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第 **1** 条，共 **12** 条

标题: Dynamic structural transformations of coordination supramolecular systems upon exogenous stimulation

作者: Li, CP (Li, Cheng-Peng); Chen, J (Chen, Jing); Liu, CS (Liu, Chun-Sen); Du, M (Du, Miao)

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摘要: Reactions in the solid state, especially single-crystal-to-single-crystal (SC-SC) transformations, provide an appealing pathway to obtain target crystalline materials with modified properties via a solvent-free green chemistry approach. This feature article focuses on the progress to date in the context of coordination supramolecular systems (CSSs), especially coordination polymers (CPs) or metal-organic frameworks (MOFs), which show interesting dynamic natures upon exposure to various exogenous stimuli, including concentration, temperature, light and mechanical force, as well as their synergic effect. In essence, dynamic CSSs normally possess crucial crystalline-reactive characteristics: (i) metal ions or clusters with unstable or metastable electronic configurations and coordination geometries; (ii) organic ligands bearing physicochemically active functional groups for subsequent reactions; (iii) polymeric networks of high flexibility for structural bending, rotation, swelling, or shrinking; (iv) guest moieties to be freely exchanged or eliminated by varying the environmental conditions. The significant changes in catalytic, sorption, magnetic, or luminescent properties accompanied by the structural transformations will also be discussed, which reveal the proof-of-concept thereof in designing new functional crystalline materials.

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第 **2** 条，共 **12** 条

标题: Lignin depolymerisation strategies: towards valuable chemicals and fuels

作者: Xu, CP (Xu, Chunping); Arancon, RAD (Arancon, Rick Arneil D.); Labidi, J (Labidi, Jalel); Luque, R (Luque, Rafael)

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摘要: Research on lignin deconstruction has recently become the center of interest for scientists and companies worldwide, racing towards harvesting fossil-fuel like aromatic compounds which are so durably put together by plants as products of millions of years of evolution. The natural complexity and high stability of lignin bonds (also as an evolutionary adaptation by plants) makes lignin depolymerization a highly challenging task. Several efforts have been directed towards a more profound understanding of the structure and composition of lignin in order to devise pathways to break down the biopolymer into useful compounds. The present contribution aims to provide an overview of key advances in the field of lignin depolymerisation. Protocols and technologies will be discussed as well as critically evaluated in terms of possibilities and potential for further industrial implementation.

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标题: Existence of entire solutions for a class of variable exponent elliptic equations

作者: Pucci, P (Pucci, Patrizia); Zhang, QH (Zhang, Qihu)
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摘要: The paper deals with the existence of entire solutions for a quasilinear equation (epsilon lambda) in R-N, depending on a real parameter A., which involves a general variable exponent elliptic operator A in divergence form and two main nonlinearities. The competing nonlinear terms combine each other. Under some conditions, we prove the existence of a critical value lambda(*) > 0 with the property that (epsilon lambda) admits nontrivial nonnegative entire solutions if and only if lambda >= lambda*. Furthermore, under the further assumption that the potential A of A is uniform convex, we give the existence of a second independent nontrivial nonnegative entire solution of (epsilon lambda), when lambda > lambda* Our results extend the previous work of Autuori and Pucci (2013) [6] from the case of constant exponents p, q and r to the case of variable exponents. More interesting, we weaken the condition max{2, p} < q < min{,r, p*) to the simple request that 1 << q << r. Furthermore, we extend the previous work of Alama and Tarantello (1996) [2] from Dirichlet Laplacian problems in bounded domains of RN to the case of a general variable exponent differential equation in the entire RN, and also remove the assumption q > 2. Hence the results of this paper are new even in the canonical case p(.) 2. (C) 2014 Elsevier Inc. All rights reserved.

