POSTERS

Abstracts

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Seunghun Hyun et al., J Org Inorg Chem 2019, Volume: 5
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REMOBILIZATION POTENTIAL OF METALLIC ELEMENTS (CU, ZN, AS, CD, AND PB) FROM AMENDED MINE SOIL UNDER UNSTEADY-STATE SEEPAGE CONDITIONS

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Remobilization potential of several metallic elements (Cu, Zn, As, Cd, and Pb) from mine soils amended with three stabilization materials (mine sludge, steal slag, and limestone) was evaluated by consecutive batch leaching, sequential extraction, and 1-D seepage flow experiments. Metallic elements were effectively immobilized by amendments treatment for one month, as proved by the decrement (10.6–92.7%) of the labile fraction compared to non-amended soil. However, metallic elements were remobilized during 14 consecutive leaching and 400 PV of seepage. In particular, repeated wetting-drying treatments during batch leaching tests and flow interruption events during seepage flow facilitated the remobilization, as demonstrated by increase in elution mass in effluents (gm), leaching rate (*k*, min-1) to seepage water, and labile fraction in soil phase. Mechanism for increased remobilization potential as affected unsteady state soil-water interaction is being investigated

Biography

Seunghun Hyun is a Professor in the Department of Environmental Science and Ecological Engineering at Korea University since 2006. He has received a PhD degree from Purdue University in 2003. He had BS and MS degree from Korea University. His expertise is of contaminant fate/clean-up in (potentially) contaminated sites such as abandoned mines, landfill, etc. His recent research project funded by Korean Government is Assessing Long-Term Fate of Heavy Metal by Understanding Nonequilibrium Characteristics of Natural Attenuation Process.

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Srđanka Tomić et al., J Org Inorg Chem 2019, Volume: 5
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SYNTHESIS AND IMMUNOSTIMULATING ACTIVITY OF NOVEL MANNOSYLATED DESMURAMYL PEPTIDES

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Peptidoglycan fragments of well-defined structures, the best known of which are muramyl peptides, have been extensively studied as possible adjuvants for human and animal vaccines. Muramyl dipeptide (MDP, *N*-acetylmuramyl-L-alanyl-D-isoglutamine) is known as the smallest synthetic adjuvant molecule capable of replacing whole *Mycobacteria* in Freund's adjuvant. Mannose receptors (MR), present on immunocompetent cells (such as macrophages and dendritic cells) are considered to be pattern-recognition receptors biding compounds with mannose, N-acetylglucosamine or fucose as their essential parts. Therefore, they are responsible for the binding, among others, of mannosylated antigens or relevant biologically active molecules containing mannose, thus affecting the immune reactions. Up to now, our research in the field of potential adjuvants was directed towards desmuramyl peptides which contain adamantylglycine and mannosylated adamantylglycine moieties bound to the essential part of MDP, L-Ala-D-*iso*Gln. Here, we present synthesis and biological evaluation of novel mannosylated desmuramyl peptides containing glycolyl linker. Investigation of their immunostimulating activity was conducted *in vivo* in mouse model using ovalbumin as an antigen. Synthesized glycopeptides showed improved immunological activity than previously described mannosylated desmuramyl peptides with (R)-hydroxyisobutyl linker.

Biography

Srđanka Tomić has graduated Chemistry in 1974 at the Faculty of Science, University of Zagreb; PhD in Chemistry was obtained in 1978 at the Department of Chemistry and Biochemistry, Southern Illinois University, USA. She has professional experience as: an Assistant, Faculty of Science, University of Zagreb, (1974/75); Research Assistant, Southern Illinois University (1975-1978); Research Assistant, "Ruđer Bošković" Institute (1978-1984), Zagreb; an Associate Researcher, Institute of Immunology, Zagreb (1984-1993); an Associate Professor (1984-1993) and Full Professor (2003-), Department of Chemistry, Faculty of Science, University of Zagreb. From 1995-2005, she was the Head of the Division of Organic Chemistry and from 2007-2011, the Head of the Department of Chemistry at the Faculty of Science, University of Zagreb. From 2012-2014, she was a Vice Dean for research and graduate studies at the Faculty of Science, University of Zagreb. Major research interests are in the field of Organic Synthesis of Bioactive Compounds. She published over 70 scientific papers.

