

**FIELD: physics, multidisciplinary**

**IMPROVED VALUE FOR THE GAMOW-TELLER STRENGTH OF THE Sn-100 BETA DECAY**

*Physical review letters, IF =9.227*

*(international consortia)*

Lubos, D., Park, J., Faestermann, T., Gernhauser, R., Krucken, R., Lewitowicz, M., Nishimura, S., Sakurai, H., Ahn, D. S., Baba, H., Blank, B., Blazhev, A., Boutachkov, P., Browne, F., Celikovic, I., de France, G., Doornenbal, P., Fang, Y., Fukuda, N., Giovinazzo, J., Goel, N., Gorska, M., Ilieva, S., Inabe, N., Isobe, T., Jungclaus, A., Kameda, D., Kim, Y. K., Kojouharov, I., Kubo, T., Kurz, N., Kwon, Y. K., Lorusso, G., Moschner, K., Murai, D., Nishizuka, I., Patel, Z., Rajabali, M. M., Rice, S., Schaffner, H., Shimizu, Y., Sinclair, L., Soderstrom, P.-A., Steiger, K., Sumikama, T., Suzuki, H., Takeda, H., Wang, Z., Warr, N., Watanabe, H., Wu, J. and Xu, Z., PHYSICAL REVIEW LETTERS, (2019), 122, 22, 222502 DOI: 10.1103/PhysRevLett.122.222502.

100Sn is the heaviest doubly magic N=Z nucleus, that is particle stable and that decays via a pure and Superallowed Gamow-Teller (GT)  $\beta$  decay. It has the smallest  $\log(ft)$  value throughout the nuclear chart. The 100Sn region is located close to the end of the astrophysical rapid proton capture process path, making this region of particular interest concerning fundamental challenges in both nuclear physics and astrophysics. In this experiment, a record number of 100Sn nuclei was detected, around order of magnitude larger than all previous experiments. Both the half-life and the  $\beta$ -decay end point energy of 100Sn were measured more precisely than the literature values which revealed a dramatic effect on the precision of the GT strength allowing a quantitative comparison with various theoretical models for the first time.

**PRECISION HIGGS PHYSICS AT CEPC**

*Chinese Physics C, IF = 5.861*

*(international consortia)*

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海军), Ying Yang(杨迎), Weiming Yao(姚为民), Dan Yu(于丹), Kaili Zhang(张凯栗), Zhaoru Zhang(张照茹), Mingrui Zhao(赵明锐), Xianghu Zhao(赵祥虎), Ning Zhou(周宁)  
Chinese Physics C, Volume 43, Number 4

The most important pillar in the physics case of the future machine in high energy physics is the physics case of the Higgs boson. The main goal of the paper is probing the potential for the precision measurement of the properties of the Higgs boson and new physics associated with the Higgs boson at future Circular Electron Positron Collider (CEPC), China. The paper represent the comprehensive study showing the capability of CEPC, as a Higgs boson factory, for high precision measurements of the Higgs boson.

Analysis were performed by CEPC invitation to the authors.

The specific study of the charged current Higgs decay to the multijet final state, was previously performed for the two colliders ILC and CLIC, thus making the author/institution the single one in the world that performed studies of Higgs boson on three future Higgs factories, CepC, China, ILC, Japan and CLIC, CERN.

**FIELD: Astronomy & Astrophysics, Physics, Particles & Fields**  
**CONSTRAINING NON-LOCAL GRAVITY BY S2 STAR ORBITS**  
*Phys. Rev. D, IF=4.394*

K. F. Dialektopoulos, D. Borka, S. Capozziello, V. Borka Jovanović, P. Jovanović. Phys. Rev. D, 99(4), 044053 (2019).

Nonlocal theories of gravity have recently drawn a lot of attention because they can suitably represent the behavior of gravitational interaction in the ultraviolet regime. Furthermore, at infrared scales, they give rise to notable cosmological effects which could be important to describe the dark energy behavior. In particular, exponential forms of the distortion function seem particularly useful for this purpose. Using Noether symmetries, it can be shown that the only nontrivial form of the distortion function is the exponential one, which is working not only for cosmological minisuperspaces, but also in a spherically symmetric spacetime. Taking this result into account, we study the weak-field approximation of this type of nonlocal gravity, and comparing with the orbits of the S2 star around the Galactic center (NTT/VLT data), we set constraints on the parameters of the theory. Nonlocal effects do not play a significant role on the orbits of S2 stars around Sgr A\* but give richer phenomenology at cosmological scales than the  $\Lambda$ CDM model. Also, we show that the nonlocal gravity model gives better agreement between theory and astronomical observations than Keplerian orbits.

**FIELD: Nuclear Science & Technology**

**THE INFLUENCE OF MONOMER/SOLVENT FEED RATIO ON POEGDMA THERMORESPONSIVE HYDROGELS: RADIATION-INDUCED SYNTHESIS, SWELLING PROPERTIES AND VPTT**

*Radiation Physics and Chemistry, IF=1.984*

E. Suljovrujic, Z. Miladinovic, M. Micic, D. Suljovrujic, D. Milicevic. Radiation Physics and Chemistry 2019; 158: 37-45.

In the paper we dealt with the investigation of the properties of polymeric biomaterials (PLLA) and smart hydrogels (POEGDMA) because of their possible wide application in medicine, pharmacy, agriculture and environmental protection. A special emphasis was on the use of high-energy radiation for synthesis, processing and sterilization of these biomaterials

**FIELD: Optics, Physics, Atomic, Molecular & Chemical**

**NONLINEAR SYMMETRY BREAKING OF AHARONOV-BOHM CAGES**

*Phys.Rev.A, IF=2.907*

Gligorić Goran, Beličev P. Petra, Laykam Daniel, Maluckov Aleksandra. Phys.Rev.A 99 2019:013823, doi.org/10.1103/PhysRevA.99.013826.

We study the influence of mean-field cubic nonlinearity on Aharonov-Bohm caging in a diamond lattice with synthetic magnetic flux. For sufficiently weak nonlinearities, the Aharonov-Bohm caging persists as periodic nonlinear breathing dynamics. Above a critical nonlinearity, symmetry breaking induces a sharp transition in the dynamics and enables stronger wave-packet spreading. This transition is distinct from other flatband networks, where continuous spreading is induced by effective

nonlinear hopping or resonances with delocalized modes and is in contrast to the quantum limit, where two-particle hopping enables arbitrarily large spreading. This nonlinear symmetry-breaking transition is readily observable in femtosecond laser-written waveguide arrays.

**FIELD: Nanoscience & Nanotechnology, Materials Science, Ceramics, Composites, Multidisciplinary, Metallurgy & Metallurgical Engineering Chemistry, Inorganic & Nuclear**

**99mTc, 90Y AND 177Lu LABELLED IRON OXIDE NANOFLOWERS DESIGNED FOR POTENTIAL USE IN DUAL MAGNETIC HYPERTHERMIA/RADIONUCLIDE CANCER THERAPY AND DIAGNOSIS**

*ACS Appl. Mater. Interfaces*, **IF=8.456**

Miloš Ognjanović, Magdalena Radović, Marija Mirković, Željko Prijović, Maria del Puerto Morales, Miran Čeh, Sanja Vranješ-Đurić, Bratislav Antić. *ACS Appl. Mater. Interfaces*, 2019, 11, 41109-41117.

Development of a complex based on iron oxide nanoparticles (IONPs) for diagnosis and dual magnetic hyperthermia/radionuclide cancer therapy accomplishing high yields of radiolabeling and great magnetic heat induction is still a challenge. We report here the synthesis of citric acid, poly(acrylic acid) (PAA) and poly(ethylene glycol) coated IONPs and their labeling with three radionuclides, namely, technetium (<sup>99m</sup>Tc), yttrium (<sup>90</sup>Y), and lutetium (<sup>177</sup>Lu), aiming at potential use in cancer diagnosis and therapy. Polyol-synthesized IONPs are a flowerlike structure with 13.5 nm spherically shaped cores and 24.8 nm diameter. PAA-coated nanoparticles (PAA@IONP) showed the best characteristics such as easy radiolabeling with very high yields (>97.5%) with all three radionuclides, and excellent in vitro stabilities with less than 10% of radionuclides detaching after 24 h. Heating ability of PAA@IONP in an alternating external magnetic field showed intrinsic loss power value of 7.3 nH m<sup>2</sup>/kg, which is one of higher reported values. Additionally, PAA@IONP itself presented no significant cytotoxicity to the CT-26 cancer cells, reaching IC<sub>50</sub> at 60 μg/mL. However, under the external magnetic field, they show hyperthermia-mediated cells killing, which correlated with the magnetic field strength and time of exposure. Since PAA@IONP are easy to prepare, biocompatible, and with excellent magnetic heat induction, these nanoparticles radiolabeled with high-energy beta emitters <sup>90</sup>Y and <sup>177</sup>Lu have valuable potential as agent for dual magnetic hyperthermia/radionuclide therapy, while radiolabeled with <sup>99m</sup>Tc could be used in diagnostic imaging.

**99mTc–BISPHOSPHONATE–COATED MAGNETIC NANOPARTICLES AS POTENTIAL THERANOSTIC NANOAGENT**

*Materials Science and Engineering C*, **IF=4.959**

Marija Mirković, Magdalena Radović, Dragana Stanković, Zorana Milanović, Drina Janković, Milovan Matović, Marija Jeremić, Bratislav Antić, Sanja Vranješ-Đurić, *Materials Science and Engineering: C*, 2019, 102, 124-133.

Novel theranostic nanoplatform is expected to integrate imaging for guiding and monitoring of the tumor therapy with great therapeutic efficacy and fewer side effects. Here we describe the preparation of a multifunctional <sup>99m</sup>Tc–bisphosphonate–coated magnetic nanoparticles (MNPs) based on Fe<sub>3</sub>O<sub>4</sub> and coated with two hydrophilic bisphosphonate ligands, i.e., methylene diphosphonate (MDP) and 1–hydroxyethane-1,1- diphosphonate (HEDP). The presence of the bisphosphonates on the MNPs surface, enabled their biocompatibility, colloidal stability and

successful binding of the radionuclide. The morphology, size, structure, surface charge and magnetic properties of obtained bisphosphonate-coated Fe<sub>3</sub>O<sub>4</sub> MNPs were characterized by transmission electron microscopy, X-ray powder diffraction, dynamic light scattering, laser Doppler electrophoresis, Fourier transform infrared spectroscopy and vibrating sample magnetometer. The specific power absorption values for Fe<sub>3</sub>O<sub>4</sub>-MDP and Fe<sub>3</sub>O<sub>4</sub>-HEDP were 113 W/g and 141 W/g, respectively, indicated their heating ability under applied magnetic field. Coated MNPs were radiolabeled with <sup>99m</sup>Tc using stannous chloride as the reducing agent in a reproducible high yield (95% for Fe<sub>3</sub>O<sub>4</sub>-MDP and 97% for Fe<sub>3</sub>O<sub>4</sub>-HEDP MNPs) and were remained stable in saline and human serum for 24 h. Ex vivo biodistribution studies presented significant liver and spleen uptake in healthy Wistar rats after intravenous administration at all examined time points due to the colloidal nature of both <sup>99m</sup>Tc-MNPs. Results of scintigraphy studies are in accordance with ex vivo biodistribution studies, demonstrating high in vivo stability of radiolabeled MNPs and therefore results of both methods were proved as accurate information on the biodistribution profile of investigated MNPs. Overall, in vitro and in vivo stability as well as heating ability, indicate that biocompatible radiolabeled bisphosphonate magnetic nanoparticles exhibit promising potential as a theranostic nanoagent.

#### **INVESTIGATION OF <sup>177</sup>Lu LABELED HEDP, DPD, AND IDP AS POTENTIAL BONE PAIN PALLIATION AGENTS**

*Journal of Radiation Research and Applied Science, IF=2.963*

Marija Mirković, Zorana Milanović, Dalibor Stanković, Đorđe Petrović, Sanja Vranješ-Đurić, Drina Janković, Magdalena Radović. Journal of Radiation Research and Applied Science, 2019, 13, 27-36.