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KeyWords Plus: NONSTANDARD GROWTH-CONDITIONS; P(X)-LAPLACIAN EQUATIONS; DIFFERENTIAL-EQUATIONS; IMAGE-RESTORATION; SOBOLEV SPACES; R-N; NONLINEARITIES; FUNCTIONALS; INEQUALITY; SYSTEMS
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第 **4** 条，共 **12** 条

标题: Toxicity of ionic liquids: Database and prediction via quantitative structure-activity relationship method

作者: Zhao, YS (Zhao, Yongsheng); Zhao, JH (Zhao, Jihong); Huang, Y (Huang, Ying); Zhou, Q (Zhou, Qing); Zhang, XP (Zhang, Xiangping); Zhang, SJ (Zhang, Suojiang)

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摘要: A comprehensive database on toxicity of ionic liquids (ILs) is established. The database includes over 4000 pieces of data. Based on the database, the relationship between IL's structure and its toxicity has been analyzed qualitatively. Furthermore, Quantitative Structure Activity relationships (QSAR) model is conducted to predict the toxicities (EC50 values) of various ILs toward the Leukemia rat cell line IPC-81. Four parameters selected by the heuristic method (HM) are used to perform the studies of multiple linear regression (MLR) and support vector machine (SVM). The squared correlation coefficient (R-2) and the root mean square error (RMSE) of training sets by two QSAR models are 0.918 and 0.959, 0.258 and 0.179, respectively. The prediction R-2 and RMSE of QSAR test sets by MLR model are 0.892 and 0.329, by SVM model are 0.958 and 0.234, respectively. The nonlinear model developed by SVM algorithm is much outperformed MLR, which indicates that SVM model is more reliable in the prediction of toxicity of ILs. This study shows that increasing the relative number of O atoms of molecules leads to decrease in the toxicity of ILs. (C) 2014 Elsevier B.V. All rights reserved.

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标题: Divergent Kinetic and Thermodynamic Hydration of a Porous Cu(II) Coordination Polymer with Exclusive CO2 Sorption Selectivity

作者: Du, M (Du, Miao); Li, CP (Li, Cheng-Peng); Chen, M (Chen, Min); Ge, ZW (Ge, Zhi-Wei); Wang, X (Wang, Xi); Wang, L (Wang, Lei); Liu, CS (Liu, Chun-Sen)

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摘要: Selective adsorption and separation of CO2 are of great importance for different target applications. Metal organic frameworks (MOFs) represent a promising class of porous materials for this purpose. Here we present a unique MOF material, [Cu(tba)(2)](n) (tba = 4-(1H-1,2,4-triazol-1-yl)benzoate), which shows high CO2 adsorption selectivity over CH4/H-2/O-2/Ar/N-2 gases (with IAST selectivity of 41-68 at 273 K and 33-51 at 293 K). By using a critical point dryer, the CO2 molecules can be well sealed in the ID channels of [Cu(tba)(2)](n) to allow a single-crystal X-ray analysis, which reveals the presence of not only C delta+-H center dot center dot center dot O delta- bonds between the host framework and CO2 but also quadrupole quadrupole (CO2 delta-center dot center dot center dot delta+CO2) interactions between the CO2 molecules. Furthermore, [Cu(tba)(2)](n) will suffer divergent kinetic and thermodynamic hydration processes to form its isostructural hydrate {[Cu(tba)(2)](H2O)}(n) and a mononuclear complex [Cu(tba)(2)(H2O)(4)] via single-crystal to single-crystal transformations.

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地址: [Du, Miao; Li, Cheng-Peng; Ge, Zhi-Wei; Wang, Xi; Wang, Lei] Tianjin Normal Univ, Coll Chem, Tianjin Key Lab Struct & Performance Funct Mol, MOE Key Lab Inorgan Organ Hybrid Funct Mat Chem, Tianjin 300387, Peoples R China.
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第 **6** 条，共 **12** 条

标题: Electrolyte and composition effects on the performances of asymmetric supercapacitors constructed with Mn3O4 nanoparticles-graphene nanocomposites

作者: Xiao, YH (Xiao, Yuanhua); Cao, YB (Cao, Yongbo); Gong, YY (Gong, Yuyin); Zhang, AQ (Zhang, Aiqin); Zhao, JH (Zhao, Jihong); Fang, SM (Fang, Shaoming); Jia, DZ (Jia, Dianzeng); Li, F (Li, Feng)

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摘要: Nanocomposites of Mn3O4 nanoparticles and graphene (GR) nanosheets - Mn3O4@GR can be made by growing Mn3O4 nanoparticles directly on the surfaces of GR in solvothermal reactions. The asymmetric supercapacitors constructed with Mn3O4@GR as positive and activated carbon (AC) as negative electrodes, respectively, show highly enhanced performances in energy storage. It was found that the electrolytes employed in constructing electrodes of the devices can influence the performances of Mn3O4@GR supercapacitors dramatically. Compared to their energy density in KOH electrolyte, the devices exhibit improved charge storage performances in Na2SO4 electrolyte. Furthermore, the charge storage abilities of the devices are closely related to the amount of Mn3O4 nanoparticles loaded onto the surface of GR nanosheets. The performances of Mn3O4@GR//AC asymmetric supercapacitors can be optimized by carefully tailoring the composition of electrode materials and adjusting the electrolytes for making the devices. (C) 2013 Elsevier B.V. All rights reserved.