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HEADSPACE SCREENING OF ALGA COLPOMENIA SINUOSA (MERTENS EX ROTH) DERBÈS & SOLIER, 1851 VOLATILES

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Colpomenia sinuosa (Mertens ex Roth) Derbès & Solier, 1851 is thallus bladder-like, smooth, slick, hollow, crisp, spherical to sac-like, irregularly expanded or somewhat lobed, to 30 cm diameter, 10 cm high. This golden-brown alga belongs to *Scytosiphonaceae* family. The sample was collected in the Adriatic Sea close to Island Vis (43° 03' 47" N, 16° 11' 15" E). Volatiles of fresh *C. sinuosa* were extracted by headspace solid-phase microextraction (HS-SPME) and analysed by gas chromatography and mass spectrometry (GC-MS). In this investigation of alga headspace volatile organic compounds (VOCs), two fibers were used: namely polydimethylsiloxane/ divinylbenzene (PDMS/DVB) and divinylbenzene/carboxene/polydimethylsiloxane (DVB/CAR/PDMS). The major *C. sinuosa* volatile compounds (PDMS/DVB; DVB/CAR/PDMS) were: dictyopterene D (6-[(Z)-1-butenyl]-1,4-cycloheptadiene) (26.7%; 10.9%), Dictyopterene C' (6-Butyl-1,4-cycloheptadiene) (11.4%, 2.7%), dimethyl sulfid (8.4%; 18.3%), tridecanal (5.1%; 6.3%), pentadecanal (5.0%; 2.4%), 1-pentene-3-on (2.2%; 3.4%), octan-1-ol (1.2%; 3.1%), -Ionone (3,8%; 5,8%) and S-methyl thioacetate (-; 3.3 %). Application of headspace solid-phase microextraction enables identification of low-molecular organic compounds. Among those volatiles, biologically active compound can be found such as allelochemicals, defensive compounds, sex attractants or pheromones.

Sample of *Colpomenia sinuosa* collected in the port of Vis

Biography

Marina Zekić has graduated in 2005 at Faculty of Chemistry and Technology, University of Split. She obtained her PhD in 2013 at Faculty of Chemical Engineering and Technology, University of Zagreb. In 2007, she started to work as an Assistant at the Department of Organic Chemistry, Faculty of Chemistry and Technology in Split, where she is currently employed. She was elected as an Assistant Professor in 2017 (Natural Sciences, Field Chemistry). She has published 10 scientific papers cited by Current Contents. She has been involved in realization of three research projects. Currently, she is a Member of Project Bioprospecting of Adriatic Sea. K.K. 01.1.1.01.0002.

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Lu-Yin Lin et al., J Org Inorg Chem 2019, Volume: 5
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SYNTHESIZING NICKEL-BASED TRANSITION BIMETALLIC OXIDE VIA NICKEL PRECURSOR-FREE HYDROTHERMAL REACTION FOR BATTERY SUPER-CAPACITOR HYBRID DEVICES

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The Ni foam can act as the source of nickel ions and current collector for synthesizing Ni-based compounds using a hydrothermal reaction especially in acid condition. Using Ni foam as the Ni^{2+} source can grow materials on the substrate directly and uniformly since nickel ions are released from substrate thoroughly. Nickel-based bimetallic oxides are intensively investigated as battery-type materials for battery supercapacitor hybrid devices (BSHD) because of high electrical conductivities and abundant transition states for inducing multiple redox reactions. In this study, Mo, Mn, Al, and W precursors are simply added in Ni precursor-free acid solution for hydrothermal reaction using nickel foam as source of nickel ions and current collector to synthesize Ni-based bimetallic oxide electrodes for BSHD. The morphology of nickel-based bimetallic oxide prepared with and without incorporating structure-directing agent is also carefully discussed. The highest specific capacitance (C_F) of 1.80 F/cm^2 corresponding to the capacity of 4.54 mAh/cm^2 at 5 mA/cm^2 is attained for nickel molybdenum oxide (Ni-Mo oxide) electrode, while the Ni-Mo oxide-based BSHD shows a potential window of 1.8 V, a C_F value of 223.53 mF/cm^2 corresponding to the capacity of 1.45 mAh/cm^2 at 5 mA/cm^2, the maximum energy density of 4.60 Wh/kg at power density of 0.21 kW/kg, and the C_F retention of 90% after 6000 times charging/discharging process.

