

1. Заглавие Polysulfonate-doped polyanilines – oxidation of ascorbic acid and dopamine in neutral solution

Автори V. Lyutov, V. Tsakova

Резюме The redox behavior of polyaniline (PANI) doped with polysulfonic acids is studied in slightly acidic and neutral solutions (from pH 4 to pH 7). The dopants used are polystyrene sulfonic acid (PSSA), poly(2-acrylamido-2-methyl-1-propanesulfonic acid) (PAMPSA) and poly-(4,4'-(2,2'-disulfonic acid)-diphenylene-tere-phthalamide) (t-PASA). Thin PANI layers are used in order to identify clearly the redox peak structure. Based on deconvolution of the reductive currents the pH dependence of the constituent peaks is studied and pathways of the reductive transitions are suggested. With increasing pH a loss of electroactivity is observed for all three dopants but to a different extent: the largest for PAMPSA- and the smallest PSSA-doped PANIs. In the same time a stabilization of the conductive emeraldine salt state is observed at pH 7 for all PANIs with largest extent of stabilization in the PANI/PAMPSA case. The electrocatalytic properties of the polysulfonic acids-doped PANIs are comparatively studied for ascorbic acid (AA) and dopamine (DA) oxidation at pH 7. It is found that all three types of PANI are good electrocatalysts for both reactions with advantage of the PAMPSA- doped layers showing higher absolute oxidative currents for both reactions. The results concerning DA oxidation demonstrate the possibility to involve polysulfonic acid-doped PANIs in electrocatalytic reactions in neutral solutions occurring at high positive potentials beyond the peak potential of the PANI oxidative transition.

Списание [J Solid State Electrochem 24 \(2020\) 3113](#)

2. Заглавие Moisture-responsive polymer films on flexible substrates for optical sensing of humidity

Автори K. Lazarova, S. Bozhilova, S. Ivanova, D. Christova, T. Babeva

Резюме In this paper, the possibility to design flexible humidity sensors by spin-coating of moisture-sensitive polymer on three types of substrates—poly(ethylene terephthalate) (PET), polylactide (PLA) and composite polysiloxane is investigated. The optical properties, surface morphology and roughness of the substrates covered with polymer are studied by transmittance measurements and surface profiling, respectively. Thin polymer films of amphiphilic copolymer obtained by partial acetalization of poly(vinyl alcohol) are used as humidity sensitive media. The sensing properties are probed through transmittance measurements at different levels of relative humidity (RH). The influence of substrate type is studied by comparing the hysteresis of flexible sensors with those that are deposited on glass substrates.

Списание [Eng Proc 2\(1\) \(2020\) 19](#)

3. Заглавие NMR profiling of North Macedonian and Bulgarian honeys for detection of botanical and geographical origin

Автори D. Gerginova, S. Simova, M. Popova, M. Stefova, J. Stanoeva, V. Bankova

Резюме Bulgaria and North Macedonia have a long history of the production and use of honey; however, there is an obvious lack of systematic and in-depth research on honey from both countries. The oak honeydew honey is of particular interest, as it is highly valued by consumers because of its health benefits. The aim of this study was to characterize honeydew and floral honeys from Bulgaria and North Macedonia based on their NMR profiles. The 1D and 2D ¹H and ¹³C-NMR spectra were measured of 16 North Macedonian and 22 Bulgarian honey samples. A total of 25 individual substances were identified, including quinovose, which was found for the first time in honey. Chemometric methods (PCA—principal component analysis, PLS-DA—partial least squares discriminant analysis, ANOVA—analysis of variance) were used to detect similarities and differences between samples, as well as to determine their botanical and geographical origin. Semiquantitative data on individual sugars and some other constituents were obtained, which allowed for the reliable classification of honey samples by botanical and geographical origin, based on chemometric approaches. The results enabled us to distinguish oak honeydew honey from other honey types, and to determine the country of origin. NMR was a rapid and convenient method, avoiding the need for other more time-consuming analytical techniques.

Списание [Molecules 25 \(20\) \(2020\) 4687](#)

4. Заглавие Role of the various surface sites and species in CO hydrogenation over alumina-supported Co-Pd catalysts

Автори M. Shopska, I. Shtereva, H. Kolev, K. Tenchev, S. Todorova, G. Kadinov

Резюме The paper is focused on evaluation of active centres and adsorbed species type impact on 10%Co+0.5%Pd)/Al₂O₃ catalyst system performance aiming selectivity optimization. Application of different sets of precursor pretreatment and reductions resulted in catalysts exhibiting high CO conversion or high methane selectivity. Sample of high selectivity was prepared by pretreatment in hydrogen and the performance was determined by lower amount of strongly adsorbed CO, strongly adsorbed carbonate species, higher amount of reduced metal and bimetallic particles. A more active system was formed by pretreatment in air leading to larger amount of unreduced metal and CO-bridged species on the surface, stable coverage of hydroxyl groups on the support, and medium-strength sites for adsorption of carbonates. Ratios of adsorbed H/CO and strongly/weakly CO species appeared as important criteria for catalyst efficiency together with supported metal state, amount of unreduced ions, bimetallic particle formation, and alumina's ability to adsorb CO and CO₂.

