electrochemically-induced deposition (ED). The formation behavior of apatite on OCP and OCP/protein coatings immersed in simulated body fluid (SBF) was investigated in physicochemical aspects. It is indicated that soaked in SBF, the OCP and OCP/protein coatings are possible to induce relevant apatite formation on their surface, and the apatite-forming behavior in body environment is dependent on the chemical composition and structure of the coatings. The apatite formed on OCP/protein composite coating possesses carbonated structure, needle-like crystals in nano scale, lower Ca/P ratio and higher degree of the preferred c-axis orientation, which are similar to the mineral composition and structure in natural bone, and hence called as bone-like apatite. (C) 2008 Elsevier B. V. All rights reserved.
Title: Ammonium iron(III) phosphate(V) fluoride, (NH4)(0.5)[(NH4)(0.375)K-0.125]FePO4F, with ammonium partially substituted by potassium

Source: ACTA CRYSTALLOGRAPHICA SECTION E-STRUCTURE REPORTS ONLINE, 65: I4-U118 Part 1 JAN 2009

Language: English

Abstract: The title compound, ammonium potassium iron(III) phosphate fluoride, (NH4)(0.875)K0.125FePO4F, is built from zigzag chains (1)(infinity){[FeO4F2](7-)}, with Fe3+ in a distorted octahedral coordination, extending along both the [011] and [0 (1) over bar1] directions. These chains are made up of alternating trans-[FeO4F2] and cis-[FeO4F2] octahedra via shared F-atom corners, and are linked by PO4 tetrahedra, resulting in an open-framework structure with channels along the [010] and [100] directions. There are two crystallographically independent ammonium sites: one in the [010] channels and the other, partially substituted by K+ ions, in the [100] channels. The ammonium in the [010] channels is fixed to the framework via eight hydrogen bonds (six N-H center dot center dot center dot O and two N-H center dot center dot center dot F).

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Record 31 of 52

Author(s): Zheng, JF (Zheng, Jian-Feng); Jiang, LJ (Jiang, Li-Jiao); Ye, JL (Ye, Jian-Liang)
Title: (3S,7aR)-7-Methoxy-7a-methyl-3-phenyl-2,3-dihydropyrrolo[2,1-b]oxazol-5(7aH)-one
Language: English

Abstract: In the title chiral butterfly-like bicyclic lactam, C14H15NO3, the phenyl and methyl groups are syn with respect to each other. The dihydropyrrrole ring adopts a boat conformation, whereas the oxazole ring has a slightly distorted boat conformation. The packing of molecules in the crystal structure is stabilized by intermolecular C-H center dot center dot center dot O hydrogen bonds.

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Record 32 of 52

Author(s): Cao, WZ (Cao, Wenzhi); Bowden, WB (Bowden, William B.); Davie, T (Davie, Tim); Fenemor, A (Fenemor, Andrew)
Title: Modelling Impacts of Land Cover Change on Critical Water Resources in the Motueka River Catchment, New Zealand
Source: WATER RESOURCES MANAGEMENT, 23 (1): 137-151 JAN 2009
Language: English

Abstract: After the SWAT (Soil and Water Assessment Tool) model was calibrated and validated to historic flow records for the current land use conditions, two additional land cover scenarios (a prehistoric land cover and a potential maximum plantation pine cover) were used to evaluate the impacts of land cover change on total water yields, groundwater flow, and quick flow in the Motueka River catchment, New Zealand. Low-flow characteristics and their potential impacts on availability for water abstraction and for support of in-stream habitat values were focused on. The results showed that the annual total water yields, quick flow and baseflow decreased moderately in the two scenarios when compared with the current actual land use. The annual water balance for the pine potential land cover scenario did not differ substantially from the prehistoric scenario for the catchment as whole. However, there were more notable differences among individual tributary catchments, which could be attributed to the relative area of land cover altered and location of those catchments. Simulated low flows for the prehistoric and potential pine cover scenarios were less than observed, indicating a potential constraint to water abstraction in the future.
land cover scenarios were both significantly lower than the low flows for the current land use. In summary, under the current land use conditions, both annual water yield and low flow are higher than was the case before human intervention in the area or in a maximum commercial reforestation scenario.