Biography

Lu-Yin Lin has completed her PhD from the Department of Chemical Engineering in National Taiwan University, under the Supervision of Professor Kuo-Chuan Ho. Her research is on Dye-sensitized solar cells. She has continued her Postdoctoral studies in Department of Chemistry in UC Berkley University, under the Supervision of Professor Pei-Dong Yang. She is currently an Associate Professor in the Department of Chemical Engineering in National Taipei University of Technology, Taiwan. Her research is focused on Electrochemistry, including energy generation and storage devices. She has published more than 80 SCI journal papers in reputed journals.

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SAXAGLIPTIN REPAIRS RENAL ISCHEMIA/REPERFUSION INJURY: ROLE OF KIM-1/STAT- 3 SIGNALING

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Saxagliptin, a 2009 FDA-approved dipeptidyl peptidase-4 (DPP-4) inhibitor, is currently used to treat type 2 diabetes mellitus either as monotherapy or in combinations; however, its potential role against the renal ischemia/reperfusion (I/R) insult has not been fully studied. Saxagliptin (10 and 30 mg/kg; p.o) was administered after acute renal ischemia (1 hour)/reperfusion (120 hours) at 1, 24, 48, 72, and 96 hours after reperfusion in male Wistar rats. Assessing the renal tissues revealed that saxaglipitin repaired renal damage caused by I/R via a kidney injury molecule-1 (Kim-1)- dependent mechanism. Kim-1, which is a type-1 membrane protein, was able to activate the signal transducer and activator of transcription 3 (STAT3) by phosphorylation at tyrosine 705, and the latter activated hypoxia inducible factor-1 alpha (HIF-1α), and its downstream vascular endothelial growth factor (VEGF). This led to enhancing the neovascularization repair of renal tissue, as well as improving the histological structure of the I/R-damaged renal glomeruli and tubules. Neovascularization involved the formation of new renal blood vessels, either from already existing vasculature, in a process termed angiogenesis, or the *de novo* formation of new vessels, in a process termed vasculogenesis. This may indicate a possible usefulness of clinical application of saxagliptin in renal transplantation surgeries during which I/R injury commonly occurs

Biography

Nada Mohamed Kamel Mohamed is currently working as a Pharmacology and Toxicology Teaching Assistant at the Faculty of Pharmacy, Cairo University. Her Master's degree is based on a study to decrease mortality rates and organ rejection after transplantation surgeries. For this study, she used Wistar rats and renal ischemia/reperfusion model.

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EFFECTS OF THE ANION NATURE OF CATIONIC POLYMETHINE DYES ON PHOTOVOLTAIC AND SPECTRAL-LUMINESCENT PROPERTIES OF THIN-FILM POLYMER PHOTOCONDUCTIVE COMPOSITES

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The aim of this work was to study the effects of the nature of the anion on the photovoltaic properties of film photosemiconducting composites (PCs) with a free surface, based on a photoconductive oligomer and symmetric cationic PDs with various anions. The samples were prepared on the basis of a cooligomer of glycidylcarbazole with butyl glycidyl ether (GCBE) and symmetric cationic polymethines 1–7 as shown in Figure 1. The cooligomer is characterized by hole-type conductivity and has good film forming and optical properties. Dyes 1–7 have the same chromophore (cation) and different anions in their structure: BF4-, $ClO4^-$, PF_6^- Cl^-, Br^-, I^-, $C_6H_4SO_3Me^-$ (Tos^-). The samples were prepared in the form of structures with a free surface of PC films: glass substrate/ITO/PC film, where ITO was a transparent electroconductive layer of In_2O_3:SnO_2. It has been found that the nature of the anion of cationic polymethine dyes in polymer solar cells affects phototovoltage. A study of the spectral and luminescent properties has revealed that polymethines in these samples form contact ion pairs. It has been shown that the photovoltaic properties of structures based on ionic organic dyes are determined not only by the chromophore structure, but also the nature of the counter ion. The key role here is played by the redox properties of the counterion. They are responsible for its ability for photoinduced electron transfer in ion pairs of the dyes, leading to the formation of radical species involved in photoprocesses in solar cells. These features of ionic organic dyes should be taken into consideration in the development of photovoltaic solar energy converters based on such dyes.