Application of bone seeking radiopharmaceuticals is one of modalities in the management of metastatic bone pain. The present study aimed to investigate the potential of <sup>177</sup>Lu-labeled phosphate/phosphonate ligands: 1-hydroxyethane 1,1-diphosphonic acid (HEDP), 2,3-dicarboxypropane-1,1-diphosphonic acid (DPD), and imidodiphosphate tetrasodium salt (IDP), as bone pain palliation agents. HEDP, DPD and IDP were radiolabeled with <sup>177</sup>Lu in high radiolabeling yield (98.49%, 93.31% and 90.69% respectively), forming in vitro stable radiolabeled complexes in saline and human serum after 96 h. Biodistribution was followed by imaging studies and ex vivo measurement of radioactivity in organs in healthy Wistar rats. Significant bone accumulation and long retention even after 96 h (3.85±0.91 %ID/g), as well as, relatively low uptake in soft tissue such as liver and spleen (< 1%ID/g), was observed for <sup>177</sup>Lu-HEDP. Two other radiolabeled ligands showed lower accumulations in bone (<1 % ID/g) and higher accumulations in liver and spleen at examined time points (>1.5 % ID/g). Obtained results suggest that difference in the chemical structure of phosphonates/phosphates, influence the rate of bone incorporation of <sup>177</sup>Lu- radiolabeled complexes. Desirable biodistribution pattern of <sup>177</sup>Lu-HEDP makes it suitable for its further preclinical investigations as potential bone pain palliation agent.

## **SELF-LIMITING INTERACTIONS IN 2D-0D SYSTEM: A CASE STUDY OF GRAPHENE OXIDE AND 12-TUNGSTOPHOSPHORIC ACID NANOCOMPOSITE.**

*Carbon, IF=7.466*

Z. Jovanović, Ž. Mravik, D. Bajuk-Bogdanović, S. Jovanović, S. Marković, M. Vujković, J. Kovač, D. Vengust, S. Uskoković-Marković, I. Holclajtner-Antunović., Carbon 156 (2020) 166-178.

In this paper, composites of graphene oxide and heteropolyacids were investigated with emphasis on the nature of their interactions. It has been found that there is an optimal component ratio that allows their maximum interaction.

## **INVESTIGATION OF THE GRAPHENE THERMAL MOTION BY RAINBOW SCATTERING**

*Carbon, IF=7.466*

Marko Ćosić, Milivoje Hadžijojić, Srđan Petrović, Stefano Bellucci. Carbon 145 (2019) 161-174.

The thermal motion of graphene atoms was investigated using rainbow scattering effect. It was shown how rainbow pattern can be used for extraction of the covariance matrix from the corresponding rainbow patterns in the general case, when atoms perform fully anisotropic and correlated motion.

## **RADIATION STABILITY AND THERMAL BEHAVIOUR OF MODIFIED UF RESIN USING BIORENEWABLE RAW MATERIAL-FURFURYL ALCOHOL**

*Composites Part B: Engineering, IF=6.86*

Suzana Samaržija-Jovanović, Vojislav Jovanović, Branka Petković, Slaviša Jovanović, Gordana Marković, Slavica Porobić, Milena Marinović-Cincović. Composites Part B: Engineering, 167 (2019)161-166.

The thermal stability of organic-inorganic nano-composites prepared by a two-stage polymerization of urea-formaldehyde resin (UF) with furfuryl alcohol (FA) and TiO<sub>2</sub> before and after irradiation has been researched. The two resins of urea-formaldehyde-TiO<sub>2</sub> composites, named: UF/TiO<sub>2</sub> and UF/TiO<sub>2</sub>/FA, were synthesized. The thermal stability of obtained materials was studied by non-isothermal thermo-gravimetric analysis (TG), differential thermal gravimetry (DTG) and differential thermal analysis (DTA). UF hybrid composites have been irradiated (50 kGy) and after that their radiation stability was evaluated on the basis of thermal behavior. The free formaldehyde (HCOH) percentage in all prepared samples was determined. The minimum percentage values of free formaldehyde (0.04% and 0.03%) for UF/TiO<sub>2</sub> and UF/TiO<sub>2</sub>/FA, respectively, after irradiation dose of 50 kGy are detected. The shift of temperature values for selected mass losses (T10%) to a high temperature indicates the increase in thermal stability of samples based on UF resin modified with FA.

**EFFICIENT CAPTURE AND PHOTOTHERMAL ABLATION OF PLANKTONIC BACTERIA AND BIOFILMS USING REDUCED GRAPHENE OXIDE-POLYETHYLENEIMINE FLEXIBLE NANOHEATERS**

*Journal of Materials Chemistry B*, *IF=5.047*

M. Budimir, R. Jijie, R. Ye, A. Barras, S. Melinte, A. V Silhanek, Z. Markovic, S. Szunerits, R. Boukherroub., *Journal of Materials Chemistry B*, 7 (2019) 2771-2781.

In the present work, we developed a simple and efficient strategy for effective bacteria capture and their subsequent eradication through photothermal killing. The developed device consists of a flexible nanoheater, comprising a Kapton/Au nanoholes substrate, coated with reduced graphene oxide-polyethyleneimine (K/Au NH/rGO-PEI) thin films. The Au NH plasmonic structure was tailored to feature strong absorption in the near infrared (NIR) region, where most of biological matter has limited absorption, while PEI was investigated for its strong binding with bacteria through electrostatic interactions. The K/Au NH/rGO-PEI device was demonstrated to capture and eliminate effectively both planktonic Gram-positive *S. aureus* and Gram-negative *E. coli* bacteria after 10 min of NIR (980 nm) irradiation and even more to destroy and eradicate *S. epidermidis* biofilms after 30 min irradiation. The technique developed herein is simple and quite universal with potential applications for eradication of different microorganisms.

**Fe<sub>0.36(4)</sub>Pd<sub>0.64(4)</sub>Se<sub>2</sub>: MAGNETIC SPIN-GLASS POLYMORPH OF FeSe<sub>2</sub> AND PdSe<sub>2</sub> STABLE AT AMBIENT PRESSURE**

*Inorganic Chemistry*, *IF = 4.850*

J. Tian, V. N. Ivanovski, D. Szalda, H. Lei, A. Wang, Y. Liu, W. Zhang, V. Koteski, C. Petrovic *Inorganic Chemistry* 58(5) (2019) 3107–3114.

We report the synthesis and characterization of Fe<sub>0.36(4)</sub>Pd<sub>0.64(4)</sub>Se<sub>2</sub> with a pyrite-type structure. Fe<sub>0.36(4)</sub>Pd<sub>0.64(4)</sub>Se<sub>2</sub> was synthesized using ambient pressure flux crystal growth methods even though the space group Pa<sub>3</sub> is high-pressure polymorph for both FeSe<sub>2</sub> and PdSe<sub>2</sub>. Combined experimental and theoretical analyses reveal magnetic spin glass state below 23 K in 1000 Oe that stems from random Fe/Pd occupancies on the same atomic site. The frozen-in magnetic randomness contributes significantly to electronic transport. Electronic structure calculations confirm dominant d-electron character of hybridized bands and large density of states near the Fermi level. Flux-grown single crystal alloys in Pd–Fe–Se atomic system therefore open new pathway for exploring different polymorphs in crystal structures and their novel properties.

**THE QUEST FOR OPTIMAL WATER QUANTITY IN THE SYNTHESIS OF METAL-ORGANIC FRAMEWORK MOF5**

*Microporous & Mesoporous Materials*, *IF=4.182*

Marjetka Savić Biserčić, B. Marjanović, B. Nedić Vasiljević, S. Mentus, B. A. Zasońska, G. Ćirić Marjanović, *Microporous & Mesoporous Materials* 278 (2019) 23-29.

Metal-organic frameworks (MOFs) are highly porous crystalline materials which have attracted a great interest due to their applicability in gas storage, separation, catalysis, and sensing. Efficient and simple room temperature synthesis of pure phase metal-organic framework MOF-5 has been developed. Crucial influence of water on a reaction pathway was revealed. All existing preparative procedures of MOF-5 could be substantially improved (regarding purity and yield) by using anhydrous zinc acetate as a precursor in the presence of 0.25–0.50 mol of water per mole of zinc salt instead of using commercially available zinc salts hydrates (e.g., zinc acetate-2-hydrate) as precursors. Our findings open up new perspectives not only in the synthesis of MOF-5 but in the syntheses of numerous other MOFs sensitive to water.

### **INTERFACIAL CHARGE-TRANSFER TRANSITIONS IN COLLOIDAL TiO<sub>2</sub> NANOPARTICLES FUNCTIONALIZED WITH SALICYLIC ACID AND 5-AMINOSALICYLIC ACID: A COMPARATIVE PHOTOELECTRON SPECTROSCOPY AND DFT STUDY**

*J. Phys. Chem. C, IF=4.31*

D. Božanić, G. Garcia, L. Nahon, D. N. Sredojević, V. Lazić, I. Vukoje, P. S. Ahrenkiel, V. Đoković, Z. Šljivančanin, J. Nedeljković. *J. Phys. Chem. C* 123 (2019) 29057-29066.

Interfacial charge transfer (ICT) complexes between wide-band-gap metal oxides and small colorless organic molecules have promising use in a variety of applications. The possibility to control optical properties and alignment of energy levels by a proper combination of inorganic and organic parts of ICT complexes is the main advantage of such materials. We used vacuum-ultraviolet electron imaging photoelectron spectroscopy (VUV PES) to determine the ionization potentials of isolated TiO<sub>2</sub> nanoparticles surface-modified with salicylic acid (SA) and 5-aminosalicylic acid (5-ASA). The VUV PES measurements indicated a shift of the photoemission onset from 7.2 eV, observed for pristine TiO<sub>2</sub> nanoparticles, to 6.5 and 5.9 eV for the surface modified ones, with SA and 5-ASA, respectively. These results are consistent with the red shift of the absorption onset observed upon surface modification of TiO<sub>2</sub> colloids. To obtain a detailed description of the optical properties of surface-modified TiO<sub>2</sub> with SA and 5-ASA, density functional theory (DFT) calculations were performed with periodic boundary conditions (PBCs) and with a finite-size TiO<sub>2</sub> cluster. The PBC model provides a qualitatively good description of electronic states of oxide surfaces functionalized with small organic molecules, while an excellent agreement between experimentally determined and calculated band gap values using a finite-size model was found.

### **SURVEY OF ELECTRONIC PROPERTIES AND LOCAL STRUCTURES AROUND Fe IN SELECTED MULTINARY CHALCOGENIDES**

*Journal of Alloys and Compounds, IF=4.175*

I. Radisavljevića, N. Novakovića, H.–E. Mahnke, V. Andrića, S. Kurkoa, D. Milivojevića, N. Romčević, N. Ivanovića. *Journal of Alloys and Compounds* 782 (2019) 160–169.

Paper presents detailed studies of local and electronic structure around Fe in selected CdTe-based multinary chalcogenides by means of X-ray absorption fine structure (XAFS), X-ray magnetic circular dichroism (XMCD) and electron paramagnetic resonance (EPR)



measurements. In addition, electronic consequences of Fe incorporation into CdTe semiconductor host were studied by means of first principles calculations. In order to improve accuracy of the calculated total energies, the band gaps and the band edge positions, special attention is paid to the treatment of exchange –correlation interaction and the description of highly localized Fe 3d states. Also, the Bader theory of the topological properties of the electron charge density is used to access details of the nature, strength and distribution of the (next) nearest neighbour bonds. Along with the crystal field effect, the spin–orbit interaction has proven to play decisive role in determining the nature of Fe doped CdTe systems. While the systems with higher Fe concentration (25 at.%) are intrinsic insulators, in systems with only 3.125 at.% Fe one spin channel contributes to the density of states at the Fermi level, which makes them suitable for spin–selective electronic transport applications.