Списание [Croatia Chem. Acta 93\(2\) \(2020\) 121](#)

5. Заглавие Sol–gel tantalum pentoxide thin films with tunable refractive index for optical sensing applications

Автори R. Georgiev, B. Georgieva, K. Lazarova, M. Vasileva, T. Babeva

Резюме Present study aims at development of thin films of sol–gel Ta₂O₅ with tunable refractive index that could be used as an active medium for volatile organic compound (VOCs) optical detection. In order to tune the refractive index, mesoporosity is introduced through soft templating approach where series of co-polymers (Pluronics) are utilized as structuredirecting agents. Thin films are prepared by spin-coating method using tantalum sol synthesized from TaCl₅ as a precursor and ethanol as a solvent. The temperature annealing at 320 °C finalizes the tantalum oxide lattice formation and decomposes the template being used. The morphology and elemental composition of the films are studied by transmission electron microscopy (TEM) and energy dispersive X-ray spectroscopy in STEM, respectively, and the amorphous status of the films is confirmed by selected area electron diffraction. Non-linear curve fitting method and non-destructive UV–Vis reflectance measurements are used for determination of optical parameters of the films. The free volume fraction in the films is estimated through modeling of refractive index by Bruggeman effective medium approximation. The films are exposed to acetone vapors as a commonly studied VOC. The reaction of the film due to vapors' exposure is recorded as a change in the reflection spectra of the film and the adsorbed acetone quantity is estimated. The influence of template composition on optical and sensing properties of Ta₂O₅ films is revealed and discussed.

Списание [Opt Quant Electron 52\(10\) \(2020\) 437](#)

6. Заглавие Simultaneous Synthesis and Nitrogen Doping of Free-Standing Graphene Applying Microwave Plasma

Автори D. Tsyganov, N. Bundaleska, J. Henriques, E. Felizardo, A. Dias, M. Abrashev, J. Kisoovski, A. Botelho do Rego, A. Ferraria, E. Tatarova

Резюме An experimental and theoretical investigation on microwave plasma-based synthesis of free-standing N-graphene, i.e., nitrogen-doped graphene, was further extended using ethanol and nitrogen gas as precursors. The in situ assembly of N-graphene is a single-step method, based on the introduction of N-containing precursor together with carbon precursor in the reactive microwave plasma environment at atmospheric pressure conditions. A previously developed theoretical model was updated to account for the new reactor geometry and the nitrogen precursor employed. The theoretical predictions of the model are in good agreement with all experimental data and assist in deeper understanding of the complicated physical and chemical process in microwave plasma. Optical Emission Spectroscopy was used to detect the emission of plasma-generated “building units” and to determine the gas temperature. The outlet gas was analyzed by Fourier-Transform Infrared Spectroscopy to detect the generated gaseous by-products. The synthesized N-graphene was characterized by Scanning Electron Microscopy, Raman, and X-ray photoelectron spectroscopies.

Списание [Materials 13\(18\) \(2020\) 4213](#)

7. Заглавие Experimental and theoretical study of bidirectional photoswitching behavior of 5,50-diphenylhydantoin Schiff bases: synthesis, crystal structure and kinetic approaches

Автори P. Todorov, S. Georgieva, P. Peneva, R. Rusew, B. Shivachev, A. Georgiev

Резюме Herein, the synthesis and characterization of four novel 5,50 -diphenylhydantoin Schiff bases containing different aromatic species are presented. Their structure–property relationship was studied by X-ray, optical and electrochemical methods as well as DFT calculations in terms of their E/Z photoisomerization and enol/keto phototautomerization. The big challenge in photoinduced motion is achieving control and stability over the two isomers. Solvent-driven bidirectional photoswitching behavior was studied in nonpolar 1,4-dioxane and polar aprotic DMF. T-type photochromism in 1,4-DOX and opposite behavior in DMF as P- type switches (bistable system) were observed. The obtained results lead to a conclusion that by variation of the solvent environment a direct control over the bidirectional switching behaviour from T-type to P-type can be achieved.

Списание [New J Chem 44 \(2020\) 15081](#)

8. Заглавие ^{13}C CPMAS NMR as a tool for full structural description of 2-Phenyl substituted imidazoles that overcomes the effects of fast tautomerization

Автори N. Burdzhiev, A. Ahmedova, B. Borrisov, R. Graf

Резюме Tautomerization of 2-phenylimidazolecarbaldehydes has not been studied in detail so far, although this process is a well-known phenomenon for imidazole derivatives. That is why we focus our study on a series of 2-phenylimidazolecarbaldehydes and their parent alcohols that were synthesized and studied by detailed ^1H and ^{13}C NMR in solution and in the solid state. The apparent problem is that the fast tautomerization impedes the full structural description of the compounds by conventional ^{13}C NMR measurements. Indeed, the ^{13}C NMR spectra in solution exhibit poor resolution, and in most cases, signals from the imidazole ring are not detectable. To avoid this problem, we used ^{13}C CP-MAS NMR as an alternative spectroscopic method for unambiguous spectroscopic characterization of the studied series of 2-phenylimidazoles. The data were analyzed in combination with quantum chemical DFT- GIAO methods by considering the tautomerization process and the intermolecular interactions. The DFT (B3LYP/6-31G(d,p)) calculations allowed to identify and suggest the preferred tautomer in the gas phase and in DMSO solvent, which for alcohols are (2-phenyl-1H-imidazol-4-yl)methanol and its analogs, and for the aldehydes are the 2-phenyl-1H-imidazole-5-carbaldehydes. The gas-phase calculated energy differences between the two possible tautomeric forms are in the range 0.645–1.415 kcal/mol for the alcohols and 2.510–3.059 kcal/mol for the aldehydes. In the DMSO solvent, however, for all compounds, the calculated energy differences go below 1.20 kcal/mol. These data suggest that both tautomeric forms of the studied 2-phenylimidazoles can be present in solution at room temperature. Our data from detailed 2D NMR measurements in the solid state (^1H - ^{13}C HETCOR and ^1H - ^1H double-quantum coherence MAS NMR) suggested that also in the solid state both tautomers coexist in different crystalline domains. This fact does not obscure the ^{13}C CP-MAS NMR spectra of the

studied 2-phenyl substituted imidazoles and suggests this spectroscopic method as a powerful tool for a complete structural description of tautomeric systems with aromatic conjugation.