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**Times Cited:** 0

**ISSN:** 0920-4741

**DOI:** 10.1007/s11269-008-9268-2

**Subject Category:** Engineering, Civil; Water Resources

---

**Record 33 of 52**

**Author(s):** Deng, YB (Deng, Yongbiao); Shen, YM (Shen, Yuemao)

**Title:** Clavicorolides A and B, Sesquiterpenoids from the Fermentation Products of Edible Fungus Clavicorona pyxidata

**Source:** ORGANIC LETTERS, 11 (1): 109-112 JAN 1 2009

**Language:** English

**Abstract:** Clavicorolides A (1) and B (2), two sesquiterpenoids possessing a novel backbone named as Clavicoronane-type, together with one new and two known Protoilludane-type sesquiterpenoids, namely, Tsugicolines M (3), A (4), and C (5), and Sterpurane (6), and Lactarane-type sesquiterpenoid Lactarorufin A (7), were isolated from the fermentation products of Clavicorona pyxidata YB2005. Their structures including relative and absolute configurations were elucidated on the basis of NIVIR data and analysis of X-ray single crystal diffraction.

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**Times Cited:** 0

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**DOI:** 10.1021/ol8024549

**Subject Category:** Chemistry, Organic

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**Record 34 of 52**

**Author(s):** Kumar, P (Kumar, Pankaj); Han, BC (Han, B. C.); Shi, Z (Shi, Z); Jia, J (Jia, J.); Wang, YP (Wang, Y. P.); Zhang, YT (Zhang, Y. T.); Liang, L (Liang, L.); Liu, QF (Liu, Q. F.); Ji, ZL (Ji, Z. L.); Chen, YZ (Chen, Y. Z.)

**Title:** Update of KDBI: Kinetic Data of Bio-molecular Interaction database

**Source:** NUCLEIC ACIDS RESEARCH, 37: D636-D641 Sp. Iss. SI JAN 2009

**Language:** English

**Abstract:** Knowledge of the kinetics of biomolecular interactions is important for facilitating the study of cellular processes and underlying molecular events, and is essential for quantitative study and simulation of biological systems. Kinetic Data of Bio-molecular Interaction database (KDBI) has been developed to provide information about experimentally determined kinetic data of protein-protein, protein nucleic acid, protein-ligand, nucleic acid-ligand binding or reaction events described in the literature. To accommodate increasing demand for studying and simulating biological systems, numerous improvements and updates have been made to KDBI, including new ways to access data by pathway and molecule names, data file in System Biology Markup Language format, more efficient search engine, access to published parameter sets of simulation models of 63 pathways, and 2.3-fold increase of data (19 263 entries of 10 532 distinctive biomolecular binding and 11 954 interaction events, involving 2635 proteins/protein complexes, 847 nucleic acids, 1603 small molecules and 45 multi-step processes). KDBI is publicly available at http://bidd.nus.edu.sg/group/kdbi/kdbi.asp.

Deletion of Shp2 Tyrosine Phosphatase in Muscle Leads to Dilated Cardiomyopathy, Insulin Resistance, and Premature Death

Author(s): Princen, F (Princen, Frederic); Bard, E (Bard, Emilie); Sheikh, F (Sheikh, Farah); Zhang, SS (Zhang, Sharon S.); Wang, J (Wang, Jing); Zago, WM (Zago, Wagner M.); Wu, DM (Wu, Dongmei); Trelles, RD (Trelles, Ramon Diaz); Bailly-Maitre, B (Bailly-Maitre, Beatrice); Kahn, CR (Kahn, C. Ronald); Chen, Y (Chen, Yan); Reed, JC (Reed, John C.); Tong, GG (Tong, Gary G.); Mercola, M (Mercola, Mark); Chen, J (Chen, Ju); Feng, GS (Feng, Gen-Sheng)

Title: Deletion of Shp2 Tyrosine Phosphatase in Muscle Leads to Dilated Cardiomyopathy, Insulin Resistance, and Premature Death