## **SYNTHESIS AND THERMAL PROPERTIES OF ARYLAZO PYRIDONE DYES**

*Dyes Pigments, IF=4.018*

S.J. Porobić, A.D. Krstić, D.J. Jovanović, J.M. Lađarević, Đ.B. Katnić, D.Ž. Mijin, M. Marinović-Cincović. *Dyes Pigments*, Volume 168, 2019, pp. 12-27.

Thermal degradation properties of 5-(4-substitutedphenylazo)-3-amido-6-hydroxy-4-methyl-2-pyridones and 5-(4-substitutedphenylazo)-3-cyano-6-hydroxy-4-methyl-2-pyridones dyes, differing in electron withdrawing and electron donating substituents in para-position of diazo components were examined. The structure of the synthesized compounds has been confirmed by <sup>1</sup>H NMR, <sup>13</sup>C NMR, FTIR, UV–Vis and XRD analysis techniques. The results obtained with thermogravimetric analysis (TGA) – derivative thermogravimetry (DTG) and differential thermal analysis (DTA) were combined with GC-mass spectral fragmentation to obtain thermal decomposition mechanism. Non-isothermal kinetics were monitored by application of TGA-DTG-DTA. For Kinetic behavior of the investigated dyes during their degradation in an inert atmosphere, Kissinger, Ozawa, Flynn-Wall-Ozawa (FWO) and Kissinger-Akahira-Sunose (KAS) isoconversional (model-free) methods were applied. It was found that different thermal stabilities of investigated dyes are the consequence of their different chemical structures, including diverse substituents.

## **EFFECT OF FE<sup>3+</sup> ION DOPING ON PHOTOCATALYTIC ABILITY OF NANOZIRCONIA CERAMIC TO DEGRADE 2, 4, 6- TRICHLOROPHENOL**

*Ceramics International, IF=3.450*

Milica V. Carević, Tatjana D. Savić, Nadica D. Abazović, Miloš D. Mojović, Tatjana B. Novaković, Mirjana I. Čomor. *Ceramics International*.  
<https://doi.org/10.1016/j.ceramint.2019.11.175>.

Series of Fe – doped zirconia samples is synthesized and characterized in detail. It was shown that doped samples, especially zirconia sample doped with 1% wt. of iron ions show excellent ability to degrade chlorinated phenol under simulated Solar light, which recommend these samples for application in real water systems remediation.

## **GREEN AND FACILE MICROWAVE ASSISTED SYNTHESIS OF (METAL-FREE) N-DOPED CARBON QUANTUM DOTS FOR CATALYTIC APPLICATIONS**

*Ceramics International*, IF=3.450

Jovana Prekodravac, Bojana Vasiljević, Zoran Markovića, Dragana Jovanović, Duška Kleut, Zdenko Špitalský, Matej Mičušik, Martin Danko, Danica Bajuk–Bogdanović, Biljana Todorović–Marković. *Ceramics International* 45 (2019) 17006–17013.

Industrialization today leads to a significant increase in the environmental pollution, with number of phenols, pesticides, paints, solvents and other organic pollutants with potentially carcinogenic effect in natural resources. Investigation of some new semiconductor materials and their photocatalytic properties for removal of pollutants is a challenging effort. In presented work, we demonstrated time saving and economically affordable method for synthesis of N-doped carbon quantum dots using microwave assisted method under mild conditions. Synthesized material showed extraordinary properties for photocatalytic application in degradation of toxic organic dyes in water. At low catalyst concentration (1 mg/ml) and under visible light, N-CQDs were able to degrade Rose Bengal up to 93% under 30 min. Presented work show huge potential for application in waste and seawater treatment, which will hopefully be of great benefit in the future for flora and fauna as well as for the living community.

## **SYNTHESIS AND THERMAL PROPERTIES OF ARYLAZO PYRIDONE DYES**

*Dyes and Pigments*, IF=4.018

Slavica J. Porobić, Aleksandar D. Krstić, Dragana J. Jovanović, Jelena M. Lađarević, Đurica B. Katnić, Dušan Ž. Mijin, Milena Marinović-Cincović. *Dyes and Pigments*, 170 (2019) 107602.

Thermal degradation properties of 5-(4-substitutedphenylazo)-3-amido-6-hydroxy-4-methyl-2-pyridones and 5-(4-substitutedphenylazo)-3-cyano-6-hydroxy-4-methyl-2-pyridones dyes, differing in electron withdrawing and electron donating substituents in para-position of diazo components were examined. The structure of the synthesized compounds has been confirmed by <sup>1</sup>H NMR, <sup>13</sup>C NMR, FTIR, UV–Vis and XRD analysis techniques. The results obtained with thermogravimetric analysis (TGA) – derivative thermogravimetry (DTG) and differential thermal analysis (DTA) were combined with GC-mass spectral fragmentation to obtain thermal decomposition mechanism. Non-isothermal kinetics were monitored by application of TGA-DTG-DTA. For Kinetic behavior of the investigated dyes during their degradation in an inert atmosphere, Kissinger, Ozawa, Flynn-Wall-Ozawa (FWO) and Kissinger-Akahira-Sunose (KAS) isoconversional (model-free) methods were applied. It was found that different thermal stabilities of investigated dyes are the consequence of their different chemical structures, including diverse substituents.

## **CYCLIC OXIDATION OF Ti3Al-BASED MATERIALS**

*Ceramics International*, IF=3.450

Ivana Cvijović-Alagić, Zorica Cvijović, Dejan Zagorac, Milan T. Jovanović. *Ceramics International*. 45 (7) (2019) 9423-9438.

The microstructure variation and oxidation behavior of a hot-rolled and quenched Ti-24Al-11Nb (at.%) intermetallic alloy with and without protective Ni-20Cr (at.%) coating were studied in the air at a cyclic annealing temperature of 600 °C and 900 °C. It was found that the annealing temperature and deposited coating significantly affect the scale formation and growth. The alloy showed better oxidation resistance at 600 °C, irrespective of the protective coating application. The higher temperature promoted the formation of thicker and multi-layered scale predominantly composed of Nb-doped TiO<sub>2</sub> and Al<sub>2</sub>O<sub>3</sub> oxides, which cracked and spalled causing oxidation rate for an order of magnitude higher than that at 600 °C.

### **LOCAL STRUCTURE STUDY OF Hf DOPANTS IN Zr<sub>2</sub>Pd AND ZrPd<sub>2</sub> INTERMETALLICS**

*Intermetallics*, IF=3.353

R. Sewaka, C.C. Deya, S.K. Deya, J. Belošević- Čavorc, A. Kapidžić. *Intermetallics* 107 (2019) 93.

The importance of this paper is that through the study of the local structure of the Zr<sub>2</sub>Pd and ZrPd<sub>2</sub> compounds, it offers one of the possible explanations for their completely different hydrogen absorption capacities (Zr<sub>2</sub>Pd easily forms several hydrides, while ZrPd<sub>2</sub> doesn't form hydride at all, even at high pressure) despite having the same crystal structure and chemical composition. It was found that the electric field gradient, property closely related to the local structure, has different temperature dependence in the two compounds, weak in the ZrPd<sub>2</sub> and strong in the Zr<sub>2</sub>Pd, meaning that in the later large changes in local structure occur with temperature rise.

### **A NEW ENDODONTIC MIXTURE BASED ON CALCIUM ALUMINATE CEMENT OBTAINED BY HYDROTHERMAL SYNTHESIS**

*Ceramics International*, IF=3.450

Čolović B, Janković O, Živković S, Žižak Ž, Besu Žižak I, Jokanović V. *Ceram. Int.* 2019;45:9211-9218.

The synthesis of a new endodontic mixture based on calcium aluminate cement is reported. Physico-chemical and mechanical properties of the mixture were investigated before and after various hydration periods. Phase analysis of the mixture was performed using X-ray diffraction (XRD), while morphological analysis was performed by scanning electron microscopy (SEM) equipped with EDS which revealed elemental composition of the mixture sample. Investigations of mechanical properties showed that this new endodontic mixture possessed good mechanical properties (compressive strength after 28 days aging was 94 MPa) and relatively short setting time (2 h). Additionally, cytotoxicity of the mixture was investigated by MTT assay, while genotoxicity was investigated by Comet assay, using MRC-5 cell line. The obtained results make this material very promising for potential application in dental practice.

## **CYCLIC OXIDATION OF Ti3Al-BASED MATERIALS**

*Ceramics International*, IF=3.450

Ivana Cvijović-Alagić, Zorica Cvijović, Dejan Zagorac, Milan T. Jovanović. *Ceramics International*, 45 (7) (2019) 9423-9438.

The microstructure variation and oxidation behavior of a hot-rolled and quenched Ti-24Al-11Nb (at.%) intermetallic alloy with and without protective Ni-20Cr (at.%) coating were studied in the air at a cyclic annealing temperature of 600 °C and 900 °C. It was found that the annealing temperature and deposited coating significantly affect the scale formation and growth. The alloy showed better oxidation resistance at 600 °C, irrespective of the protective coating application. The higher temperature promoted the formation of thicker and multi-layered scale predominantly composed of Nb-doped TiO<sub>2</sub> and Al<sub>2</sub>O<sub>3</sub> oxides, which cracked and spalled causing oxidation rate for an order of magnitude higher than that at 600 °C.

## **DENSIFICATION BEHAVIOR OF 316L-NiB STAINLESS STEEL POWDER AND SURFACE MORPHOLOGY DURING SELECTIVE LASER MELTING PROCESS USING PULSED Nd:YAG LASER**

*Rapid Prototyping Journal*, IF=2.801

Jelena Stašić, Dušan Božić., *Rapid Prototyping Journal*, 25 (2019) 47-54.

Selective laser melting is one of the techniques of additive manufacturing, i.e. manufacturing layer-by-layer, based on consolidation of starting powders by laser energy. The aim of this work was to obtain 316L-1 wt.% NiB by selective laser melting of powder mixture using pulsed, millisecond Nd:YAG system. Compared to laser melting of pure 316L steel powder, the addition of 1 wt.% NiB provided certain improvements. Better wetting of the molten material was achieved and therefore easier obtaining of high density 3D compacts. Also, structural defects were significantly reduced: porosity was minimized, surface roughness lowered, balling and crack formation disabled.

## **FIELD: Chemistry, Analytical**

### **PHASE AND MICROSTRUCTURAL STUDY OF URINARY STONES**

*Microchemical Journal*, IF=3.206

Miljana Mirković, Anja Došen, Suzana Erić, Predrag Vulić, Branko Matović, Aleksandra Rosić. *Microchemical Journal*, 152 (2020) 104429.

In this paper the phase and morphological characteristics of urinary stones from more than 600 Serbian patients were presented. The study included XRD analysis, SEM-EDS analysis as well as statistical analysis of urinary stones found in both men and women over the period of three years. Results indicate that there are several different types of urinary stones that vary in mineral composition, chemistry and morphology. This was the first comprehensive and systematic study on phase composition of urinary stones found in Serbian patients.

**FIELD: Chemistry, Applied; Polymer Science; Chemistry Multidisciplinary**  
**ANTIBACTERIAL ABILITY OF IMMOBILIZED SILVER NANOPARTICLES IN**  
**AGAR-AGAR FILMS CO-DOPED WITH MAGNESIUM IONS**

*Carbohydrate Polymers*, **IF=6.044**

S. Davidović, V. Lazić, M. Miljković, M. Gordić, M. Sekulić, M. Marinović-Cincović, I.S. Ratnayake, S.P. Ahrenkiel, J.M. Nedeljković. *Carbohydrate Polymers*, 224 (2019) 115187.