Списание [Molecules 25\(17\) \(2020\) 3770](#)

9. Заглавие Investigation of photophysical, electrochemical and electroluminescent properties of Iridium(III)bis[2-phenylbenzo[d]thiazolato-N,C2']-quinolin-8-olate for white organic light emitting diodes application

Автори P. Ivanov, P. Petrova, R. Tomova

Резюме The complex Iridium(III)bis[2-phenylbenzo[d]thiazolato-N,C2']-quinolin-8-olate ((bt)2Irq) was synthesized and identified by ¹H NMR and IR spectroscopy. Its photophysical, electrochemical and electroluminescent properties for White Organic Light-Emitting Diodes (WOLED) application were investigated. It was established that (bt)2Irq irradiates yellow-orange light in CH₂Cl₂ (DCM) solution and solid film with maximum peaks, respectively, at 578 and 666 nm and shoulders at 628 and 720 nm. The complex was used as stand-alone emitter and a dopant in the matrixes of hole transporting layer (HTL) or electroluminescent layer (EL) in the range from 0 to 16.5 w%. The base OLED structure was Anode/HTL/EL/ETL/Cathode, where HTL is N,N'-bis(3-methylphenyl)-N,N'-diphenylbenzidine (TPD) included in a matrix of poly(N-vinylcarbazole) (PVK), EL is Aluminium (III) bis(2-methyl-8-quinolinato)-4-phenylphenolate (BALq) and ETL is an electron transporting layer of Tris-(8-hydroxyquinoline) aluminium (Alq₃) or Zinc (II) bis(2-(hydroxyphenyl) benzothiazole (Zn(bt)₂). It is found that the electroluminescent spectra of both types OLEDs were the sum of the greenish-blue and yellow-orange emissions of BALq and Ir complex and CIE coordinates of the emitted light remain within the white range over wide dopant concentrations. The best current efficiency and CIE coordinates close to the ideal white (0.3300; 0.3300) demonstrate devices with 2 wt% doped HTL (6 Cd/A, (0.2735; 0.3613)) and 16.5 w% doped EL (5.1 Cd/A, (0.2721; 0.3284)). It was found that both types of doped devices operate through a charge trapping mechanism.

Списание [J Mater Sci: Mater Electron 31 \(2020\) 15707](#)

10. Заглавие Prospects for microwave plasma synthesized N-graphene in secondary electron emission mitigation applications

Автори N. Bundaleska, A. Dias, N. Bundaleski, E. Felizardo, J. Henriques, D. Tsyganov, M. Abrashev, E. Valcheva, J. Kisoovski, A. Ferraria, A. Botelho do Rego, A. Almeida, J. Zavašnik, U. Svelbar, O. Teodoro, T. Strunskus, E. Tatarova

Резюме The ability to change the secondary electron emission properties of nitrogen-doped graphene (N-graphene) has been demonstrated. To this end, a novel microwave plasma-enabled scalable route for continuous and controllable fabrication of free-standing N-graphene sheets was developed. High-quality N-graphene with prescribed structural qualities was produced at a rate of 0.5 mg/min by tailoring the high energy density plasma environment. Up to 8% of nitrogen doping levels were achieved while keeping the oxygen content at residual amounts (~1%). The synthesis is accomplished via a single step, at atmospheric conditions, using

ethanol/methane and ammonia/methylamine as carbon and nitrogen precursors. The type and level of doping is affected by the position where the N-precursor is injected in the plasma environment and by the type of precursors used. Importantly, N atoms incorporated predominantly in pyridinic/pyrrolic functional groups alter the performance of the collective electronic oscillations, i.e. plasmons, of graphene. For the first time it has been demonstrated that the synergistic effect between the electronic structure changes and the reduction of graphene π -plasmons caused by N doping, along with the peculiar “crumpled” morphology, leads to sub-unitary (< 1) secondary electron yields. N-graphene can be considered as a prospective low secondary electron emission and plasmonic material.

Списание [Sci Rep 10 \(2020\) 13013](#)

11. Заглавие Indirect solvent assisted tautomerism in 4-substituted phthalimide 2-hydroxy-Schiffbases

Автори D. Yordanov, V. Deneva, A. Georgiev, A. Crochet, K. Fromm, L. Antonov

Резюме The paper presents the synthesis and characterization of two 4-substituted phthalimide 2-hydroxy-Schiff bases containing salicylic (4) and 2-hydroxy-1-naphthyl (5) moieties. The structural differences of 2-hydroxyaryl substituents, resulting in different enol/keto tautomeric behaviour, depending on the solvent environment were studied by absorption UV–Vis spectroscopy. Compound 5 is characterized by a solvent-dependent tautomeric equilibrium (KT in toluene = 0.12, acetonitrile = 0.22 and MeOH = 0.63) while no tautomerism is observed in 4. Ground state theoretical DFT calculations by using continuum solvation in MeOH indicate an energy barrier between enol/keto tautomer 5.6 kcal mol⁻¹ of 4 and 0.63 kcal mol⁻¹ of 5, which confirms the experimentally observed impossibility of the tautomeric equilibrium in the former. The experimentally observed specific solvent effect in methanol is modeled via explicit solvation. The excited state intramolecular proton transfer (ESIPT) was investigated by steady state fluorescence spectroscopy. Both compounds show a high rate of photoconversion to keto tautomers hence keto emissions with large Stokes shifts in five alcohols (MeOH, EtOH, 1-propanol, 1-butanol, and 1-pentanol) and various aprotic solvents (toluene, dichloromethane, acetone, AcCN). According to the excited state TDDFT calculations using implicit solvation in MeOH, it was found that enol tautomers of 4 and 5 are higher in energy compared to the keto ones, which explains the origin of the experimentally observed keto form emission.