Abstract: The intracellular signaling mechanisms underlying the pathogenesis of cardiac diseases are not fully understood. We report here that selective deletion of Shp2, an SH2-containing cytoplasmic tyrosine phosphatase, in striated muscle results in severe dilated cardiomyopathy in mice, leading to heart failure and premature mortality. Development of cardiomyopathy in this mouse model is coupled with insulin resistance, glucose intolerance, and impaired glucose uptake in striated muscle cells. Shp2 deficiency leads to upregulation of leukemia inhibitory factor-stimulated phosphatidylinositol 3-kinase/Akt, Erk5, and Stat3 pathways in cardiomyocytes. Insulin resistance and impaired glucose uptake in Shp2-deficient mice are at least in part due to impaired protein kinase C-zeta/lamba and AMP-kinase activities in striated muscle. Thus, we have generated a mouse line modeling human patients suffering from cardiomyopathy and insulin resistance. This study reinforces a concept that a compound disease with multiple cardiovascular and metabolic disturbances can be caused by a defect in a single molecule such as Shp2, which modulates multiple signaling pathways initiated by cytokines and hormones.

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Direct Preparation Kinetics of 1,3-Dichloro-2-propanol from Glycerol Using Acetic Acid Catalyst

Author(s): Luo, ZH (Luo, Zheng-Hong); You, XZ (You, Xiao-Zi); Li, HR (Li, Hua-Rong)

Title: Direct Preparation Kinetics of 1,3-Dichloro-2-propanol from Glycerol Using Acetic Acid Catalyst

Source: INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH, 48 (1): 446-452 JAN 7 2009

Abstract: Direct preparation of 1,3-dichloro-2-propanol from glycerol is carried out in a batch reactor using acetic acid catalyst at 363-393 K. The analytical technique, gas chromatography, is employed in order to follow the time evolution of the reagents. The kinetic model of the process is developed. Furthermore, the model parameters of the process are also determined by data fitting. The results show that direct preparation follows the S(N)2 mechanism. A kinetic model corresponding to the mechanism is proposed in this work. The experimental results show that the kinetic model agrees well with the experiments.

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Culturable bacteria in glacial meltwater at 6,350 m on the East Rongbuk Glacier, Mount Everest

Abstract: Culturable bacteria in the glacial meltwater in the ablation zones of glacier at high altitude (6,350 m) on Mt Everest were isolated and identified by 16S rRNA amplification and sequencing. The obtained sequences revealed the presence of members of alpha, beta, and gamma-Proteobacteria, Actinobacteria, and Firmicutes, with the Actinobacteria dominant in the studied habitat. All 16S rRNA sequences were similar to previously determined sequences, ranging from 97 to 99% identical values. The strains isolated from meltwater were distinctly different from those recovered from a cryoconite hole and under glacier habitat. The majority of the isolates' nearest neighbors were from the permafrost, dust, soil, plant, and aqueous environments. The Biolog bioassay and growth test under different temperatures suggested that the culturable bacteria in glacial meltwater could be divided into three categories in terms of their survival strategies: Group I sensitive to temperature change but versatile in utilization of carbon substrates (capable of utilization of about 70% of the Biolog carbon substrates); Group II tolerant to variable temperature and less capable of carbon utilization (less than half of the Biolog carbon species can be used); Group III slow in growth and weak in carbon utilization (only a few Biolog carbon substrates can be used).

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Lateral Flow Immunoassay Using Europium Chelate-Loaded Silica Nanoparticles as Labels

Abstract: BACKGROUND: Despite their ease of use, lateral flow immunoassays (LFIs) often suffer from poor quantitative discrimination and low analytical sensitivity. We explored the use of a novel class of europium chelate-loaded silica nanoparticles as labels to overcome these limitations.

METHODS: Antibodies were covalently conjugated onto europium chelate-loaded silica nanoparticles with dextran as a linker. The resulting conjugates were used as labels in LFIA for detection of hepatitis B surface antigen (HBsAg). We performed quantification with a digital camera and Adobe Photoshop software. We also used 286 clinical samples to compare the proposed method with a quantitative ELISA.

RESULTS: A detection limit of 0.03 μg/L was achieved, which was 100 times lower than the colloidal gold-based LFIs and lower than ELISA. A precise quantitative dose-response curve was obtained, and the linear measurement range was 0.05-3.13 μg/L, within which the CVs were 2.3%-10.4%. Regression analysis of LFIA on ELISA results gave: log (LFIA) = -0.14 log (ELISA) + 1.03 μg/L with r = 0.99 for the quantification of HBsAg in 35 positive serum samples. Complete agreement was observed for the qualitative comparison of 286 clinical samples assayed with LFIA and ELISA.