The antibacterial ability of in situ prepared nanometer-sized silver particles, immobilized in agar-agar films, was studied as a function of the concentration of co-dopant, magnesium ions. The complete microbial reduction of Gram-positive bacteria *Staphylococcus aureus* was observed for all agar-silver films, while satisfactory results were observed for Gram negative bacteria *Pseudomonas aeruginosa* ( $\geq 99.6\%$ ). The release of  $\text{Ag}^+$  ions is suppressed by the increase of the concentration of  $\text{Mg}^{2+}$  ions and it was found to be significantly smaller ( $\leq 0.24\text{ppm}$ ) than the harmful ecological level (1ppm).

**CONJUGATES OF GOLD NANOPARTICLES AND ANTITUMOR GOLD(III)**  
**COMPLEXES AS A TOOL FOR THEIR AFM AND SERS DETECTION IN**  
**BIOLOGICAL TISSUE**

*International journal of molecular sciences*, **IF=4.183**

Bondzic Aleksandra M, Leskovac Andreja R, Petrovic Sandra Z, Vasic-Anicijevic Dragana D, Luce Marco, Massai Lara, Generosi Amanda, Paci Barbara, Cricenti Antonio, Messori Luigi, Vasic Vesna M. *International Journal of Molecular Sciences*, (2019), vol. 20 br. 24.

Citrate-capped gold nanoparticles (AuNPs) were functionalized with three distinct antitumor gold(III) complexes, e.g.,  $[\text{Au}(\text{N,N})(\text{OH})_2][\text{PF}_6]$ , where (N,N)=2,2'-bipyridine;  $[\text{Au}(\text{C,N})(\text{AcO})_2]$ , where (C,N)=deprotonated 6-(1,1-dimethylbenzyl)-pyridine;  $[\text{Au}(\text{C,N,N})(\text{OH})][\text{PF}_6]$ , where (C,N,N)=deprotonated 6-(1,1-dimethylbenzyl)-2,2'-bipyridine, to assess the chance of tracking their subcellular distribution by atomic force microscopy (AFM), and surface enhanced Raman spectroscopy (SERS) techniques. An extensive physicochemical characterization of the formed conjugates was, thus, carried out by applying a variety of methods (density functional theory—DFT, UV/Vis spectrophotometry, AFM, Raman spectroscopy, and SERS). The resulting gold(III) complexes/AuNPs conjugates turned out to be pretty stable. Interestingly, they exhibited dramatically increased resonance intensity in the Raman spectra induced by AuNPs. For testing the use of the functionalized AuNPs for biosensing, their distribution in the nuclear, cytosolic, and membrane cell fractions obtained from human lymphocytes was investigated by AFM and SERS. The conjugates were detected in the membrane and nuclear cell fractions but not in the cytosol. The AFM method confirmed that conjugates induced changes in the morphology and nanostructure of the membrane and nuclear fractions. The obtained results point out that the conjugates formed between AuNPs and gold (III) complexes may be used as a tool for tracking metallodrug distribution in the different cell fractions.

**FIELD: Electrochemistry**

**ELECTROCHEMICAL INVESTIGATION OF IONIC LIQUID-DERIVED POROUS CARBON MATERIALS FOR SUPERCAPACITORS: PSEUDOCAPACITANCE VERSUS ELECTRICAL DOUBLE LAYER**

*Electrochimica Acta*, *IF*=5.383

Nikola Zdolsek, Raquel P. Rocha, Jugoslav Krstić, Tatjana Trtić-Petrović, Biljana Šljukić, José L. Figueiredo, Milica J. Vujković. *Electrochimica Acta* 298 (2019) 541-551.

This paper presents direct carbonization of ionic liquids as a new simple, one-step and template free route to produce doped-carbon materials with desirable physicochemical properties opens up a new possibility for industrial, large-scale synthesis and application of carbon materials in electrochemistry.

**FIELD: Spectroscopy**

**OPTICAL EMISSION OF GRAPHITE PLASMA GENERATED IN AMBIENT AIR USING LOW-IRRADIANCE CARBON DIOXIDE LASER PULSES**

*Spectrochimica Acta Part B: Atomic Spectroscopy*, *IF*=3.101

Kuzmanović M, Ranković D, Trtica M, Ciganović J, Petrović J, Savović J. *Spectrochim. Acta* 2019;157:37. doi: 10.1016/j.sab.2019.05.006.

In this paper, studies of graphite plasma induced by pulsed carbon dioxide laser (TEA CO<sub>2</sub>) are reported. The research aimed to develop laser-induced plasma spectroscopy technique (LIBS) for elemental analysis of materials with significant carbon content, such as different types of organic materials, coal, incompletely burned fossil fuel ash, soot and others. In addition, the small molecule (C<sub>2</sub> and CN) emission spectra detected in the plasma opened the possibility to identify the presence of organic compounds in different types of carbon-containing materials. Given that one of the special features of the LIBS technique is the ability to analyze samples at a distance, the special significance of the described studies is reflected in the possible application of LIBS based on a TEA CO<sub>2</sub> laser for the remote detection of traces of explosives or for the indication of the presence of some hazardous substances (e.g. chemical agents).

**FIELD: Engineering, Mechanical, Chemical**

**THE INFLUENCE OF ALUMINA CRYSTAL STRUCTURES ON THE MORPHOLOGY AND SURFACE EROSION OF PMMA COMPOSITE MATERIALS EXPOSED TO CAVITATION TESTING**

*Wear*, *IF*=2.950

Marija M. Vuksanović, Nataša Z. Tomić, Maja Gajić-Kvašček, Veljko R. Djokić, Marina Dojčinović, Tatjana Volkov Husović, Radmila Jančić Heinemann, *Wear*, Vol. 436-437 No. 15 (2019) 203033.

PMMA, was used as the polymer matrix reinforced with alumina particles. The reinforcement content of all the samples was 3 wt. %. The results showed that the alumina crystal structure

resulting at different calcination temperatures influences the defect morphology, cavitation resistance and the hardness of the composites.

**IMPROVED SINGLE-STEP EXTRACTION PERFORMANCE OF AQUEOUS BIPHASIC SYSTEMS USING NOVEL SYMMETRIC IONIC LIQUIDS FOR THE DECOLORISATION OF TOXIC DYE EFFLUENTS**

*Journal of Industrial and Engineering Chemistry, IF=4.978*

Aleksandra Dimitrijević, Ana Jocić, Nebojša Zec, Aleksandar Tot, Snežana Papović, Slobodan Gadžurić, Milan Vraneš, Tatjana Trtić-Petrović. *J. Ind. Eng. Chem.* 76 (2019) 500-507.

This paper presents the design and synthesis of new ionic liquids as green solvents with improved color removal properties from wastewater effluents.

**MULTIFUNCTIONAL USE OF MAGNETITE-COATED TUFF GRAINS IN WATER TREATMENT: REMOVAL OF ARSENATES AND PHOSPHATES**

*Advanced Powder Technology, IF=3.250*

Andrija B. Savić, Dj. Čokeša, M.Savić Biserčić, I.Častvan-Janković, R.Petrović, Lj.S.Živković, *Advanced Powder Technology*, 30 (2019) 1687-1695.

Natural filtration material tuff, T (0.6-1.9 mm grain fraction) was modified by coating with nano-sized magnetite. This modification changed pore structure and specific surface area. Specific surface area was increased by cca 35%. Batch experiments proved that magnetite modified tuff (MMT) was 4-5 times more efficient in removal of phosphates than tuff before modifying.

**VOLTAMMETRIC SENSOR BASED ON PT NANOPARTICLES SUPORTED MWCNT FOR DETERMINATION OF PESTICIDE CLOMAZONE IN WATER SAMPLES**

*Journal of the Taiwan Institute of Chemical Engineers, IF=3.763*

Marjan S. Randelović, Milan Z. Momčilović, Jelena S. Milicević, Rada D. Đurovic-Pejčev, Sajjad S. Mofarah, Charles C. Sorrel. *Journal of the Taiwan Institute of Chemical Engineers* 105 (2019) 115–123.

Pesticide clomazone is stable, readily soluble in water, and it is often found in water sources. Hence, its determination in the environment is of utmost importance. Herein, for clomazone assay in aqueous media novel electrochemical sensor based on Pt supported multiwalled carbon nanotubes is applied in differential pulse stripping voltammetry (DPSV). Pesticide is determined in 0.1 M phosphate buffer solution at pH 7.0 in the concentration range of 0.61–20.56 ng cm<sup>-3</sup>, with LOQ = 0.61 and LOD = 0.38.

**FIELD: Energy & Fuels, Thermodynamics**

**MATHEMATICAL MODELLING AND OPTIMISATION OF LIGNITE AND WHEAT STRAW CO-COMBUSTION IN 350 MWE BOILER FURNACE**

*Applied Energy*, **IF=8.426**

Aleksandar Milićević, Srdjan Belošević, Nenad Crnomarković, Ivan Tomanović, Dragan Tucaković. *Applied Energy*, Volume 260, 15 February 2020, Article 114206 (<https://doi.org/10.1016/j.apenergy.2019.114206>, Available online 14 December 2019).

In this paper pulverised lignite-fired 350 MWe boiler furnace is selected for numerical simulations performed by using in-house developed computer code to deepen understanding of complex processes during direct co-firing with wheat straw. The code is significantly upgraded and the fuel devolatilization model improved to accommodate simulation of lignite and wheat straw particle reactions and interactions with gas phase, and to allow analysis of particles behavior under real conditions inside the furnace. The results of parametric analysis could support implementation of biomass co-firing technology in existing coal-fired power plants, to increase energy efficiency and mitigate environmental pollutants.

**FULL-SCALE CFD INVESTIGATION OF GAS-PARTICLE FLOW, INTERACTIONS AND COMBUSTION IN TANGENTIALLY FIRED PULVERIZED COAL FURNACE**

*Energy*, **IF=5.537**

Srdjan Belošević, Ivan Tomanović, Nenad Crnomarković, Aleksandar Milićević. *Energy*, 179 (2019), pp. 1036-1053.

In order to provide better understanding of reactive gas-particle turbulent flow and interphase exchanges in full-scale energy conversion systems, numerical investigation was done in pulverized coal utility boiler tangentially fired furnace, by using an in-house developed combustion code. Results demonstrated remarkable complexity of the two-phase flow phenomena, such as turbulence modulation, particles dispersion and energy transfer between phases. Diagrams based on numerical predictions were proposed to enable efficient estimation of the combustion and flame characteristics in the case-study furnace, for different coals, particle mass fractions and distributions of coal particle size classes over the burner tiers.

**NEW APPLICATION METHOD OF THE ZONAL MODEL FOR SIMULATIONS OF PULVERIZED COAL-FIRED FURNACES BASED ON CORRECTION OF TOTAL EXCHANGE AREAS**

*International Journal of Heat and Mass Transfer*, **IF=4.346**

Nenad Crnomarkovic, Srdjan Belosevic, Ivan Tomanovic, Aleksandar Milicevic. *International Journal of Heat and Mass Transfer*. Vol. 149, March 2020, Article 119192 (doi: [10.1016/j.ijheatmasstransfer.2019.119192](https://doi.org/10.1016/j.ijheatmasstransfer.2019.119192), Available online 20 December 2019).

Improvement of the zonal model application in the numerical simulations of the processes inside pulverized coal-fired furnaces is described in the paper. New method of the zonal model application, called continual corrections of the total exchange areas (CCTEA), provides values of



the wall variables by single run of the numerical simulation. The method is based on the corrections of the total exchange areas according to the changes of the surface zone emissivities during the iterative calculation and summation rules of the total exchange areas. The CCTEA method is an improvement of the previously developed method based on multiple run of numerical simulation, as it reduces the computation time.

### **NUMERICAL MODELING OF IN-FURNACE SULFUR REMOVAL BY SORBENT INJECTION DURING PULVERIZED LIGNITE COMBUSTION**

*International Journal of Heat and Mass Transfer, IF=4.346*

Ivan Tomanović, Srdjan Belošević, Nenad Crnomarković, Aleksandar Milićević, Dragan Tucaković. *International Journal of Heat and Mass Transfer*, 128 (2019), pp. 98-114 (doi: 10.1016/j.ijheatmasstransfer.2018.08.129).