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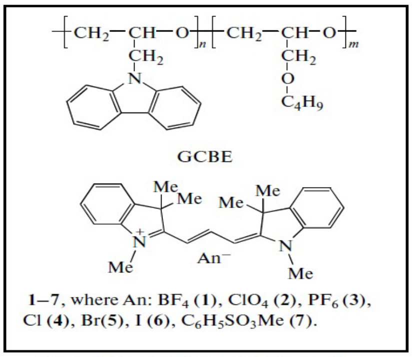

Fig 1. Structural formulas of molecules

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PLANT EXTRACTS AS A GREEN AND SAFE CORROSION INHIBITOR FOR STEEL ALLOY IN AQUEOUS SOLUTIONS

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Corrosion control of mild steel in saline water solution by pomegranate leaf extract (PLE) is investigated at different inhibitor concentration and temperature by using weight loss method. Inhibitor performance is enhanced with decrease of temperature and increases with the raise of inhibitor concentration. Adsorption follows Langmuir adsorption isotherm with negative values of adsorption heat, signifying a stable and spontaneous process of inhibition. Mathematical models were suggested to construct a relationship between the corrosion rate data and independent variables with high correlation coefficients. Quantum chemical parameters of inhibitor were calculated by using the AM1-SCF method to simulate the adsorption of the *PLE* molecules on steel surface.

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L1CAM GENE OVEREXPRESSION IS ASSOCIATED WITH PLATINUM RESISTANCE IN HIGH-RISK ENDOMETRIAL CARCINOMA

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Introduction: L1 cell adhesion molecule (L1CAM) expression has been reported to be associated with high-grade disease and non-endometrioid histology, as well as poor prognosis, in endometrial carcinoma (EC). These high-risk EC types have already spreaded outside the uterus when diagnosed and, after an extensive surgery, are often treated with chemo and radiation therapy. We hypothesized that L1CAM gene expression could discriminate, among poor outcome EC patients, those who do and who do not respond to adjuvant platinum-based chemotherapy.

Experimental Model: Using an efficient multiplex qRT-PCR, we studied L1CAM mRNA expression on 117 EC and 16 normal endometrial (NE) flash-frozen tissues, with HPRT1 and PPIA as reference genes.

Results: L1CAM mRNA was significantly overexpressed in EC compared to NE tissues ($p=0.02$), significantly upregulated in G3 *vs*. G1-2 ECs ($p<0.001$) and in non-endometrioid vs. endometrioid ECs ($p< 0.001$). Our analysis showed no difference in L1CAM expression of stage I-II vs. stage III-IV ECs ($p=0.5$). Of the initial 117 EC patients, 47 received chemotherapy on adjuvant setting and were classified as platinum-sensitive and platinum-resistant patients, based on PFI>12 months and <6 months, respectively. L1CAM gene was significantly overexpressed in resistant vs. sensitive EC ($p=0.001$). Moreover, by means of a multivariate logistic regression model, we found L1CAM gene overexpression as an independent indicator of the probability to harbor a platinum-resistant EC ($p=0.047$, OR=3.5). In addition, univariate and multivariate survival analysis showed L1CAM gene upregulation is associated with poor outcome, in terms of progression-free survival and disease-specific survival.

Conclusions: Our results suggest L1CAM gene expression as a potential prognostic marker and a predictive biomarker of platinum response in high-risk EC patients.