Списание [Spectrochim Acta A Mol Biomol Spectrosc \(SAA\) 237 \(2020\) 118416](#)

12. Заглавие Terbium-doped calcium germanate (Ca₂GeO₄) as a potential candidate for LED application

Автори Koseva, P. Tzvetkov, P. Ivanov, P. Petrova, R. Tomova, A. Yordanova, V. Nikolov

Резюме Powder samples of Ca₂GeO₄ doped with 0.5, 1, 2 and 3 at.% Tb³⁺ were prepared via solid-state synthesis technique. The obtaining of pure phase at all dopant concentrations was proved through XRD analyses. In the emission and excitation spectra of the obtained powders, the characteristic peaks of Tb³⁺ ion were observed. The Tb³⁺ excitation spectrum in the range

from 300 to 500 nm shows characteristic transitions of Tb^{3+} , attributed to the f–f transitions. The strongest peak is located at 379 nm corresponding to the ${}^7F_6 \rightarrow {}^5D_3$ transition. The main emission peak of Tb^{3+} is ${}^5D_4 \rightarrow {}^7F_5$ transitions at 545 nm, corresponding to green color. Other transitions are located at 416 (${}^5D_3 \rightarrow {}^7F_5$), 437 (${}^5D_3 \rightarrow {}^7F_4$), 458 (${}^5D_3 \rightarrow {}^7F_3$), 488 (${}^5D_4 \rightarrow {}^7F_6$), 588 (${}^5D_4 \rightarrow {}^7F_4$), 621 (${}^5D_4 \rightarrow {}^7F_3$), 651 (${}^5D_4 \rightarrow {}^7F_2$) and 675 (${}^5D_4 \rightarrow {}^7F_1$) nm. The optimum emission is observed for 2 at.% Tb^{3+} ion concentration. At this concentration dominate also (${}^5D_4 \rightarrow {}^7F_4$) and (${}^5D_4 \rightarrow {}^7F_3$) transitions. CIE coordinates of the samples show different emission colors depending on the active ion concentration. The obtained results confirm that as-prepared terbium-doped materials could be used like green, yellow and reddish phosphors.

Списание [J Opt 49 \(2020\) 403](#)

13. Заглавие Fluoride etching of AlZSM-5 and GaZSM-5 zeolites

Автори Т. Todorova, P. Shestakova, T. Petrova, M. Popova, H. Lazarova, Y. Kalvachev

Резюме The post-synthesis treatment of AlZSM-5 and GaZSM-5 zeolites by etching with buffer solution of ammonium fluoride and 0.25 M HF acid was carried out. The treatment is applied in order to obtain secondary pores in crystals and to provide easier access to the catalytically active zeolite centers. Hydrothermal synthesis of these zeolites was performed from systems containing tetrapropylammonium bromide as a template. The reaction parameters of synthesis conditions for both zeolites were optimized in order to obtain pure crystalline phases. The zeolites obtained were characterized by X-ray diffraction, IR spectroscopy, scanning electron microscopy, physical adsorption–desorption of nitrogen and solid-state NMR spectroscopy. It has been found that the result materials remain with high crystallinity while new mesoporous are created in their structure. The volume due to the presence of mesopores increases by up to 67% from the total volume, which is a drastic increase compared with the parent solids. The investigations with FTIR spectroscopy of low-temperature CO adsorption and solid-state NMR spectroscopy show that the treatment is slightly selective toward dissolution of heteroatom (aluminum or gallium). This phenomenon is observed for the first time for gallium-substituted zeolites. In order to study the influence of the metal atom in zeolite structure and the efficacy of the acid attack on the catalytic activity, the samples obtained were tested in reaction of m-xylene and toluene transformation.

Списание [J Mater Sci 55 \(2020\) 13799](#)

14. Заглавие Effect of hydrogen induced decrepitation on the hydrogen sorption properties of MmNi5

Автори S. Todorova, V. Rangelova, L. Mihaylov, T. Spassov

Резюме MmNi5 hydrogen storage alloy with an average particle size of 120 μm was subjected to hydriding treatment at 50oC, under 40 atm. pure hydrogen atmosphere. As a result, a large density of particle cracks was formed, which led to an increase in the particle surface area. The enlarged particles surface, in turn, led to substantially improved hydrogen sorption kinetics compared to the as-received (untreated) alloy. It was also found that hydrogen-induced

decrepitation of the MmNi5 powder results in enhancement of the hydrogen diffusivity mainly due to shortening of its diffusion distances.

Списание [Int J Electrochem Sci 15 \(2020\) 4900](#)

15. Заглавие Coarse Quantization in Dynamic Speckle Metrology at Non-uniform Illumination

Автори E. Stoykova, D. Nazarova, L. Nedelchev, K. Oh, J. Park

Резюме Analysis of dynamic speckle patterns enables visualization of faster or slower changes for 3D objects. Compression of data in this type of metrology by coarse quantization at non-uniform illumination is studied by simulation and experiment.