This paper presents results of SO<sub>2</sub> emission reduction study from utility boiler by means of the calcium-based sorbent direct injection into the boiler furnace. Analysis is based on the numerical simulations of complex processes during combustion and sorbent reactions in turbulent reactive two-phase flow obtained on the full scale utility boiler furnace model. In order to predict the desulfurization process, models of the sorbent calcination/sintering/sulfation reactions are improved and incorporated into the developed comprehensive computer code. The performed analysis may help a great deal in optimization of the SO<sub>2</sub> reduction method under realistic operating conditions.

### **THE INFLUENCE OF MECHANICAL MILLING PARAMETERS ON HYDROGEN DESORPTION FROM MgH<sub>2</sub>-WO<sub>3</sub> COMPOSITES**

*International Journal of Hydrogen Energy, IF=4.229*

Tijana Pantić, Igor Milanović, Miodrag Lukić, Jasmina Grbović Novaković, Sandra Kurko, Nikola Biliškov, Sanja Milošević Govedarović. *International Journal of Hydrogen Energy*, 2019, Article in press, doi:10.1016/j.ijhydene.2019.07.167.

The influence of different milling conditions obtained using two high-energy mills on hydrogen desorption from MgH<sub>2</sub>-WO<sub>3</sub> composites was investigated. The morphology, particle and crystallite size were studied as a function of milling speed, vial's volume, and ball-to-powder ratio. The vial's fill level, the number, and type of milling balls and additive's content kept constant. Changes in morphology and microstructure were correlated to desorption properties of materials. Higher milling speed reduced particle size but, there is no significant crystallite size reduction. On the other hand, additive distribution is similar regardless of the energy input. It has been noticed that different energy input on milling blend, which is the result of combined effects of above-mentioned factors, reflects on desorption temperature but not on the kinetics of desorption. In fact, desorption mechanism changes from 2D to 3D growth with constant nucleation rate, despite obtained changes in microstructure or chemical composition of the material.

## **INFLUENCE OF DEFECTS ON THE STABILITY AND HYDROGEN-SORPTION BEHAVIOR OF Mg-BASED HYDRIDE**

*ChemPhysChem*, IF=3.077

Jasmina Grbović Novaković, Nikola Novaković, Sandra Kurko, Sanja Milošević Govedarović Tijana Pantić, Bojana Paskaš Mamula, Katarina Batalović, Jana Radaković, Jelena Rmuš, Marina Shelyapina, Nataliya Skryabina, Patricia de Rango, Daniel Fruchart. A review. *ChemPhysChem*, 20 (2019) 1216-1247.

The review deals with the destabilization methods for improvement of storage properties of metal hydrides. Both theoretical and experimental approaches were used to point out the influence of various types of defects on structure and stability of hydrides. As a case study, Mg, and Ni based hydrides has been investigated. Theoretical studies, mainly carried out within various implementations of DFT, are a powerful tool to study mostly MgH<sub>2</sub> based materials. By providing an insight on metal-hydrogen bonding that governs both thermodynamics and hydrogen kinetics, they allow us to describe phenomena to which experimental methods have a limited access. The influence of ion irradiation and mechanical milling with and without additives has been discussed. Ion irradiation is the way to introduce a well-defined concentration of defects (Frankel pairs) at the surface and sub-surface layers of a material. Defects at the surface play the main role in sorption reaction since they enhance the dissociation of hydrogen. On the other hand, ball-milling introduce defects through the entire sample volume, refine the structure and thus decrease the path for hydrogen diffusion. Two Severe Plastic Deformation techniques were used to better understand the hydrogenation/dehydrogenation kinetics of Mg- and Mg<sub>2</sub>Ni-based alloys: Equal-Angular-Channel-Pressing and Fast-Forging.

## **DFT STUDY OF BORON DOPED MgH<sub>2</sub>: BONDING MECHANISM, HYDROGEN DIFFUSION AND DESORPTION**

*Inter.Journal of Hydrogen Energy*, IF=4.229

Sandra Kurko, Bojana Paskaš Mamula, Jasmina Grbović Novkaović, Nikola Novaković. *Inter.Journal of Hydrogen Energy*, 2019, Article in press. doi: 10.1016/j.ijhydene.2019.05.015.

The impact of boron doping on MgH<sub>2</sub> bonding mechanism, hydrogen diffusion and desorption was calculated using density functional theory (DFT). Atomic interactions in doped and non-doped system and its influence on hydrogen and vacancy diffusion were studied in bulk hydride. Slab calculations were performed to study hydrogen desorption energies from (110) boron doped surface and its dependence on the surface configuration and depth position. To study kinetics of hydrogen diffusion in boron vicinity and hydrogen molecule desorption activation energies from boron doped and non-doped (110) MgH<sub>2</sub> surface Nudged Elastic Band (NEB) method was used. Results showed that boron forms stronger, covalent bonds with hydrogen causing the destabilization in its first and second coordination. This leads to lower hydrogen desorption energies and improved hydrogen diffusion, while the impact on the energy barriers for H<sub>2</sub> desorption from hydride (110) surface is less pronounced.

## **THE IMPROVED PHOTOVOLTAIC RESPONSE OF COMMERCIAL MONOCRYSTALLINE SI SOLAR CELL UNDER NATURAL AND ARTIFICIAL LIGHT BY USING WATER FLOW LENS (WFL) SYSTEM**

*International Journal of Energy Research, IF=3.343*

Lojpur V, Mitrić M, Validžić I Lj. Int. J. Energy Res. 2019;43:3507. doi: 10.1002/er.4491.

The performances of a photovoltaic system based on high-efficiency commercial monocrystalline Si solar cell associated with the water flow lens (WFL) system are investigated. This system enables the cooling of the surface of the cell, indirectly cooling the surrounding, and, on the other hand, it allows us to investigate, depending on the position of the cell and the WFL system, the influence of larger and smaller intensities of the light with the inevitable change in the spectrum. All of these effects are very important and can greatly contribute to the better photovoltaic performance of the used cells. Indoor characterization at higher and lower light intensities is performed using both different spectra and intensity of the light. The obtained results show that at low/lower light intensity, spectra are more dominant than the intensity of light itself and that the used WFL system always improves the photovoltaic response leading to a higher efficiency of the tested solar cell. It was found that the ratios of the short circuit current ( $I_{sc}$ ) and the input light energy ( $P_{input}$ ) are 4.42 and 8.96 without and with the use of the WFL system in the measurements, respectively. The same Si solar cell is also tested in outdoor condition, but this time using the WFL system to concentrate sunlight to produce a larger amount of power and water flow for cooling the surface of the solar cell. Again, a higher efficiency (an increase from 25.7% to 33.5%) by using the WFL system was obtained.

## **NUMERICAL AND EXPERIMENTAL ANALYSIS OF PHOTOVOLTAIC CELLS UNDER A WATER LAYER AND NATURAL AND ARTIFICIAL LIGHT**

*IEEE Journal of Photovoltaics, IF=3.398*

Marco Tina G, Rosa-Clot M, Lojpur V, Validžić I Lj. IEEE J. Photov. 2019;3:733. doi: 10.1109/JPHOTOV.2019.2896669.

The possibility to use photovoltaic (PV) modules under a water layer has been explored under different forms: submerged, covered by a water layer, and under a transparent box that contains water. All these test conditions have in common the use of water as a filter for solar radiation to reduce the warming of the PV cells. The effect of the change of the solar spectrum impinging on the PV cells depends highly on the PV technology. A numerical analysis to evaluate the photoelectric efficiency of different PV cells under water is given. Further indoor experimental measurements of PV cells stroked by the artificial light of a halogen lamp that passes through the water-flow-lens (WFL) system are also presented. The connection between the band gap, intensity of light, and distribution of light for a different approach for filtering solar radiation is discussed. The influence of light intensity, halogen spectrum, as well as the WFL system used and their influence on the short-circuit current (ISC) and the open-circuit voltage (VOC) are also investigated.

**FIELD: Food Science & Technology, Nutrition & Dietetics**  
**UV-C LIGHT IRRADIATION ENHANCES TOXIC EFFECTS OF CHLORPYRIFOS AND ITS FORMULATIONS**

*Food Chemistry, IF=5.399*

Jasmina Z. Savić, Sandra Ž. Petrović, Andreja R. Leskovac, Tamara D. Lazarević Pašti, Branislav J. Nastasijević, Brankica B. Tanović, Slavica M. Gašić, Vesna M. Vasić. *Food Chemistry* 271 (2019) 469–478.

UV-C irradiation is widely used in the food industry. However, the health effects from dietary exposure to the irradiated pesticide residues retained in foodstuffs are underestimated. In this study, technical chlorpyrifos (TCPF) and its oil in water (EW) and emulsifiable concentrate (EC) formulations were irradiated by UV-C, and their photodegradation products were subjected to toxicity assessment, including determination of acetylcholinesterase (AChE) activity, genotoxicity and oxidative stress using human blood cells as a model system. Toxicity studies were performed using the chlorpyrifos concentrations in the range of those proposed as the maximum residue levels in plant commodities. TCPF, EW and EC photodegradation products induced DNA damage and oxidative stress, and their genotoxicity did not decrease as a function of irradiation time. Irradiated TCPF and EC are more potent AChE inhibitors than irradiated EW. Accordingly, the application of UV-C irradiation must be considered when processing the plants previously treated with chlorpyrifos formulations.

**ESTRADIOL AMELIORATES ANTIOXIDANT AXIS SIRT1-FOXO3A-MNSOD/CATALASE IN THE HEART OF FRUCTOSE-FED OVARIECTOMIZED RATS**

*Journal of Functional Foods, IF=3.470*

Maja Boskovic, Maja Bundalo, Maja Zivkovic, Jelena Stanisic, Milan Kostic, Goran Koricanac, Aleksandra Stankovic. *Journal of Functional Foods* 52 (2019) 690–698.

We added knowledge of fructose-rich diet harmful effect on SIRT1-FoxO3a-MnSOD/catalase axis in the heart and benefits of estradiol replacement. Regulation of investigated molecules are rather complex, and although the AMPK and SIRT are regulatory connected within a circle, our results suggest the possibility of their independent response to treatment.

**LOW INTENSITY EXERCISE IN THE PREVENTION OF CARDIAC INSULIN RESISTANCE-RELATED INFLAMMATION AND DISTURBANCES IN NOS AND MMP-9 REGULATION IN FRUCTOSE-FED OVARIECTOMISED RATS**

*Appl Physiol Nutr Metab, IF=3.455*

Stanisic J, Koricanac G, Kostic M, Stojiljkovic M, Culafic T, Romic S, Tepavcevic S. *Appl Physiol Nutr Metab*. 2019 Nov;44(11):1219-1229.

Results of this study shed new light on the molecular mechanisms responsible for effects of low-intensity exercise, as nonpharmacological treatment, on prevention of cardiac insulin action disturbances and reduction of cardiovascular risk in high fructose-fed ovariectomized rats.

**FIELD: Microscopy**

**APPLICATION OF GRAY LEVEL CO-OCCURRENCE MATRIX ANALYSIS AS A NEW METHOD FOR ENZYME HISTOCHEMISTRY QUANTIFICATION**

*Microsc Microanal*, IF=2.673

Dragić M, Zarić M, Mitrović N, Nedeljković N, Grković I. *Microsc Microanal* 2019; 25: 690-698.

Enzyme histochemistry is a histological method which provides a connection between morphology, activity, and spatial localization of investigated enzymes. It is widely used for qualitative pathohistological diagnostics. By applying textural analysis - angular second moment, contrast, correlation, inverse difference moment, and entropy we demonstrated that it is possible to perform reliable quantification of enzymatic histochemistry results on ecto-5'-nucleotidase activity in healthy hippocampus and tissue with pronounced neurodegeneration. Our results strongly argue that co-occurrence matrix analysis could be used for the determination of fine differences in the enzyme activities with the possibility to ascribe those differences to regions or specific cell types. In addition, it emerged that inverse difference moment and contrast are especially useful parameters for this type of enzyme histochemistry analysis.