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第 **7** 条，共 **12** 条

标题: Design and construction of coordination polymers with mixed-ligand synthetic strategy

作者: Du, M (Du, Miao); Li, CP (Li, Cheng-Peng); Liu, CS (Liu, Chun-Sen); Fang, SM (Fang, Shao-Ming)

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摘要: The rational construction of coordination polymers (CPs), normally existing as infinite crystalline lattices extended from inorganic vertices and organic struts, essentially benefits from the development of crystal engineering strategies. In this review, we summarily comment on the key advances in the design of CPs using mixed-ligand synthetic strategy and discuss the relationship between the specifically selected mixed organic ligands and the resulting CPs. Significantly, fine tuning on the structural features of organic ligands, such as spacers, positional isomers, and substituents, can lead to a delicate regulation of the diverse network structures of CPs. Additionally, such mixed-ligand coordination assemblies may also be heavily affected by metal ion, synthetic route, and some other external stimuli such as solvent and pH condition, etc. The advantages of mixed-ligand systems as promising approaches to construct CPs-based crystalline materials with interesting structures and useful properties will also be demonstrated. (C) 2012 Elsevier B.V. All rights reserved.

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作者关键词: Coordination polymers; Crystal engineering; Mixed-ligand synthetic strategy; Structural diversity and regulation; Structure-property correlation
KeyWords Plus: METAL-ORGANIC FRAMEWORKS; GAS-ADSORPTION PROPERTIES; R-ISOPHTHALATE R; CRYSTAL-STRUCTURES; SORPTION PROPERTIES; BUILDING-BLOCKS; STRUCTURAL DIVERSIFICATION; CO-LIGANDS; SUPRAMOLECULAR ISOMERISM; CARBOXYLATE FRAMEWORKS

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第 **8** 条，共 **12** 条

标题: 3D Hierarchical Co3O4 Twin-Spheres with an Urchin-Like Structure: Large-Scale Synthesis, Multistep-Splitting Growth, and Electrochemical Pseudocapacitors

作者: Xiao, YH (Xiao, Yuanhua); Liu, SJ (Liu, Shaojun); Li, F (Li, Feng); Zhang, AQ (Zhang, Aiqin); Zhao, JH (Zhao, Jihong); Fang, SM (Fang, Shaoming); Jia, DZ (Jia, Dianzhen)

来源出版物: ADVANCED FUNCTIONAL MATERIALS 卷: 22 期: 19 页: 4052-4059 **DOI:** 10.1002/adfm.201200519 出版年: OCT 10 2012

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摘要: Novel, 3D hierarchical Co3O4 twin-spheres with an urchin-like structure are produced successfully on the large scale for the first time by a solvothermal synthesis of cobalt carbonate hydroxide hydrate, Co(CO3)0.5(OH)center dot 0.11H2O, and its subsequent calcination. The morphology of the precursor, which dominates the structure of the final product, evolves from nanorods to sheaf-like bundles, to flower-like structures, to dumbbell-like particles, and eventually to twin-spheres, accompanying a prolonged reaction time. A multistep-splitting growth mechanism is proposed to understand the formation of the 3D hierarchical twin-spheres of the precursor, based on the time effect on the morphologies of the precursor. The 3D hierarchical Co3O4 twin-spheres are further used as electrode materials to fabricate supercapacitors with high specific capacitances of 781, 754, 700, 670, and 611 F g-1 at current densities of 0.5, 1, 2, 4, and 8 A g-1, respectively. The devices also show high charge-discharge reversibility with an efficiency of 97.8% after cycling 1000 times at a current density of 4 A g-1.