Списание [Imaging and Applied Optics Congress, OSA Technical Digest \(2020\) HTh5H.5](#)

16. Заглавие Polarization Holographic Gratings with Improved Polarization Properties

Автори L. Nedelchev, B. Blagoeva, G. Mateev, D. Nazarova, E. Stoykova

Резюме Characteristics of polarization holographic gratings (PHG) in non-covered azopolymer thin films and azopolymer films covered with glass slide are compared. An improvement of the polarization properties of the PHG in the covered films is established.

Списание [Imaging and Applied Optics Congress, OSA Technical Digest \(2020\) JTh2A.19](#)

17. Заглавие DNA delivery systems based on copolymers of poly (2-methyl-2-oxazoline) and polyethyleneimine: Effect of polyoxazoline moieties on the endo-lysosomal escape

Автори E. Haladjova, M. Smolíček, I. Ugrinova, D. Momekova, P. Shestakova, Z. Kroneková, J. Kronek, S. Rangelov

Резюме Poly(2-methyl-2-oxazoline)-polyethylenimine (PMeOx-co-PEI) copolymers differing by degree of polymerization (DP = 50 and 200) and PEI content (from 37 to 99 mol%) were synthesized by living cationic ring-opening polymerization of 2-methyl-2-oxazoline, followed by partial hydrolysis. Upon mixing with DNA in a wide range of N/P ratios, they formed well-defined polyplex particles of small size (typically below 100 nm) and narrow size distribution. The polyplexes demonstrated good colloidal stability and very low in vitro cytotoxicity. The copolymers exhibited buffering capacity of over 50% relative to that of the reference PEI implying effective endo-lysosomal escape of the polyplexes. Increased cellular internalization of both PCR fragments and plasmid DNA, attributable to the strongly positive ζ potential and small size of the polyplexes, was observed. In spite of these favorable prerequisites, the transfection efficiency was low (below 20% relative to the control PEI) and was attributed to retarded swelling of the polyplex particles, endo-lysosomal rupture, and DNA release.

Списание [J Appl Polym Sci 137 \(45\) \(2020\) 49400](#)

18. Заглавие Poly(vinyl alcohol)-based thin films for optical humidity sensing

Автори K. Lazarova, S. Bozhilova, D. Christova, T. Babeva

Резюме The optical and humidity-sensing properties are studied of hydrophobically modified PVA, namely poly(vinyl alcohol-co-vinyl acetal)s of varied copolymer composition. Copolymers are synthesized by reacting PVA with acetaldehyde in aqueous solution, thus introducing cyclic acetal functionalities in the polymer chain. Thin polymer films are deposited by spin-coating and their optical properties are studied as a function of the copolymer composition, i.e., degree of acetalization. Reflectance measurements at different relative humidities in the range 5 – 95 % RH are conducted in order to probe the sensing behavior. The comparison with neat PVA thin films confirms the influence of the copolymer's acetal fraction on the optical and sensing properties and degree of hysteresis. The feasibility of applying poly(vinyl alcohol-co-vinyl acetal) thin films for optical sensing of humidity is demonstrated and discussed.

Списание [J Phys: Conf Ser 1492 \(2020\) 012040](#)

19. Заглавие Atomic layer deposited Al-doped ZnO thin films for display applications

Автори D. Dimitrov, C. Tsai, V. Marinova, S. Petrov, D. Petrova, B. Napoleonov, B. Blagoev, V. Strijkova, K. Hsu, S. Lin

Резюме The integration of high uniformity, conformal and compact transparent conductive layers into next generation indium tin oxide (ITO)-free optoelectronics, including wearable and bendable structures, is a huge challenge. In this study, we demonstrate the transparent and conductive functionality of aluminum-doped zinc oxide (AZO) thin films deposited on glass as well as on polyethylene terephthalate (PET) flexible substrates by using an atomic layer deposition (ALD) technique. AZO thin films possess high optical transmittance at visible and near-infrared spectral range and electrical properties competitive to commercial ITO layers. AZO layers deposited on flexible PET substrates demonstrate stable sheet resistance over 1000 bending cycles. Based on the performed optical and electrical characterizations, several applications of ALD AZO as transparent conductive layers are shown—AZO/glass-supported liquid crystal (LC) display and AZO/PETbased flexible polymer-dispersed liquid crystal (PDLC) devices.

Списание [Coatings 10 \(6\) \(2020\) 539](#)

20. Заглавие Raman spectroscopy of alpha-FeOOH (goethite) near antiferromagnetic to paramagnetic phase transition

Автори M. Abrashev, V. Ivanov, B. Stefanov, N. Todorov, J. Rosell, V. Skumryev

Резюме Synthetic powder, ore samples, and mineral single crystals of goethite (α -FeOOH) were investigated with polarized Raman spectroscopy at temperatures from 293 K to 473 K. The symmetry of the vibrational modes, observed in different scattering configurations, was determined unequivocally. The assignment of the Raman-active modes to definite atomic