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DRUG SURFACTANT INTERACTION: THERMO-ACOUSTIC INVESTIGATION OF SODIUM DODECYL SULFATE AND ANTIMICROBIAL DRUG (LEVOFLOXACIN) FOR POTENTIAL PHARMACEUTICAL APPLICATION

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At present, the advantages of surfactant micelles as vehicle are taken into consideration and the impact of potential antimicrobial drug (levofloxacin) on micellar system of anionic surfactant (SDS) has been studied. It would therefore be interesting to evaluate the region of micelle formation in order to design such system which could prove valuable in pharmaceutical formulations. In this context, conductance study, critical micelle concentration (CMC), standard thermodynamic parameters of micellization namely, $\Delta H^o_{m,}$ $\Delta G^o_{m,}$ and $\Delta S^o_{m,}$ have been evaluated at four different temperatures (298.15 to 313.15) K. Molar volume and compressibility measurements have also been carried out to evaluate the apparent molar volume and apparent molar adiabatic compression of drug-surfactant complex and discussed in terms of the solute-solute and solute-solvent interactions. In addition, spectroscopic analysis (FTIR and ^{1}H–NMR) confirmed the presence of intermolecular interaction between levofloxacin-SDS moiety within studied concentration. Conclusively, this study provides an indication to assess and develop surfactant immobilized levofloxacin for better biological action.

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COMPARATIVE EVALUATION OF DOMESTIC AND FOREIGN APPROACHES TO THE DEVELOPMENT OF ADVANCED REACTOR TECHNOLOGIES AND THE FUEL CYCLE IN NUCLEAR POWER

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In the development of nuclear energy in Russia and the world, there are three stages, separated by major accidents at nuclear power plants: Three Mile Island (USA, 1979). Chernobyl nuclear power-plant (USSR Ukraine, 1986) and Fokuma-1 nuclear power plant (Japan, 2011). On the first and second stages (with a slight delay in 80's years) and up to 1990, there was a rapid development of nuclear power, when in the year (20's)-30 blocks were introduced and their number increased to 391, with a total capacity 321 W, followed by a sharp decline (after 90's), removing many of the blocks out of operation, reached the maximum term of 40 years. So for the post-Fukushima period from 2011-2016, 24 units were introduced, and 17 withdrawn (5 years added 7 blocks). As a result, on 01.12.2016, the total installed capacity of 450 units was 392 GW. At the same time, the prices for uranium and gas decreased and the latter led to the excess of the competitiveness of gas thermal power plants (PSU with an efficiency of up to 55-60%). The introduction of new technologies began to develop wind and solar power. It is projected that by 2035, the share of elektroprovodka on the "clean" energy sources (hydro, CCGT, nuclear and renewables) will be more than 50%. The share of world electricity production at nuclear power plants fell from 17.6% (1995) to 10.7% (2015). To improve the competitiveness of nuclear power plants required a significant increase in safety while simplifying and reducing the cost of the actual projects, primarily the reactor compartment (nuclear island-NW), the cost of power unit equipment, construction and installation on site, reducing operating costs. The result was developed and have built water cooled reactors "Generation-3+". These are reactors of Westing house (USA) AR-1000, ARR-1400 (Korea), boiling-General Electric (USA) ESBWR-1650, Areva (France) EPR (1600mw), and also in Russia Rosatom-NPP-2006 (1200mw) and VVER-TOI (1250 MW). The paper presents the results of comparing the economic efficiency of these projects. The pace of development of nuclear power has significantly decreased, proven uranium reserves have increased to 5.7 million tons with a cost of less than $130/kg (these reserves with the existing structure of nuclear power will be enough for ~70 years) and up to 7.6 million tons with a cost of less than $260/kg (these reserves are estimated to last for ~120 years), in this case, the need to solve fuel supply problems by implementing a closed fuel cycle (ZTC) in the nuclear power industry may move to ~2050. This report discusses the features of the development of nuclear power, the implementation of ZTC in different countries and mainly in Russia, the stages, timing of their implementation, emerging problems. The use of supercritical pressure water cooled reactors (SCWR) with a fast neutron spectrum in the near future and in systems with ZTC is substantiated.