**FIELD: Neurosciences, Neuropharmacology, Translational Psychiatry**

**SPATIAL DISTRIBUTION AND EXPRESSION OF ECTONUCLEOTIDASES IN RAT HIPPOCAMPUS AFTER REMOVAL OF OVARIES AND ESTRADIOL REPLACEMENT**

*Molecular Neurobiology*, IF=5.076

Grković I, Mitrović N, Dragić M, Adžić M, Drakulić D, Nedeljković N. *Mol Neurobiol*. 2019; 56: 1933-1945.

Purinergic signaling is the main synaptic and non-synaptic signaling system in brain. ATP acts as a fast excitatory transmitter, while adenosine sets a global inhibitory tone within hippocampal neuronal networks. ATP and adenosine are interconnected by ectonucleotidase enzymes, which convert ATP to adenosine. Existing data point to the converging roles of ovarian steroids and purinergic signaling in synapse formation and refinement and synapse activity in the hippocampus. Therefore, in the present study, we have used enzyme histochemistry and expression analysis to obtain data on spatial distribution and expression of ecto-enzymes NTPDase1, NTPDase2, and ecto-5'-nucleotidase (eN) after removal of ovaries (OVX) and estradiol replacement (E2) in female rat hippocampus. The results show that target ectonucleotidases are predominantly localized in synapse-rich hippocampal layers. Investigated ectonucleotidases are differentially modulated by OVX and E2 replacement. Also, analysis of the enzymes in the synaptic and astrocytic compartments showed their different expression pattern and sensitivity to hormonal manipulation. Since ovarian steroids shape hippocampal synaptic networks and regulate ectonucleotidase activities, it is possible that cognitive deficits seen after ovary removal may arise from the loss of E2 modulatory actions on ectonucleotidase expression in the hippocampus.

## **ROLE OF ECTONUCLEOTIDASES IN SYNAPSE FORMATION DURING BRAIN DEVELOPMENT: PHYSIOLOGICAL AND PATHOLOGICAL IMPLICATIONS**

*Current Neuropharmacology, IF=4.568*

Grković I, Drakulić D, Martinović J, Mitrović N.. *Curr Neuropharmacol.* 2019; 17: 84-98.

In this review, as a result of our long-term study and the results of other authors, we review the expression and role of four ectonucleotidase families, their role in synapse formation during development, as well as changes in ectonucleotidase activity and expression in pathological conditions during development, which have been described in the literature.

## **PROGESTERONE PROTECTS PREFRONTAL CORTEX IN RAT MODEL OF PERMANENT BILATERAL COMMON CAROTID OCCLUSION VIA PROGESTERONE RECEPTORS AND AKT/ERK/ENOS**

*Cellular and Molecular Neurobiology, IF=3.895*

Stanojlović M, Guševac Stojanović I, Zarić M, Martinović J, Mitrović N, Grković I, Drakulić D. *Cellular and Molecular Neurobiology* 2019, DOI: 10.1007/s10571-019-00777-2.

Sustained activation of pro-apoptotic signaling due to a sudden and prolonged disturbance of cerebral blood circulation governs the neurodegenerative processes in prefrontal cortex of rats whose common carotid arteries are permanently occluded. The adequate neuroprotective therapy should minimize the activation of toxicity pathways and increase the activity of endogenous protective mechanisms. Several neuroprotectants have been proposed, including progesterone. The obtained results indicate that potential amelioration of histological changes in cortex might be associated with the absence of activation of Bax/caspase 3 signaling cascade and the decline of DNA fragmentation. The study also provides the evidence that P4 treatment in repeated regiment of administration might be effective in neuronal protection against ischemic insult due to re-establishment of the compromised action of Akt/Erk/eNOS-mediated signaling pathway and the upregulation of progesterone receptors.

## **TIANEPTINE ANTAGONIZES THE REDUCTION OF PARVALBUMIN AND GAD67 CELLS NUMBER IN LAYERS OF HIPPOCAMPAL SUBREGIONS OF SOCIALLY ISOLATED RATS**

*Progress in Neuro-psychopharmacology and Biological Psychiatry, IF=4.315*

Perić I, Stanisavljević A, Inta D, Gass P, Lang E.U, Borgwardt S, Filipović D. 2019. *Progress in Neuro-psychopharmacology and Biological Psychiatry* 89:386-399.

Contemporary studies have shown that reduced GABA (&#947;-aminobutyric acid) neurotransmission, the main inhibitory neurotransmitter in the brain, is involved in the pathophysiology of depression. In recent years, parvalbumin (PV) positive (+) GABA interneurons have been in the research focus of the therapy of depressive disorders. The detrimental effect of six weeks of social isolation in adult male rats was studied, as well as the protective effect of the antidepressant tianeptin (10 mg/kg/day) on the number of PV + interneurons in the dorsal hippocampal subregions. Analysis of the results showed that tianeptin

increased the number of PV+ GABA interneurons, preferentially of interneurons located in SP layers of CA fields and ML-GCL of DG of the hippocampus in isolated rats, thereby it re-establishes the inhibitory regulation of the neurons. Our results are indicative of the overlapping GABAergic and glutamatergic hypothesis of depression.

**GLUCOCORTICOID RECEPTOR ALPHA TRANSLATIONAL ISOFORMS AS MEDIATORS OF EARLY ADVERSITIES AND NEGATIVE EMOTIONAL STATES**

*Progress in Neuro-psychopharmacology and Biological Psychiatry, IF=4.315*

Adzic M, Glavonic E, Nestic MJ, Milosavljevic M, Mihaljevic M, Petrovic Z, Pavlovic Z, Brkic Z, Francija E, Soldatovic I, Mitic M, Radulovic J, Maric NP. Prog Neuropsychopharmacol Biol Psychiatry. 2019 Mar 2;90:288-299.

Childhood trauma (CT) increases the risk for psychopathology through disturbed acquisition and extinction of fear. The effects of CT are mediated by abnormalities of the hypothalamic-pituitary-adrenal axis and glucocorticoid receptor (GR). Our data emphasized that the association between CT and adult negative affects (NA) in non-clinical subjects are mediated by the GR $\alpha$  translational isoforms, in particular 40-kDa GR $\alpha$ , and emphasized its role in fear extinction and neural plasticity.

**FIELD: Chemistry, Medicinal; Biochemistry & Molecular Biology, Biophysics**

**DISPROT: INTRINSIC PROTEIN DISORDER ANNOTATION IN 2020**

*Nucleic Acids Research, IF=11.147*

*(international consortia)*

Hatos A, Hajdu-Soltész B, Monzon AM, Palopoli N, Álvarez L, Aykac-Fas B, et al. DisProt: intrinsic protein disorder annotation in 2020. Nucleic Acids Res. 2020 Jan 8;48(D1):D269-D276.

Hatos et al. encompass Laboratory's research within international consortia, which are focused on the protein function annotation and annotation of intrinsically disordered proteins.

**EXPRESSION OF ANTIOXIDANT ENZYMES IN PATIENTS WITH UTERINE POLYP, MYOMA, HYPERPLASIA, AND ADENOCARCINOMA**

*Antioxidants, IF=4.520*

Todorović, A.; Pejić, S.; Gavrilović, L.; Pavlović, I.; Stojiljković, V.; Popović, N.; Pajović, S.B. Antioxidants 2019, 8, 97. <https://doi.org/10.3390/antiox8040097>.

The results of our study clearly showed that in the course of benign, premalignant, and malignant uterine transformation significant changes occurred in expression level of Nrf2, and consequently on transcriptional and translational levels of antioxidant enzyme (AOE). It is also evident that the impact of AOE expression on their enzyme activity depends not only on the type of the enzyme, but also on the type of endometrial transformation. Observed findings could contribute to a better insight into molecular mechanisms connecting oxidative stress with different gynecological disorders, and to a better understanding of therapeutic approaches based on altering the cellular redox status.

## **MODULATION OF HIPPOCAMPAL ANTIOXIDANT DEFENSE SYSTEM IN CHRONICALLY STRESSED RATS BY LITHIUM.**

*Oxidative Medicine and Cellular Longevity*, IF=4.936

Popović N, Stojiljković V, Pejić S, Todorović A, Pavlović I, Gavrilović L, Pajović SB. *Oxidative Medicine and Cellular Longevity*. 2019, Vol. 2019, Article ID 8745376, 11 pages <https://doi.org/10.1155/2019/8745376>.

We found that lithium induced modulation of hippocampal antioxidant status and attenuation of oxidative stress stabilized behavior in animals with high anxiety index. In addition, reduced oxidative stress was followed by the changes of both turnover of dopamine and levels of brain-derived neurotrophic factor protein in chronically stressed rats treated with lithium. These findings may be important in preclinical research of the effects of lithium on oxidative stress level in pathological conditions.

## **CHEMISTRY AND REACTIVITY OF RUTHENIUM(II) COMPLEXES: DNA/PROTEIN BINDING MODE AND ANTICANCER ACTIVITY ARE RELATED TO THE COMPLEX STRUCTURE**

*Coord Chem Rev*, IF=14.50

A Rilak-Simović, R Masnikosa, I Bratsos, E Alessio. *Coord Chem Rev* (2019), 398, Article 113011.

In this review we summarize our work on development of Ru complexes with potential antitumor activity, which was performed over the last few years. In order to establish the structure-activity relationship for Ru(II) compounds, we have designed, synthesized and thoroughly studied several Ru(II) complexes, which were divided in three main groups: i) organometallic Ru(II)-arene complexes, ii) Ru(II) half-sandwich coordination complexes bearing neutral face-capping macrocyclic ligands, such as 1,4,7-trithiacyclononane ([9]aneS3) and 1,4,7-triazacyclononane ([9]aneN3), and iii) Ru(II)-polypyridyl complexes. Our most recent experiments moved toward synthesis, chemistry and reactivity of the heteronuclear ruthenium(II)/ferrocene complexes. The first part of the present review gives a brief overview of the structural features and anticancer activity of ruthenium complexes. The second part is focused mainly on the results obtained from the kinetic and mechanistic studies of the reactions between Ru(II) complexes and guanine derivatives, such as 9-methylguanine (9MeG), guanosine (Guo) and guanosine-5'-monophosphate (5'-GMP), as well as on structural characterization of the final products of these reactions. In the final part we deal with the reactions of Ru(II) complexes with DNA, which is widely accepted as a potential target for cytotoxic ruthenium compounds. We have also described the interactions of Ru(II) compounds with the most abundant transport proteins from human serum: human serum albumin (HSA) and transferrin (Tf). We believe that a systematic review of the aforementioned studies will not only contribute to the future development of ruthenium complexes as potential antitumor agents, but will also help to understand the potential toxicity of ruthenium-based drugs.



**NOVEL ELECTROPHILIC AMIDES AMENABLE BY THE UGI REACTION PERTURB THIOREDOXIN SYSTEM VIA THIOREDOXIN REDUCTASE 1 (TRXR1) INHIBITION: IDENTIFICATION OF DVD-445 AS A NEW LEAD COMPOUND FOR ANTICANCER THERAPY**

*European Journal of Medicinal Chemistry, IF 4.833*

Jovanović M, Zhukovsky D, Podolski-Renić A, Domračeva I, Žalubovskis R, Senčanski M, et al.. Eur J Med Chem. 2019 Nov 1;181:111580.

In the research published in the Jovanović et al., Laboratory's team applied various computational chemistry tools and the most significant results include design and synthesis of new inhibitors of TrxR1 enzyme, which is important in regulation of cellular response to oxidative stress and represents an important hemiotherapeutic target in cancer.

**GRAPHENE OXIDE SIZE AND STRUCTURE PRO-OXIDANT AND ANTIOXIDANT ACTIVITY AND PHOTOINDUCED CYTOTOXICITY RELATION ON THREE CANCER CELL LINES**

*J. Photoch. Photobio B, IF=4.067*

M, Mičušík M, Jovanović DJ, Kleinová A, Špitalský Z, Pavlović VB, Todorović Marković BM. *J. Photoch. Photobio B* 200 (2019) 111647.