vibrations is supported by two types of lattice-dynamical calculations: empirical shell model and *ab initio* density functional theory. The temperature dependencies of the line shape parameters of some Raman-active vibrations at temperatures near to the antiferromagnetic–paramagnetic phase transition infers for a significant spin–lattice coupling in this compound. The most informative in this aspect is the *B3g* phonon at 387cm^{-1} – 1387cm^{-1} , which overlays a broad scattering background and displays a pronounced asymmetric Fano-line shape. The asymmetry increases in the paramagnetic state above the Néel temperature ($T_N=393\text{K}$), indicating a strong interaction of this mode with the underlying excitation continuum. The origin of the excitation background is discussed in light of our experimental results and the existing data for the magnetic structure and transport properties of α -FeOOH. By using the molecular-orbital dimer approach, we calculate the spin–phonon coupling constants for the *B3g* mode as $J'=-0.2\text{eV}/\text{\AA}$ and $J''=+0.18\text{eV}/\text{\AA}^2$, respectively. Thus, we rationalize that, most probably, the scattering background stems from magnetic excitations, and the asymmetric shape of the *B3g* band is a result of a linear spin–phonon coupling of this mode with the Fe–O–Fe spin dimers. Another mechanism, a phonon interaction with thermally activated charge carriers above T_N , is also considered.

Списание [J Appl Phys 127 \(2020\) 205108](#)

21. Заглавие $\text{Ni}_{0.5}\text{M}_{0.5}\text{Fe}_2\text{O}_4$ (M = Cu, Zn) Ferrites Hosted in Nanoporous Carbon from Waste Materials as Catalysts for Hydrogen Production

Автори T. Tsoncheva, I. Spassova, G. Issa, R. Ivanova, D. Kovacheva, D. Paneva, D. Karashanova, N. Velinov, B. Tsyntsarski, B. Georgieva, M. Dimitrov, N. Petrov

Резюме This work is focused on the preparation of $\text{Ni}_{0.5}\text{M}_{0.5}\text{Fe}_2\text{O}_4$ mixed ferrites (M=Zn or Cu), supported on nanoporous carbons materials. The carbon supports are obtained from various waste residues, such as peach stones from the canning industry and by-products from the low rank coals pyrolysis. X-ray diffraction (XRD), nitrogen physisorption, high-resolution transmission electron microscopy (HRTEM), Moessbauer spectroscopy and temperature programmed reduction (TPR) analyses as well as mesoporous silica with tridimensional structure type KIT-6 silica based reference samples are used for detail characterization of the obtained materials. It was established that the loaded on the carbon supports phase is a complex mixture of finely dispersed ferrite, substituted magnetite, metal (Cu, Fe, FeNi alloy) and ZnO particles. Their dispersion and composition depend on the texture characteristics of the carbon support, which could be easily controlled by the waste precursor used. The existence of mesoporosity in the carbon host matrix provokes the formation of more finely dispersed and easily reducible spinel particles, which ensures higher initial catalytic activity, but fast deactivation of the catalysts. The formation of activated carbon mesoporosity is facilitated by the presence of cellulose and hemicellulose in the biomass or the addition of furfural to the coal tar pitch precursor. The $\text{Ni}_{0.5}\text{Zn}_{0.5}\text{Fe}_2\text{O}_4$ modifications demonstrate higher potential as catalysts for hydrogen production via methanol decomposition.

Списание [Waste Biomass Valor 12 \(2021\) 1371](#)

22. Заглавие Influence of the Size of Coal Ash FAU Zeolites Used as Dopants on the Sensing Properties of Nb₂O₅ Thin Films

Автори K. Lazarova, S. Boycheva, M. Vasileva, D. Zgureva, T. Babeva

Резюме In this study, solid waste from coal combustion in thermal power plants (TPPs) was used for the synthesis of zeolite Na-X samples. They were prepared by the long-term alkaline atmospheric conversion of coal ash collected from the electrostatic precipitators in the TPP “AES Galabovo”. When used in the form of thin films/layers, the optical detection of volatile organic compounds (VOCs) is possible due to a change in their reflectance spectra and color. In order to improve the sensing properties of synthesized zeolites, they were wet milled for 60 s and both milled and unmilled zeolites were used as dopants for the niobium oxide matrix in the form of thin films deposited by the spin-coating method on a silicon substrate. The surface morphology and structure of both zeolite powders were studied by scanning electron microscopy, while their size was determined by dynamic light scattering (DLS) spectra. Optical constants (refractive index, n , and extinction coefficient, k) and the thickness of the films were calculated from reflectance measurements. The change in the reflection coefficient ΔR of the films was determined from measured reflectance spectra prior to and after exposure to probe acetone molecules. An increase in the reaction of the films with milled zeolites to acetone, compared to the samples with unmilled zeolites, is demonstrated.

Списание [Mater Proc 2\(1\) \(2020\) 3](#)

23. Заглавие Mathematical modeling and experimental validation of advanced alkaline water electrolyser U/j performance

Автори G. Borisov, N. Borisov, E. Petkucheva, E. Slavcheva

Резюме Hydrogen generation by water electrolysis plays an important role in the green energy cycle with zero carbon emissions. The recent development in the classical alkaline electrolysis including the development of new electrode materials, novel cell architecture and system design, offers possibilities for enhanced kinetics and improved energy efficiency. At the same time, the mathematical modeling and simulations of the reaction mechanisms are more and more often used to predict the response of the system to varying operating conditions which in turn, speeds up additionally the progress of this clean energy converting technology. This paper presents a simple modeling of advanced alkaline water electrolyser using the theoretical thermodynamic functions and electrochemical equations by means of free Scilab 6.0 software. The model allows the calculation of the U/j characteristics as well as parameters such as reversible potential, activation and ohmic losses of the electrochemical process. It is validated using real experimental data obtained in a single electrolysis cell with Ni-based electrodes and Zifron Perl500 diaphragm at 25 °C. Through extrapolation of the results obtained, the model is applied to predict the electrochemical performance of the cell at elevated temperatures up to 80 °C and current densities up to 1 A.cm⁻².