CONCLUSIONS: Europium chelate-loaded silica nano-particle labels have great potential to improve LFIs, making them useful not only for simple screening applications but also for more sensitive and quantitative immunoassays.

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Residues that affect human Argonaute2 concentration in cytoplasmic processing bodies

Sequence-specific gene silencing triggered by double-stranded RNA is a fundamental gene regulatory mechanism present in almost all eukaryotes. Argonaute2 (Ago2) is the central protein component of RNA-induced silencing complex (RISC), and resides in cytoplasmic processing bodies (P-bodies). In the present Study, we demonstrated one human Mutant Ago2 protein containing 6 point mutations (G32W, F128L, R196Q, P458S, T741A, S752G) failed to accumulate in P-bodies. Analysis of the different Ago2 revertants indicates the S752 as a key amino acid for P-body localization of Ago2. The S752 is evolutionary conserved in the Piwi domain of Ago2 homologs from worms, insects, plants and mammals. We further showed the single point mutation S752G interfering the interaction between Ago2 and Dcp1a, a key component of P-bodies. (C) 2008 Elsevier Inc. All rights reserved.

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Genetic Diversity and Abundance of Flavobacterial Proteorhodopsin in China Seas

Proteorhodopsin (PR) genes related to Flavobacteria were found to be highly diverse in the East and South China seas and displayed a distinct geographic pattern, which appeared to reflect cold versus warm adaptation when Global Oceanic Sampling database metagenomic data were included. Flavobacterial PR genes were more abundant offshore than nearshore, implying that inheritance of the PR gene could be important for Flavobacteria living in the oligotrophic environment.

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Author(s): Chen, CM (Chen, Chang-Ming); Liu, F (Liu, F.); Anh, V (Anh, V.)
Title: A Fourier method and an extrapolation technique for Stokes' first problem for a heated generalized second grade fluid with fractional derivative
Language: English
Abstract: In this article, we consider Stokes' first problem for a heated generalized second grade fluid with fractional derivative (SFP-HGSGF). Implicit and explicit numerical approximation schemes for the SFP-HGSGF are presented. The stability and convergence of the numerical schemes are discussed using a Fourier method. In addition, the solvability of the implicit numerical approximation scheme is also analyzed. A Richardson extrapolation technique for improving the order of convergence of the implicit scheme is proposed. Finally, a numerical test is given. The numerical results demonstrate the good performance of our theoretical analysis. (C) 2008 Elsevier B.V. All rights reserved.
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Record 42 of 52
Author(s): Zhang, Y (Zhang, Yong); Cai, KH (Cai, Kunhuang); Li, C (Li, Cheng); Chen, SY (Chen, Songyan); Lai, HK (Lai, Hongkai); Kang, JY (Kang, Junyong)
Title: Strain relaxation in SiGe layer during wet oxidation process
Source: APPLIED SURFACE SCIENCE, 255 (6): 3701-3705 JAN 1 2009
Language: English
Abstract: The strain relaxation in SiGe layer on silicon substrate during wet oxidation at 1000 degrees C was investigated. It was proposed that the competition between Ge accumulation and diffusion led to different strain-relaxation behaviors. At the very beginning, Ge atoms at the oxidizing interface were quickly accumulated due to the high oxidation rate resulting in the additional nucleation of misfit dislocations (therefore a lot of threading dislocations) to relieve stress after the thickness of the Ge condensed layer was larger than the critical value. And then, when the Ge accumulation rate was less than the diffusion rate, Ge content started to decrease from a maximum value and the strain in the SiGe layer was mainly relieved through surface roughing and the degree of strain relaxation reached a maximum. When the samples were further oxidized, Ge accumulation could be neglected because of the self-limiting oxidation and the Ge diffusion dominated the consequent processes. As a result, Ge content at the interface was reduced, with the contribution of the strain relaxation in SiO2 viscously, leading to the decrease of degree of strain relaxation in the SiGe layers slowly. (C) 2008 Elsevier B.V. All rights reserved.
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Record 43 of 52
Author(s): Wu, GY (Wu, Guo-yang); Hasenberg, T (Hasenberg, Till); Magdeburg, R (Magdeburg, Richard); Bonninghoff, R (Boenninghoff, Roderich); Sturm, JW (Sturm, Joerg W.); Keese, M (Keese, Michael)
Title: Association Between EGF, TGF-beta 1, VEGF Gene Polymorphism and Colorectal Cancer
Language: English
Abstract: Up to the present, EGF 61 A/G, TGF-beta 1 -509 T/C, and VEGF 936 T/C gene polymorphisms have been analyzed in other cancer entities than colorectal cancer. We have now investigated the frequency of these gene polymorphisms among colorectal cancer patients.