Photoactive materials called photosensitizers can be used for treatment of different types of cancer in combination with light source. In this paper, we have investigated pro-oxidant and antioxidant potentials of four graphene based nanomaterials (graphene oxide-GO, graphene quantum dots-GQDs, carbon quantum dots-CQDs and N-doped carbon quantum dots-N-CQDs) depending on the presence/absence of visible light source. Structural and optical properties of these materials and their potentials for reactive oxygen species generation/quenching are investigated by applying different microscopy and spectroscopy techniques (transmission electron microscopy, FTIR, UV-Vis, photoluminescence, electron paramagnetic resonance). Results show that all types of quantum dots has pro-oxidant and antioxidant potentials whereas GO demonstrated only moderate antioxidant effect. The best free radical scavenger is CQDs sample in the absence of light. CQDs are the best singlet oxygen generator under blue light irradiation as well. To check photo-cytotoxicity of these materials, photo-cytotoxic concentrations of the GO, GQDs, CQDs and N-CQDs were determined for three cellular lines: human rhabdomyosarcoma (RD), cell line derived from human cervix carcinoma Hep2c (HeLa) and fibroblast cell line from murine (L<sub>2</sub>OB). Cytotoxicity test has indicated that all samples are much less photocytotoxic than cis-diamminedichloroplatinum (cis-DPP). The production method and doping of quantum dots affect the photodynamic activity of tested samples very much.

**ENDOTHELIAL DYSFUNCTION IN DYSLIPIDAEMIA: MOLECULAR MECHANISMS AND CLINICAL IMPLICATIONS**

*Current Medicinal Chemistry, IF=3.894*

Bozidarka Zaric, Milan Obradovic, Andreja Trpkovic, Maciej Banach, Dimitri P. Mikhailidis, Esma R. Isenovic. *Curr Med Chem*. 2019 Sep 3. doi: 10.2174/0929867326666190903112146.

The endothelium consists of a monolayer of endothelial cells (ECs) which form the inner cellular lining of veins, arteries, capillaries and lymphatic vessels. ECs interact with the blood and lymph. The endothelium fulfils functions such as vasodilatation, regulation of adhesion, infiltration of leukocytes, inhibition of platelet adhesion, vessel remodeling and lipoprotein metabolism. ECs synthesize and release compounds such as nitric oxide (NO), metabolites of arachidonic acid, reactive oxygen species (ROS) and enzymes that degrade the extracellular matrix. Endothelial dysfunction represents a phenotype prone to atherogenesis and may be used as a marker of atherosclerotic risk. Such dysfunction includes impaired synthesis and availability of NO and an imbalance in the relative contribution of endothelial derived relaxing factors and contracting factors such as endothelin-1 and angiotensin. This dysfunction appears before the earliest anatomic evidence of atherosclerosis and could be an important initial step in further development of atherosclerosis. Endothelial dysfunction was historically treated with vitamin C supplementation and L-arginine supplementation. Short term improvement of the expression of adhesion molecule and endothelial function during antioxidant therapy has been observed. Statins are used in the treatment of hyperlipidaemia, a risk factor for cardiovascular disease. Future studies should focus on identifying the mechanisms involved in the beneficial effects of statins on the endothelium. This may help develop drugs specifically aimed at endothelial dysfunction.

## **REDOX CONTROL OF VASCULAR BIOLOGY**

*Biofactors*, **IF=3.598**

Milan Obradovic, Magbubah Essack, Sonja Zafirovic, Emina Sudar Milanovic, Vladan P. Bajic, Christophe Van Neste, Julijana Stanimirovic, Andreja Trpkovic, Vladimir B. Bajic, and Esma R. Isenovic (2019): Redox control of vascular biology, *Biofactors*. 2019; 1–17.

Chronically elevated levels of ROS cause oxidative stress and redox may eventually lead to cardiovascular diseases. Our study analyzed the sub-compartments of the vascular system and gives an overview of how redox changes influence those different compartments and also the core aspects of redox biology, cardiovascular physiology, and pathophysiology. Moreover, the topic-specific knowledgebase DES-RedoxVasc was used to develop two case studies, one focused on endothelial cells and the other on the vascular smooth muscle cells, as a starting point to possibly extend our knowledge of redox control in vascular biology and to see new pathways for improved treatment and more adequate prevention of cardiovascular-related diseases.

## **FIELD: Cell Biology**

### **GLUTATHIONE “REDOX HOMEOSTASIS” AND ITS RELATION TO CARDIOVASCULAR DISEASE. OXIDATIVE MEDICINE AND CELLULAR LONGEVITY**

*Oxidative Medicine and Cellular Longevity*, **IF=4.936**

Vladan Bajic, Christophe Van Neste, Milan Obradovic, Sonja Zafirovic, Djordje Radak, Vladimir Bajic, Magbubah Essack and Esma R. Isenovic (2019). Special issue Chemistry, Biology, and Pharmacology of Modulators of Oxidative Stress. *Oxidative Medicine and Cellular Longevity*. <https://doi.org/10.1155/2019/5028181>.

Cardiovascular complications are thought to arise from enhanced levels of free radicals causing impaired 'Redox Homeostasis', which represents the interplay between oxidative stress (OS) and reductive stress (RS). In our study, we compile several experimental research findings that show sustained shifts towards OS will alter the homeostatic redox mechanism to cause cardiovascular complications; as well as findings that show prolonged, antioxidant state or RS, can similarly lead to such cardiovascular complications. This experimental evidence is specifically focused on the role of Glutathione, the most abundant antioxidant in the heart, in a redox homeostatic mechanism that has been shifted towards OS or RS. This may lead to impairment of cellular signaling mechanisms and elevated pools of proteotoxicity associated with cardiac dysfunction.

**FIELD: Otorhinolaryngology, Medicine, Research & Experimental**  
**A GRANULATION TISSUE WITH A SPECIFIC TRANSCRIPTOMIC SIGNATURE**  
*Laryngoscope*, IF=2.442

Jovanovic I, Zivkovic M, Djuric T, Stojkovic L, Jesic S, Stankovic A. Perimatrix of middle ear cholesteatoma. *Laryngoscope*. 2019 May 27. doi: 10.1002/lary.28084

The cholesteatoma is a clinically important complication of chronic otitis media. The presence of cholesteatoma leads to progressive erosion of the bones and can result in permanent hearing loss, vestibular dysfunction and even fatal intracranial complications. However, surgical removal is the only possible approach because the mechanism of onset is unclear and therefore non-invasive methods of treatment and prophylaxis are not available yet.

**FIELD: Genetics & Heredity**  
**THE CAFA CHALLENGE REPORTS IMPROVED PROTEIN FUNCTION PREDICTION AND NEW FUNCTIONAL ANNOTATIONS FOR HUNDREDS OF GENES THROUGH EXPERIMENTAL SCREENS**  
*Genome Biology*, IF=14.028

(international consortia)

Zhou N, Jiang Y, Bergquist TR, Lee AJ, Kacsóh BZ, Crocker AW, et al.. *Genome Biol*. 2019 Nov 19;20(1):244.

Zhou et al. encompass Laboratory's research within international consortia, which are focused on the protein function annotation and annotation of intrinsically disordered proteins.

**FIELD: Mathematical & Computational Biology**  
**DINGO: STANDALONE APPLICATION FOR GENE ONTOLOGY AND HUMAN PHENOTYPE ONTOLOGY TERM ENRICHMENT ANALYSIS**  
*Bioinformatics*, IF=4.531

Davidović R, Perovic V, Gemovic B, Veljkovic N.. *Bioinformatics*. 2019 Nov 8. pii: btz836.

Davidović et al. describes an enrichment analysis tool, DiNGO, which was developed in the Laboratory for Bioinformatics and Computational Chemistry. DiNGO, an application based on

Gene Ontology and Human Phenotype Ontology, is developed for fast processing of large datasets and it outperforms state-of-the-art tools in the field

**FIELD: Radiology & Nuclear Medicine**

**BIOLOGICAL OUTCOMES OF  $\gamma$ -RADIATION INDUCED DNA DAMAGES IN BREAST AND LUNG CANCER CELLS PRETREATED WITH FREE RADICAL SCAVENGERS**

*International Journal of Radiation Biology, IF=2.226*

Petković VD, Keta OD, Vidosavljević MZ, Incerti S, Ristić Fira AM, Petrović IM. Int J Radiat Biol. 2019 Mar; 95(3):274-285.

Investigation of effects on DNA of  $\gamma$ -irradiated human cancer cells pretreated with free radical scavengers is aimed to create reference data which would enable assessment of the relative efficiency of high linear energy transfer (LET) radiations used in hadron therapy, i.e. protons and carbon ions.

MCF-7 breast and HTB177 lung cancer cells are irradiated with  $\gamma$ -rays. To minimize indirect effects of irradiation, dimethyl sulfoxide (DMSO) or glycerol are applied as free radical scavengers. Biological response to irradiation is evaluated through clonogenic cell survival, immunocytochemical and cell cycle analysis, as well as expression of proteins involved in DNA damage response.

Examined cell lines reveal similar level of radioresistance. Application of scavengers leads to the rise of cell survival and decreases the number of DNA double strand breaks in irradiated cells. Differences in cell cycle and protein expression between the two cell lines are probably caused by different DNA damage repair mechanisms that are activated.

The obtained results show that DMSO and glycerol have good scavenging capacity, and may be used to minimize DNA damage induced by free radicals. Therefore, they will be used as the reference for comparison with high LET irradiations, as well as good experimental data suitable for validation of numerical simulations.

**FIELD: Environmental Sciences, Toxicology, Public, Environmental & Occupational Health**

**PHYSICO-CHEMICAL CHARACTERIZATION OF CARBONIZED APRICOT KERNEL SHELL AS PRECURSOR FOR ACTIVATED CARBON PREPARATION IN CLEAN TECHNOLOGY UTILIZATION**

*Journal of Cleaner Production, IF=6.395*

Bojan Janković, Nebojša Manić, Vladimir Dodevski, Ivana Radović, Milena Pijović, Đurica Katnić, Gvozden Tasić. *Journal of Cleaner Production*. Volume 238, 2019, pp. 111-128.

This paper investigates the ability of waste apricot (*Prunus armeniaca*) kernel shells (AKS) bio-char prepared by single-step carbonization process at 850 °C (residence time of 1 h) for possible removal of toxic elements and organic micro-pollutants. The experiment that was performed as well as parameters used proved to be optimal for bio-char production as adsorbing medium, where last issue is validated by multiform material characterization techniques. It has been shown that the produced bio-char possess highly-porous morphology features, with large specific surface area (328.570 m<sup>2</sup> g<sup>-1</sup>). The obtained product was characterized by various pore sizes (including super-micropores and mesopores with maximum pore size of 2.24 nm) structures. Preliminary results are indicated that obtained bio-char can shows increased affinity to possible adsorption of the small organic molecule contaminants upgraded by its physico-chemical properties. Cost estimation of AKS bio-char production substantiated its cost effectiveness and its good physical and chemical properties for future design in batch adsorption and regeneration tests. It was established that AKS produced bio-char was 2.5 times cheaper than the commercially available activated carbon. Bio-char exhibits promising removal performances for potential adsorption of heavy metal and organic micro-pollutants from wastewaters systems, as indicated by material textures and spectroscopy measurements.

**NON-THERMAL PLASMA NEEDLE AS AN EFFECTIVE TOOL IN DIMETHOATE REMOVAL FROM WATER**

*Journal of Environmental Management, IF=4.865*

Tatjana Mitrović, Saša Lazović, Branislav Nastasijević, Igor A. Pašti, Vesna Vasić, Tamara Lazarević-Pašti. *Journal of Environmental Management* 246 (2019) 63–70.