Списание [Bulg Chem Commun 52 \(Special Issue E\) \(2020\) 84](#)

24. Заглавие Impedance spectroscopy studies of the electrochemical hybrid supercapacitors based on activated carbon and iron oxides

Автори E. Lefterova, S. Veleva, A. Stoyanova

Резюме Symmetric and hybrid supercapacitors were developed and investigated by electrochemical impedance spectroscopy (EIS). Activated nanoporous carbon (commercial product, TDA Research, USA) and electrochemically active iron oxides - Fe₂O₃ (hematite) and Fe₃O₄ (magnetite) were laboratory synthesized and used as electrode materials for assembling of supercapacitor cells. LiBF₄ with an organic solvent mixture of ethylene carbonate/dimethyl carbonate (1:1) was served as an electrolyte. The results from EIS measurements show the possibility of application of magnetite and hematite as electrochemically active materials for hybrid lithium battery–supercapacitor systems and can provide guidance in selection the most suitable metal oxides, as composite electrode materials in supercapacitors.

Списание [Bulg Chem Commun 52 \(Special Issue E\) \(2020\) 88](#)

25. Заглавие Progress in the Utilization of Coal Fly Ash by Conversion to Zeolites with Green Energy Applications

Автори S. Boycheva, D. Zgureva, K. Lazarova, T. Babeva, C. Popov, H. Lazarova, M. Popova

Резюме Fly ash (FA) from lignite coal combusted in different Thermal Power Plants (TPPs) was used for the synthesis of zeolites (FAZs) of the Na-X type by alkaline activation via three laboratory procedures. FAZs were characterized with respect to their morphology, phase composition and surface properties, which predetermine their suitability for applications as catalysts and adsorbents. FAZs were subsequently modified with metal oxides (CuO) to improve their catalytic properties. The catalytic activity of non-modified and CuO-modified FAZs in the total oxidation of volatile organic compounds was investigated. FAZs were studied for their potential to retain CO₂, as their favorable surface characteristics and the presence of iron oxides make them suitable for carbon capture technologies. Thin films of FAZs were deposited by in situ crystallization, and investigated for their morphology and optical sensitivity when exposed to pollutants in the gas phase, e.g., acetone. This study contributes to the development of novel technological solutions for the smart and valuable utilization of FA in the context of the circular economy and green energy production.

Списание [Materials 13\(9\) \(2020\) 2014](#)

26. Заглавие Azomethine phthalimides fluorescent E→Z photoswitches

Автори A. Georgiev, D. Yordanov, D. Dimov, I. Zhivkov, D. Nazarova, M. Weiter

Резюме Herein, we report the synthesis and E→Z photoswitching behavior of two 4-substituted azomethine phthalimides containing anthracenyl and 4-(dimethylamino)phenyl moieties (EAMP1 and EAMP2). These compounds represent newly synthesized and unstudied photoswitches with dual fluorescence properties as E-isomers and at photostationary state (PSS)

depending on the solvent polarity. Steady-state fluorescence measurements were performed in various solvents and the results show strong sensitivity on the environmental polarity. The kinetics of E→Z photoswitching to PSS was studied in AcCN by visible light activation at 410 nm (EAMP1) and long wavelength UV-light activation at 350 nm (EAMP2). The quantitative and qualitative performance of the switching behavior was evaluated by the degree of photoisomerization (R) and the rate constant (k). It was found for EAMP1 R = 6.95 %, k = 8.87 × 10⁻⁴ s⁻¹ and EAMP2 R = 88.72 %, k = 4.00 × 10⁻⁴ s⁻¹, respectively. The reason for the lower photoconversion of EAMP1 compared to the EAMP2 was analyzed through optimization of the molecular geometry of E- and Z-isomers in the ground state (S₀) and first excited state (S₁) by DFT/ TD-DFT calculations with B3LYP/6-31+G(d,p) level of theory using IEFPCM in AcCN. It was found that E-isomers in the S₀ have nonplanar conformation, while the Z-isomer of EAMP1 prefers twisted conformation and the Z-isomer of EAMP2 T-shaped conformation is energetically advantageous compared to the twisted one. The reason is the weak H...π noncovalent interaction (NCI) between 4-(dimethylamino)phenyl moiety and phthalimide ring. Moreover, the Z-isomer of EAMP2 is unusual stable up to 600 min at room temperature in dark compared to the EAMP1, which undergoes full Z→E relaxation for less than 60 min at the same conditions. The Z→E relaxation of EAMP2 is achieved for 90 min at 60 °C. The fluorescence E→Z switching behavior was studied by emission measurements in AcCN and 1,4-DOX as E-isomers and at PSS in room and liquid nitrogen (77 K) temperatures. In the polar and nonpolar solvents, red-shifted emissions with increased fluorescence quantum (Φ_{fl}) yields have been observed at PSS compared to the E-isomers. The molecular rotor behavior was studied in the binary mixture of glycerol:ethanol and the results show a sensitivity of the emission bands depending on the environmental viscosity. Time-resolved fluorescence decay measurements were performed in AcCN and 1,4-DOX as E-isomers and at PSS to estimate the mechanism of fundamental fluorescence bands. We found that dyes at PSS have longer lifetime (τ) compared to the E-isomers, especially in less polar 1,4-DOX.