A total of 157 colorectal cancer patients and 117 cancer-free healthy people were recruited at the Surgical Department of the Universitätsklinikum Mannheim. All patients and healthy people are Caucasians. Genomic DNA was isolated from peripheral blood, and gene polymorphisms were analyzed by polymerase chain reaction-restriction fragment length polymorphism (PCR-RFLP).

The distribution of EGF 61 G/G homozygotes among colorectal cancer patients was more frequent than that in the control group (33.1% versus 11.1%; Odds Ratio [OR] = 3.962; 95% Confidence Interval [CI] = 2.036-7.708). The frequency of the "G" allele in the colorectal cancer patient group was also higher than that in the control group (51.3% versus 33.3%; OR = 2.105; 95% CI = 1.482-2.988). No difference could be found for the TGF-beta 1 and VEGF genotypes among colorectal cancer patients and healthy controls.

The EGF 61 G/G genotype and the G allele are significantly related to colorectal cancer. The TGF-beta 1 -509 T/C and VEGF 936 T/C gene polymorphisms are not related to colorectal cancer.

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Record 45 of 52

Author(s): Ohnuma, I (Ohnuma, I.); Saegusa, T (Saegusa, T.); Takaku, Y (Takaku, Y.); Wang, CP (Wang, C. P.); Liu, XJ (Liu, X. J.); Kainuma, R (Kainuma, R.); Ishida, K (Ishida, K.)

Title: Microstructural Evolution of Alloy Powder for Electronic Materials with Liquid Miscibility Gap


Language: English

Conference Title: Symposium on Phase Stability, Phase Transformation and Reactive Phase Formation in Electronic Materials VII held at the 2008 TMS Annual Meeting

Conference Date: MAR 09-13, 2008

Conference Location: New Orleans, LA

Abstract: The microstructure of powders that are applicable for electronic materials were studied for some systems in which there is a liquid miscibility gap. The characteristic morphologies of an egg-like core type and a uniform second-phase dispersion are shown in relation to the phase diagram, where thermodynamic calculations are a powerful tool for alloy design and the prediction of microstructure. Typical examples of microstructural evolution and properties of Pb-free solders and Ag-based micropowders with high electrical conductivity produced by a gas-atomizing method are presented.


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Subject Category: Engineering, Electrical & Electronic; Materials Science, Multidisciplinary; Physics, Applied

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Record 46 of 52

Author(s): Xu, XY (Xu, Xin Ying); Zhao, JN (Zhao, Jun Ning)

Title: On the Global Existence and Uniqueness of Solutions to Prandtl's System


Language: English

Abstract: In this paper, we consider the Prandtl system for the non-stationary boundary layer in the vicinity of a point where the outer flow has zero velocity. It is assumed that U(t, x, y) = x(m) U-1(t, x), where 0 <= x <= L and m >= 1. We establish the global existence of the weak solution to this problem. Moreover the uniqueness of the weak solution is proved.

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Subject Category: Mathematics, Applied; Mathematics

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Record 47 of 52

Author(s): Chen, SH (Chen, Shu Hong); Tan, Z (Tan, Zhong)

Title: The Method of A-Harmonic Approximation and Boundary Regularity for Nonlinear Elliptic Systems under the Natural Growth Condition