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METAL ORGANIC FRAMEWORKS AS VERSATILE HETEROGENEOUS CATALYSTS FOR ORGANIC TRANSFORMATIONS

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Metal organic frameworks (MOFs) are porous crystalline materials whose crystal lattice contains metal ions or metal clusters held by rigid, normally aromatic, bi- or multipodal organic linkers. MOFs are increasingly used in heterogeneous catalysisdue to their intrinsic activity derived from the presence of metal ions having coordinatively unsaturated sites or to the substituents at the organic linker, but also because MOFs can host in the pore voids catalytically active guests. One of the important features that make MOFs so appropriate in heterogeneous catalysis is their high porosity and large surface area. This high pore volume makes MOFs particularly suited to incorporate guests that can exhibit catalytic activity, the role of MOFs being as insoluble supports allowing easy recovery of the occluded guests and also providing stabilization of the guest under reaction conditions due to confinement and geometric restrictions. In the present lecture, recent developments of using MOFs as heterogeneous catalysts for organic transformations will be discussed by our group.

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MICROPLASTICS: AN EMERGING THREAT TO GLOBAL OCEANS

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Microplastics [MPs] include microbeads, fibers and fragments of plastics that are <5 mm in size. Mostly they are produced by solar UV-facilitated weathering of plastic litter in the marine environment. MPs are now ubiquitous in bodies of water worldwide. MPs are ingested by a wide range of marine organisms. Over 185 species of birds, 64 species of marine mammals and numerous plankton species are reported to ingest MPs. At some locations as much as 77% of fish sampled had MPs in their gut. Given the high plastic/water distribution coefficient, MPs tend to sorb and persistent organic pollutants (POPs) in sea water effectively. MPs derived from plastic products contain additives such as plasticizers and flame retardants (that include endocrine disruptors), used during manufacture. Ingestion thus provides a credible pathway for delivery of a variety of toxic chemicals into ingesting organisms. Weathering of plastic debris produces nanoplastics [NPs] or microparticles <micron, in addition to the MPs. Recent studies have shown that far more NPs are produced on weathering of plastics compared to MPs. Ingestion of NPs by marine organisms is even more concern because the smaller NPs can cross the gut tissue to enter their systemic circulation. Some evidence of NPs concentrating in specific organs in fish embryo have been reported, potential delivery of sorbed POPs directly to these organs magnifies their potential adverse physiological impacts. The possibility of MPs and NPs reaching the human consumer via seafood is a matter of concern. Whether this low intake of MP/NP *via* seafood is significant enough to result in health hazards is not known at this time. Even in the absence of enough data for a good risk assessment, a precautionary stance to limit the input of plastics into the oceans needs to be seriously considered.

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EVALUATION OF FATIGUE PROPERTIES OF MEDIUM CARBON LOW ALLOY FORGED STEELS QUENCHED IN POLYMER

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Medium carbon low alloy forged steels (EN18, EN19, EN24 and EN25) have been investigated with respect to their fatigue properties for untreated (Forged) and polymer quenched samples. For heat treatment solutionizing temperature of 8550C with a soaking period of 60 min followed by step tempering of 575° and 220° was used. Thereafter quenching was carried out in polymer (polyethylene glycol 10% and 30%) separately. Fatigue tests were carried for untreated and polymer quenched samples; the polymer quenched samples being superior to untreated samples. Simulation of fatigue analysis carried out using ANSYS and corroborated the experimental results for the polymer quenched samples loaded to 30% of UTS; also the specimens quenched in poly ethylene glycol exhibited the best mechanical properties. The heat treated specimens had a structure of fine tempered martensite with small amount of ferrite.