Списание [J Photochem Photobiol A Chem 393 \(2020\) 112443](#)

27. Заглавие Diffraction efficiency of polarization holographic gratings recorded in azopolymer thin films coated using different solvents

Автори В. Blagoeva, L. Nedelchev, G. Mateev, E. Stoykova, D. Nazarova

Резюме We present a study of the diffraction efficiencies of polarization holographic gratings recorded in thin films of the azopolymer PAZO (poly[1-[4-(3-carboxy-4-hydroxyphenylazo) benzenesulfonamido]-1,2-ethanediyl, sodium salt]). Two series of layers have been prepared using two different solvents – distilled water and methanol. The gratings are inscribed by two plain waves with orthogonal circular polarizations (left and right circular) from a He-Cd gas laser (442 nm) at recording angle 20°, corresponding to grating period 1.3 μm. Higher diffraction efficiency is obtained for the thin film samples spin-coated from the methanol solution for thicknesses below 600 nm. Diffraction efficiency higher than 27% was achieved, as well as surface relief height more than 500 nm.

28. Заглавие Influence of Mechanical and Chemical Modification Techniques on Zirconia Surface Roughness

Автори M. Tsanova-Stamatova, N. Manchorova-Veleva, T. Babeva

Резюме 3D profilometry is a highly technological method successfully used in dentistry for evaluating materials' roughness. The aim of our in vitro study was to estimate the effect of mechanical and chemical agents on surface roughness and microscopic structure of zirconia polycrystals by means of 3D profilometry. Seven groups of yttria-stabilized KATANA™ Zirconia (Kuraray Noritake Dental Inc.) samples were prepared: one control group (no pretreatment); four groups sandblasted with 50 μm and 250 μm Al_2O_3 particles at a pressure of 2 and 4 bars and two groups treated with HF (hydrofluoric acid) of 10% and 40% concentration. Each specimen was with diameter and thickness of 11.8 mm and 5.0 mm, respectively. 3D optical profilometry was used to study the surface topography and roughness of the samples. By comparison with control group it was demonstrated that the most suitable treatment that leads to the highest surface roughness values is sand blasting with 50 μm Al_2O_3 particles at a pressure of 4 bars. This method can be suggested as an effective method for surface pretreatment of zirconia.

Списание [Comptes Rendus Acad Bulg Sci 73\(11\) \(2020\) 1510](#)

29. Заглавие Microwave plasma-based direct synthesis of free-standing N-graphene

Автори D. Tsyganov, N. Bundaleska, A. Dias, J. Henriques, E. Felizardo, M. Abrashev, J. Kisoovski, A. M. Botelho do Rego, A. M. Ferraria, and E. Tatarova

Резюме Free-standing N-graphene was synthesized using a microwave plasma-based method at atmospheric pressure conditions through a single step and in a controllable manner. Using ethanol and ammonia as precursors, N-graphene with low relative amount of bonded oxygen and low level of saturated sp^3 carbon bonds was produced. Adjusting the injection position of the nitrogen precursor in the plasma medium leads to selectivity in terms of doping level, nitrogen configuration and production yield. A previously developed theoretical model, based on plasma thermodynamics and chemical kinetics, was further updated to account for the presence of nitrogen precursor. The important role of HCN attachment to the graphene sheets as the main process of N-graphene formation is elucidated. The model predictions were validated by experimental results. Optical Emission Spectroscopy was used to detect the emission of plasma generated "building units" and to determine the gas temperature. The plasma outlet gas was analyzed by Fourier-Transform Infrared Spectroscopy to detect the generated gaseous by-products. The synthesized N-graphene was characterized by Scanning Electron Microscopy, Raman and X-ray photoelectron spectroscopies.

Списание [Phys Chem Chem Phys 22\(8\) \(2020\) 4772](#)

30. Заглавие All niobia Bragg stacks for optical sensing of vapors

Автори R. Georgiev, K. Lazarova, M. Vasileva, T. Babeva

Резюме Vapor responsive all Nb₂O₅ Bragg stacks were prepared using spin-coating of alternating dense and porous flms with quarter-wavelength thickness. The required porosity in the flms was achieved by soft-templating method using micellar solution of Pluronic copolymer as an organic template. The surface morphology and structure of the flms were studied by transmission electron microscopy and selected area electron diffraction, respectively, while optical characterization was performed by combination of ellipsometric and reflectance measurements. Vapor sensing response of the flms was tested by reflectance measurements of the samples prior to and after exposure to acetone vapors selected as probe molecules. Incorporation of “defect” layer in the multilayered structures was firstly simulated theoretically and then realized experimentally aiming at improvement of the optical response to volatile organic compounds. Furthermore, the potential of all niobia stacks consisting of alternating dense and porous sol–gel Nb₂O₅ flms as chemical sensors with optical read-out is demonstrated and discussed.

Списание [Opt Quant Electron 52 \(114\) \(2020\) 1](#)

31. Заглавие Determination of macroelements in potable waters with cell-based inductively-coupled plasma mass spectrometry

Автори V. Lyubomirova, V. Mihaylova, R. Djingova

Резюме The accurate determination of macroelements (Na, K, Ca, Mg and Si) in potable waters with inductively-coupled plasma mass spectrometry (ICP-MS) is difficult due to their high concentrations. In the present study, optimisation of cell-based ICP-MS for application of a bandpass parameter (RPa) for signal reduction was performed to extend their linear ranges. Individual values of the RPa for each isotope have been selected. A method for the determination of macroelements without dilution using optimised RPa values has been developed and applied for potable water analysis. The accuracy was evaluated by analyses of a surface water reference material.

Списание [Spectroscopy Europe 32\(5\) 2020 18](#)