入藏号: WOS:000309404000011

语种: English

文献类型: Article

作者关键词: Co3O4; hierarchical nanostructures; twin-spheres; supercapacitors; multistep-splitting growth

KeyWords Plus: SUPERCAPACITOR ELECTRODE MATERIALS; ENERGY-STORAGE; CONTROLLABLE SYNTHESIS; THIN-FILMS; OXIDE; CAPACITORS; NANOSTRUCTURES; MORPHOLOGY; CONVERSION; METAL

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第 **9** 条，共 **12** 条

标题: Electrochemical investigation of MnO2 electrode material for supercapacitors

作者: Zhang, Y (Zhang, Yong); Li, GY (Li, Guang-yin); Lv, Y (Lv, Yan); Wang, LZ (Wang, Li-zhen); Zhang, AQ (Zhang, Ai-qin); Song, YH (Song, Yan-hua); Huang, BL (Huang, Bei-li)

来源出版物: INTERNATIONAL JOURNAL OF HYDROGEN ENERGY 卷: 36 期: 18 页: 11760-11766 **DOI:** 10.1016/j.ijhydene.2011.06.020 出版年: SEP 2011

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摘要: MnO2 electrode material is synthesized by low temperature solid state reaction between KMnO4 and MnCl2. Effects of the KMnO4:MnCl2 molar ratio on the structure, morphology and electrochemical properties of the as-prepared sample were analyzed by X-ray diffraction (XRD), scanning electron microscopy (SEM) and electrochemical tests. Results showed that the obtained MnO2 is alpha-MnO2, the average diameter is about 0.5-1.5 mu m, which are constituted of nanoparticles of 20 nm. Under 100 mA g(-1), the specific capacitances of the prepared sample is 258.7, 219.6, 215.3, 198.5 and 209.5 F g(-1) at the KMnO4/MnCl2 molar ratio of 3:2, 2:1,

1:1, 1:2 and 2:3, respectively. And the MnO2 sample with a KMnO4/MnCl2 molar ratio of 3:2 exhibits the best discharge capacitance and cycle performance. When the charge/discharge rate increases to 300 mA g(-1), the sample still remains initial discharge capacitance of 165.3 F g(-1), and the discharge capacitance is 145.9 F g(-1) after 200 cycles, the capacitance retention rate is 102.4% during the 20-200th cycles. Therefore, the MnO2 sample is an excellent material for use in supercapacitors because of its large specific capacitance and good cycle performance. Copyright (C) 2011, Hydrogen Energy Publications, LLC. Published by Elsevier Ltd. All rights reserved.

入藏号: WOS:000294982800030

语种: English

文献类型: Article

作者关键词: Supercapacitors; MnO2; Low temperature solid state reaction

KeyWords Plus: DOUBLE-LAYER CAPACITORS; AQUEOUS SUPERCAPACITORS; MANGANESE OXIDE; CARBON; PERFORMANCE; ENERGY; COMPOSITES; DENSITY; POWER; FILM

地址: [Zhang, Yong; Li, Guang-yin; Lv, Yan; Wang, Li-zhen; Zhang, Ai-qin; Song, Yan-hua; Huang, Bei-li] Zhengzhou Univ Light Ind, Dept Mat & Chem Engn, Zhengzhou 450002, Peoples R China.
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第 **10** 条，共 **12** 条

标题: Thermoresponsive copolymers: from fundamental studies to applications

作者: Liu, RX (Liu, Ruixue); Fraylich, M (Fraylich, Michael); Saunders, BR (Saunders, Brian R.)

来源出版物: COLLOID AND POLYMER SCIENCE 卷: 287 期: 6 页: 627-643 **DOI:** 10.1007/s00396-009-2028-x 出版年: JUN 2009

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摘要: Thermoresponsive copolymers have attracted considerable interest in both the polymer and biomaterial literature. They show interesting fundamental behaviour (thermally triggered contraction and aggregation) as well as potentially useful properties (reversible gelation). Biocompatible thermoresponsive copolymers are being developed for application in drug delivery and regenerative medicine. This review focuses on the fundamental aspects of thermally triggered conformational changes with an emphasis on copolymer design. Also, the ability to use these copolymers to produce thermoresponsive colloidal dispersions is discussed. Recent examples from within our group and elsewhere are considered in order to illustrate structure-property relationships. The review focuses on copolymers involving N-isopropylacrylamide. However, non-acrylamide thermoresponsive copolymers are also considered in detail. Emerging areas that appear likely to be actively pursued in the future are also discussed.