Intensive use of pesticides requires innovative approaches for their removal from the environment. Here we report the method for degradation of dimethoate in water using non-thermal plasma needle and analyze kinetics of dimethoate removal and possible degradation pathways. The effects of dimethoate initial concentration, plasma treatment time, Argon flow rate and the presence of radical promoters on the effectiveness of proposed method are evaluated. With argon flow rate of 0.5 slm (standard litres per minute) 1×10<sup>-4</sup>M dimethoate can be removed within 30 min of treatment. Using UPLC analysis it was confirmed that one of the decomposition products is dimethoate oxo-analogue omethoate, which is in fact more toxic than dimethoate. However, the overall toxicity of contaminated water was reduced upon the treatment. The addition of H<sub>2</sub>O<sub>2</sub> as a free radical promoter enhances dimethoate removal, while K<sub>2</sub>S<sub>2</sub>O<sub>8</sub> results with selective conversion to omethoate. Using mass spectrometry in combination with the theoretical calculations, possible degradation pathways were proposed. The feasibility

of the proposed method for dimethoate degradation in real water samples is confirmed. The proposed method is demonstrated as a highly effective approach for dimethoate removal without significant accumulation of undesirable toxic products and secondary waste.

**CADMIUM RETENTION AND DISTRIBUTION IN CONTAMINATED SOIL: EFFECTS AND INTERACTIONS OF SOIL PROPERTIES, CONTAMINATION LEVEL, AGING TIME AND IN SITU IMMOBILIZATION AGENTS**

*Ecotoxicology and Environmental Safety, IF=4.527*

J. Marković, M. Jović, I. Smičiklas, M. Šljivić-Ivanović, A. Onjia, K. Trivunac, A. Popović., *Ecotoxicology and Environmental Safety*. 174, 2019, 305-314.

This study aimed to increase the knowledge on the Cd behavior in the soil by investigating complex interdependence between the factors affecting its retention and mobility, as well as to test and compare the performance of the Cd stabilization agents in different soil types. The soil capacity for Cd accumulation was found positively correlated with soil pH and the cation exchange capacity (CEC). With the increase of the contamination level, the highest increase of Cd amounts was detected in the exchangeable fraction regardless of the soil properties, signifying that added Cd is principally associated with the readily accessible and mobile fraction. Prolonged aging times influenced the natural stabilization of Cd in all types of soil, but only at a low contamination level. The application of both conventional and alternative soil amendments resulted in Cd stabilization and reduction of exchangeable Cd content. The relocation of Cd between different soil fractions was significantly dependant on soil and amendment properties. The efficiency of in situ immobilization needs to be monitored for the possible re-mobilization of Cd.

**IN SEARCH OF AN OPTIMAL IN-FIELD CALIBRATION METHOD OF LOW-COST GAS SENSORS FOR AMBIENT AIR POLLUTANTS: COMPARISON OF LINEAR, MULTILINEAR AND ARTIFICIAL NEURAL NETWORK APPROACHES**

*Atmospheric Environment, IF=4.012*

Dušan B.Topalović, Miloš Davidović, Maja Jovanović, Alena Bartonova, Zoran Ristovski, Milena Jovašević-Stojanović. *Atmospheric Environment*, 213, 140-658.

The current compliance networks of automatic air-quality monitoring stations in large urban environments are not sufficient to provide spatial and temporal measurement resolution for realistic assessment of personal exposure to pollutants. Small low-cost sensor platforms with greater mobility and expected lower maintenance costs, are increasingly being used as a supplement to compliance monitoring stations. However, low-cost sensor platforms usually provide data with uncertain precision. To improve the precision, these sensor platforms require in-field calibration. Our paper aims to demonstrate that data from each individual sensor system can be corrected using that sensor system's own data to achieve much improved data quality compared to a reference. However, in this procedure, there are practical difficulties such as individual sensor outputs from the multi-sensor system not being sufficiently available due to malfunctions for instance. We explore how this can be dealt with. In our opinion, this is a novel approach, of practical importance both to users and manufacturers. We present a detailed

comparative analysis of Linear Regression (univariate), Multivariate Linear Regression and Artificial Neural Networks used with a specific aim of calibrating field-deployed low-cost CO and O<sub>3</sub> sensors. For Artificial Neural Network models, the performance of three common training algorithms was compared (Levenberg-Marquardt, Resilient back-propagation and Conjugate Gradient Powell-Beale algorithm). Data for this study were obtained from two campaigns conducted with 25 multi-sensor AQMESH v.3.5 platforms used within the activities of the CITI-SENSE project. The platforms were co-located to reference gas monitors at the Automatic Monitoring Station Stari Grad, in Belgrade, Serbia. This paper demonstrates that Multivariate Linear Regression and Artificial Neural Network calibration models can improve the output signal. This improvement can be measured by changes in the median and interquartile ranges of statistical parameters used for model evaluation. Artificial Neural Networks showed the best results compared to Linear Regression and Multivariate Linear Regression models. The best predictors for CO, in addition to CO low-cost sensor data, were PM<sub>2.5</sub> and NO<sub>2</sub>, while for O<sub>3</sub>, in addition to O<sub>3</sub> low-cost sensor data, the most suitable input predictors were NO and aH. Based on residual error analysis, we have shown that for CO and O<sub>3</sub>, a certain range of concentrations exists in which calibrated values differ by less than 10% from the reference method results. In addition, it was noted that for all models, CO sensors consistently showed lower variability between platforms compared to O<sub>3</sub> sensors.

#### **COMPARISON OF FINE PARTICULATE MATTER LEVEL, CHEMICAL CONTENT AND OXIDATIVE POTENTIAL DERIVED FROM TWO DISSIMILAR URBAN ENVIRONMENTS**

*Science of The Total Environment, IF=5.589*

Maja V.Jovanović, Jasmina Savić, Renata Kovačević, Viša Tasić, Žaklina Todorović, Svetlana Stevanović, Dragan Manojlović, Milena Jovašević-Stojanović. *Science of The Total Environment*. In Press, <https://doi.org/10.1016/j.scitotenv.2019.13520>.

Urban airborne particles contain a wide spectrum of components, known to have harmful effects on human health. This study reports a detailed investigation of fine particulate matter (PM<sub>2.5</sub>), chemical content and oxidative potential derived from two different urban environments. During summer and winter, 20-day campaigns were conducted at Belgrade city center (urban-background site – UB) and Bor (urban-industrial site – UI). Using various analytical techniques, carbonaceous compounds, water-soluble inorganic ions, major and trace elements were determined, while the oxidative potential of PM<sub>2.5</sub> was estimated by dichloro-dihydro-fluorescein diacetate (DCFH-DA) assay (OPDCFH values). The mean PM<sub>2.5</sub> concentrations in both urban environments were above the recommended daily value, and the dominant PM<sub>2.5</sub> mass contributor was organic matter (29–55%). The OC/EC ratio was significantly higher at UB site during winter, which was an indication of a considerable contribution of secondary organic carbon to the overall organic carbon (OC). Water-soluble organic carbon (WSOC) was also higher at UB than at UI site, and it probably came from the same sources as OC. In general, the different partition of secondary organic aerosol (SOA) in warm and cold periods affected the number of organic components. Sulfates and nitrates were the most abundant ions at both sites and they counted approximately 40% (summer) and 50% (winter) of total ions. Further, the concentrations of the most elements, particularly some potentially carcinogenic elements such as As, Cd and Pb were significantly higher at UI, due to the emissions from the copper smelter

complex in the vicinity. The mean OPDCFH values were similar during the summer at both sampling sites, whereas a statistically significant difference between sites was noticed in favor of UB environment in winter.

## **MEASUREMENTS OF OXIDATIVE POTENTIAL OF PARTICULATE MATTER AT BELGRADE TUNNEL; COMPARISON OF BPEANIT, DTT AND DCFH ASSAYS**

*Int J Environ Res Public Health*, **IF=2.468**

Maja V. Jovanovic , Jasmina Z. Savic , Farhad Salimi, Svetlana Stevanovic, Reece A. Brown, Milena Jovasevic-Stojanovic, Dragan Manojlovic, Alena Bartonova, Steven Bottle, Zoran D. Ristovski. 2019., *Int J Environ Res Public Health*. 16, 24, 4906. <https://doi.org/10.3390/ijerph16244906>.

To estimate the oxidative potential (OP) of particulate matter (PM), two commonly used cell-free, molecular probes were applied: dithiothreitol (DTT) and dichloro-dihydro-fluorescein diacetate (DCFH-DA), and their performance was compared with 9,10-bis (phenylethynyl) anthracene-nitroxide (BPEAnit). To the best of our knowledge, this is the first study in which the performance of the DTT and DCFH has been compared with the BPEAnit probe. The average concentrations of PM, organic carbon (OC) and elemental carbon (EC) for fine (PM<sub>2.5</sub>) and coarse (PM<sub>10</sub>) particles were determined. The results were  $44.8 \pm 13.7$ ,  $9.8 \pm 5.1$  and  $9.3 \pm 4.8$   $\mu\text{g}\cdot\text{m}^{-3}$  for PM<sub>2.5</sub> and  $75.5 \pm 25.1$ ,  $16.3 \pm 8.7$  and  $11.8 \pm 5.3$   $\mu\text{g}\cdot\text{m}^{-3}$  for PM<sub>10</sub>, respectively, for PM, OC and EC. The water-soluble organic carbon (WSOC) fraction accounted for  $42 \pm 14\%$  and  $28 \pm 9\%$  of organic carbon in PM<sub>2.5</sub> and PM<sub>10</sub>, respectively. The average volume normalized OP values for the three assays depended on both the sampling periods and the PM fractions. The OPBPEAnit had its peak at 2 p.m.; in the afternoon, it was three times higher compared to the morning and late afternoon values. The DCFH and BPEAnit results were correlated ( $r = 0.64$ ), while there was no good agreement between the BPEAnit and the DTT ( $r = 0.14$ ). The total organic content of PM does not necessarily represent oxidative capacity and it shows varying correlation with the OP. With respect to the two PM fractions studied, the OP was mostly associated with smaller particles.



**FIELD: Soil Science**

**INTERACTIONS OF ACIDIC SOIL NEAR COPPER MINING AND SMELTING COMPLEX AND WASTE-DERIVED ALKALINE ADDITIVES**

*Geoderma*, *IF=4.336*

Marija Egerić, Ivana Smičiklas, Biljana Dojčinović, Biljana Sikirić, Mihajlo Jović, Marija Šljivić-Ivanović, Dragan Čakmak. *Geoderma*, 352, (2019) 241-250.

Acidification of soil near mining and smelting complexes and the contamination with heavy metals are the issues that can be solved by liming. In this study, alternative alkalizers, waste seashells (SW) and red mud (RM) were applied in different doses to the acidic soil sampled in the vicinity of copper mining and smelting complex near Bor, Serbia. Effects of interactions between the acidic soil and waste-derived additives were evaluated. Low dose of waste seashells caused the increase in soil pH and reduction of Cu and trace metals mobility, while moderate use of red mud had the same effect onto pH and metal mobility in addition of the increase in soil phosphorus supply.

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Replacement of natural limestone with alternative soil alkalizers found among waste materials represents a step towards sustainable resource management and reduced waste storage. In this study, carbonate-rich waste seashells (SW) and oxide-based red mud (RM) were applied in different doses to improve the agrochemical properties of the soil sampled in the vicinity of mining and smelting complex. The soil was characterized by the acidic reaction, increased Cu concentration, and a very low level of P-supply. The study aimed to quantify and compare additive-induced effects onto soil physicochemical properties, the status of macronutrients, and the distribution of trace metals in various soil fractions. The results emphasize low amounts of contained trace elements and lower doses for achieving targeted effects on pH and metal mobility as the main benefits of SW treatments. Moderate and controlled use of RM provoked simultaneous pH regulation, P-supply, and reduced trace metals mobility, while higher doses of RM adversely affect soil properties by increasing its salinity and the total concentration of trace elements.