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EFFECT OF SURFACE AND INTERFACES: BAND GAP ENGINEERING TO ACHIEVE HIGH EFFICIENCY FUNCTIONAL MATERIALS AND ITS TUNABILITY

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Controlled thin film coating opens up a promising pathway for band gap engineering and designing the interface mediated defect levels generation, with significant tuneability, which leads to achieving enhanced performance of a given semiconductor in terms of their opto-electronic and electrochemical properties. For e.g., controlled growth of epitaxial graphene (EG) layers on silicon carbide (SiC) provides a novel way of tuning photocatalytic activity and bandgap narrowing in EG/SiC, yielding high efficiency photocatalyst. Results show that the quality and quantity of EG and heterojunction interface layer between EG and SiC, play a crucial role in band gap narrowing, and substantial enhancement of photocatalytic activity in EG/SiC systems. Second example is the atomic layer deposition (ALD) grown ZnO thin films (about 2 nm to 70 nm) on different templates including thin polymeric templates, which formulate a mechanism to achieve significant tunable changes in deep level emission (DLE) of ZnO from green to violet emission range, and in the ratio of DLE to near band edge emission (NBE) from about 0 to 100. The wide range notable variation of photoluminescence and UV-Vis absorption spectra of ZnO are discussed in reference to its potential use as a transparent conducting oxide material and prospective application in ultraviolet light-emitting diodes and solar cell.

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DIRECT EVIDENCE OF VIRAL INFECTION AND MITOCHONDRIAL ALTERATIONS IN THE BRAIN OF FETUSES AT HIGH RISK FOR SCHIZOPHRENIA

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There is increasing evidences that favor the prenatal beginning of schizophrenia. These evidences point toward intra-uterine environmental factors that act specifically during the second pregnancy trimester causing a direct damage to the brain of the fetus. The current available technology doesn't allow observing what is happening at cellular level since the human brain is not exposed to a direct analysis in that stage of the life in subjects at high risk of developing schizophrenia.

Methods: In 1977, we began a direct electron microscopic research of the brain of fetuses at high risk from schizophrenic mothers in order to find differences at cellular level in relation to controls.

Results: In these studies, we have observed the presence of complete and incomplete viral particles within the nuclei of neurons, that reacted in positive form with antibodies to herpes simplex hominis type I [HSV1] virus, and mitochondria alterations .

Conclusion: The importance of these findings can have practical applications in the prevention of the illness keeping in mind its direct relation to the aetiology and physiopathology of schizophrenia. A study of the gametes or the amniotic fluid cells in women at risk of having a schizophrenic offspring is considered. Of being observed the same alterations that those observed previously in the cells of the brain of the studied foetuses, it would intend to these women in risk of having a schizophrenia descendant, previous information of the results, the voluntary medical interruption of the pregnancy or an early anti HSV1 viral treatment as preventive measure of the later development of the illness.

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EFFECT OF CURCUMIN ANALOG (PAC) ON THE DNA REPAIR PATHWAY GENES EXPRESSION IN HUMAN BREAST CELLS

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Background: Breast cancer is a multifactorial disorder with genetic alteration and environmental factors as well as the most commonly diagnosed life-threatening malignancy in females. Moreover, even if there is development in BC treatments till date, there are still limitations in the efficiency of these treatments. To this end, scientists try to revisit tradition medicine, and attention has been drawn to natural products such as curcumin and their analogues due to their anti-cancer effect and their safety. In the present study, we investigated the effect of curcumin analogue 3, 5-Bis (4-hydroxy-3-methoxybenzylidene)-N-methyl-4-piperidone (PAC) on the DNA repair pathway in human breast cancer cells.

Methods: *In vitro* cultures of human MCF-7 and MDA-MB231 were exposed to PAC. Subsequently, DNA repair signalling pathways were evaluated by PCR arrays focused on genes related to DNA repair pathway, and we confirmed the PCR array results by RT-PCR.

Results: Curcumin analogue (PAC) affected the expression of multiple genes involved in the DNA repair pathway in breast cancer cell line. Our results indicate that PAC observed up-regulation of 16 genes in MDA-MB 231, six genes in MCF-7 and ERCC1, PNKP, MPG and RAD54L being upregulated in both MCF-7 and MDA-MB 231 cells.

Conclusion: Our results indicated that PAC significantly up-regulated multiple genes involved in the DNA repair pathway which certainly open new incites in cancer prevention and maintenance of genome stability. We suggest that PAC could use as a complementary treatment for cancer protection by modulation of these genes.