Language: English

Abstract: We consider the questions of boundary regularity for weak solutions of second-order nonlinear elliptic systems under the natural growth condition. We obtain a general criterion for a weak solution to be regular in the neighborhood of a given boundary point. The proof yields directly the optimal regularity for the solution in this neighborhood. This result is new for the situation under the natural growth conditions.
In this paper we study the strict localization for the p-Laplacian equation with strongly nonlinear source term. Let $u := u(x,t)$ be a solution of the Cauchy problem

$$u(t) = \text{div}(\|\nabla u\|^{p-2}\nabla u) + u^q, \quad u(x,0) = u(0)(x).$$

where $(x,t)$ is an element of $\mathbb{R}^N \times (0, T)$, $N \geq 1$ and $p \geq 2$. When $q \geq p - 1$, we prove that if the initial data $u(0)(x)$ has a compact support, then the solution $u(\cdot, t)$ has also compact support. Moreover, when $1 < q < p - 1$, we show that the solution of the Cauchy problem blows up at any point of $\mathbb{R}^N$ to arbitrary compactly supported initial data. (C) 2008 Elsevier Inc. All rights reserved.
Record 50 of 52

Author(s): Zhang, FJ (Zhang, Fuji); Chen, YC (Chen, Yi-Chiuan); Chen, ZB (Chen, Zhibo)
Title: Clique-inserted-graphs and spectral dynamics of clique-inserting
Language: English

Abstract: Motivated by studying the spectra of truncated polyhedra, we consider the clique-inserted graphs. For a regular graph G of degree \( r \geq 0 \), the graph obtained by replacing every vertex of G with a complete graph of order \( r \) is called the clique-inserted graph of G, denoted as \( C(G) \). We obtain a formula for the characteristic polynomial of \( C(G) \) in terms of the characteristic polynomial of G. Furthermore, we analyze the spectral dynamics of iterations of clique-inserting on a regular graph G. For any r-regular graph G with \( r > 2 \), let \( S(G) \) denote the union of the eigenvalue sets of all iterated clique-inserted-graphs of G. We discover that the set of limit points of \( S(G) \) is a fractal with the maximum r and the minimum -2, and that the fractal is independent of the structure of the concerned regular graph G as long as the degree r of G is fixed. It follows that for any integer \( r > 2 \) there exist infinitely many connected r-regular graphs (or, non-regular graphs with r as the maximum degree) with arbitrarily many distinct eigenvalues in an arbitrarily small interval around any given point in the fractal. We also present a formula on the number of spanning trees of any kth iterated clique-inserted-graph and other related results. (C) 2008 Elsevier Inc. All rights reserved.

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Record 51 of 52

Author(s): Chen, S (Chen, S.); Liu, F (Liu, F.); Zhuang, P (Zhuang, P.); Anh, V (Anh, V.)
Title: Finite difference approximations for the fractional Fokker-Planck equation
Language: English

Abstract: The fractional Fokker-Planck equation has been used in many physical transport problems which take place under the influence of an external force field. In this paper we examine some practical numerical methods to solve a class of initial-boundary value problems for the fractional Fokker-Planck equation on a finite domain. The solvability, stability, consistency, and convergence of these methods are discussed. Their stability is proved by the energy method. Two numerical examples are also presented to evaluate these finite difference methods against the exact analytical Solutions. (C) 2007 Elsevier Inc. All rights reserved.

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E-mail Address: fliu@qut.edu.au
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Record 52 of 52

Author(s): Miao, ZW (Miao, Zhaowei); Lim, A (Lim, Andrew); Ma, H (Ma, Hong)
Title: Truck dock assignment problem with operational time constraint within crossdocks
Source: EUROPEAN JOURNAL OF OPERATIONAL RESEARCH, 192 (1): 105-115 JAN 1 2009
Language: English

Abstract: In this paper, we consider a truck dock assignment problem with an operational time constraint in crossdocks where the number of trucks exceeds the number of docks available. The problem feasibility is affected by three factors: the arrival and departure time window of each truck, the operational time for cargo shipment among the docks, and the total capacity available to
the crossdock. The objective is to find an optimal assignment of trucks that minimizes the operational cost of the cargo shipments and the total number of unfulfilled shipments at the same time. We combine the above two objectives into one term: the total cost, a sum of the total dock operational cost and the penalty cost for all the unfulfilled shipments. The problem is then formulated as an integer programming (IP) model. We find that as the problem size grows, the IP model size quickly expands to an extent that the ILOG CPLEX Solver can hardly manage. Therefore, two meta-heuristic approaches, Tabu Search (TS) and genetic algorithm (GA), are proposed. Computational experiments are conducted, showing that meta-heuristics, especially the Tabu search, dominate the CPLEX Solver in nearly all test cases adapted from industrial applications. (C) 2007 Elsevier B.V. All rights reserved.

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