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语种: English

文献类型: Review

作者关键词: Thermoresponsive copolymer; NIPAm; LCST; Thermogelation

KeyWords Plus: POLY N-ISOPROPYLACRYLAMIDE; THERMALLY CONTROLLED ASSOCIATION; TRANSFER RADICAL POLYMERIZATION; CRITICAL SOLUTION TEMPERATURES; GENE TRANSFECTION EFFICIENCY; RESPONSIVE GRAFT-COPOLYMERS; ANGLE NEUTRON-SCATTERING; VOLUME PHASE-TRANSITION; CROSS-LINKING POLYMER; AQUEOUS-SOLUTION

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第 **11** 条，共 **12** 条

标题: Progress of electrochemical capacitor electrode materials: A review

作者: Zhang, Y (Zhang, Yong); Feng, H (Feng, Hui); Wu, XB (Wu, Xingbing); Wang, LZ (Wang, Lizhen); Zhang, AQ (Zhang, Aiqin); Xia, TC (Xia, Tongchi); Dong, HC (Dong, Huichao); Li, XF (Li, Xiaofeng); Zhang, LS (Zhang, Linsen)

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摘要: The electrode is the key part of the electrochemical capacitors (ECs), so the electrode materials are the most important factors to determine the properties of ECs. In this paper, the storage principles and characteristics of electrode materials, including carbon-based materials, transition metal oxides and conductive polymers for ECs are depicted briefly. Among them, more work has been done using microporous carbons than with the other materials and most of the commercially available devices use carbon electrodes and organic electrolytes. But the composites of pseudocapacitive and carbonaceous materials are promising electrode materials for ECs because of their good electrical conductivity, low cost and high mass density. (C) 2009 International Association for Hydrogen Energy. Published by Elsevier Ltd. All rights reserved.

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作者关键词: Electrochemical capacitor; Electrode materials; Review

KeyWords Plus: DOUBLE-LAYER CAPACITORS; ACTIVATED-CARBON CAPACITOR; COMPOSITE ELECTRODES; POSITIVE ELECTRODE; ENERGY-DENSITY; SURFACE-AREA; NICKEL-OXIDE; IONIC LIQUID; POLYMER ELECTROLYTE; POROUS CARBON

地址: [Zhang, Yong; Feng, Hui; Wu, Xingbing; Wang, Lizhen; Zhang, Aiqin; Xia, Tongchi; Dong, Huichao; Li, Xiaofeng; Zhang, Linsen] Zhengzhou Univ Light Ind, Henan Prov Key Lab Surface & Interface Sci, Zhengzhou 450002, Peoples R China.

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第 **12** 条，共 **12** 条

标题: Optimisation of ultrasound-assisted extraction of phenolic compounds from wheat bran

作者: Wang, J (Wang, Jing); Sun, BG (Sun, Baoguo); Cao, YP (Cao, Yanping); Tian, YA (Tian, Yuan); Li, XH (Li, Xuehong)

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摘要: Wheat bran, an important by-product of the cereal industry, is rich in potentially health-promoting phenolic compounds. In this paper, the phenolic compounds from wheat bran were extracted by ultrasound-assisted extraction technology. The experiments were carried out according to a five level, three variable central composite rotatable design (CCRD), and the best possible combination of solvent concentration, extraction temperature and extraction time with the application of ultrasound, for maximum extraction of phenolic compounds from wheat bran, was obtained, through response surface methodology (RSM). The optimum extraction conditions were as follows: ethanol concentration, 64%; extraction temperature, 60 degrees C and extraction time, 25 min; and the extraction time was the most significant parameter for the process. Under the above-mentioned conditions, the experimental total phenolic content was 3.12 mg gallic acid equivalents/g of wheat bran tested, which is well matched with the predicted content. (c) 2007 Elsevier Ltd. All rights reserved.

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作者关键词: central composite rotatable design; phenolic compounds; ultrasound extraction; wheat bran

KeyWords Plus: ANTIOXIDANT PROPERTIES; DIFFERENT LOCATIONS; GRAIN

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