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CHLORONIUM CATIONS AND CARBOCATIONS IN CONDENSED PHASES: STABILIZATION AND PROPERTIES

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The simple chloronium salts with exceptionally stable carborane anion, R2Cl$^+$ ($CHB^{11}Cl_{11}^-$), with R=CH_3 (see Figure), C_2H_5 and $(CH_3)_2CH$ are stable at room temperature and serve as intermediates in obtaining different carbocations. Some chemical properties of chloronium ions in dichloroethane solutions and in the solid salts at room and elevated temperatures (up to 150°C) are reported. Decomposition of chloronium salts resulted in the formation of the high purity carbocation salts. Their detailed IR spectra showed a strong discrepancy with the generally accepted theory of hyperconjugative stabilization of saturated carbocations, based on the modern ab initio calculations. We proposed a refined theory that allowed us to interpret the IR spectra of all carbocations having sp^2 carbon atom in gaseous, liquid, and solid phases. It was proved that CH_3/CH_2 groups of carbocations, which are involved in hyperconjugation, show the stretch and band vibration typical for those of corresponding groups of the neutral alkanes (that is retain their isoelectronic nature) in IR spectra. Hyperconjugation and polarization are equally important and closely linked in stabilization of carbocations: the strengthening of one effect weakens the second and vice versa. We obtained the salts of unsaturated chloronium cations and unsaturated carbocations with conjugated multiple CC bonds, which are stable at ambient conditions for the first time.

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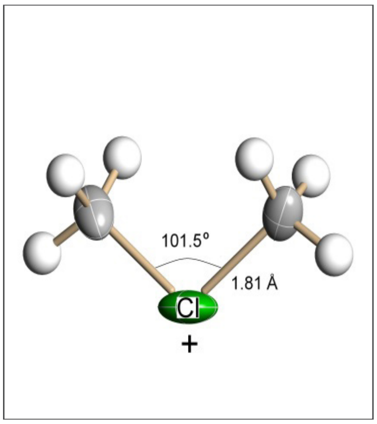

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THE CRUCIAL ROLE OF METAL-OXIDE INTERFACES IN CATALYSIS

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Nanoparticles deposited on an oxide support or nanostructured oxides grown on a metal surface may result in new efficient catalysts. We will discuss in particular the high reactivity of the oxygen atoms at the boundary region between a metal cluster and the oxide surface in CO oxidation, a prototype reaction. Au nanoparticles on TiO_2 and ZrO_2 supports will be used to provide compelling evidence that the reaction occurs at specific sites of the Au/oxide interface and that even a non-reducible oxide such as ZrO_2 can become reducible when interfaced with gold. Also the deposition of oxide ultrathin films on metals may result in completely different properties of deposited metal clusters and recent examples of this effect will be discussed for ultrathin, graphitic-like ZnO layers on Cu, Ag, Au. Controlling the metal/oxide interface is thus essential to design new catalysts with tailored properties.

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DEVELOPMENT AND VALIDATION OF SAMPLING PROCEDURES AND QUANTITATIVE DETERMINATION HPLC METHODS OF ACTIVE PHARMACEUTICAL INGREDIENT-ALPRAZOLAM RESIDUES ON PHARMACEUTICAL TECHNOLOGICAL EQUIPMENT

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The aim of this study was to validate direct swab and indirect rinse sampling procedures and demonstrate the applicability of developed HPLC method for quantitative estimation of residues of active pharmaceutical ingredient-alprazolam residues as a high potent and practically insoluble compound in water in cleaning control samples collected from pharmaceutical equipment surfaces after manufacturing of alprazolam 1 mg uncoated tablets. The swab and rinse sampling procedures were developed in order to obtain a suitable and good recovery (> 90%). The sampling procedures were qualified in respect to the validation parameters. The known amounts of alprazolam at three different concentration levels are spiked onto representative surfaces, which are disinfected and cleaned, then dried, sampled using swabbing and rinsing and analysed using the validated HPLC method. Additionally, the robustness of sampling procedures was assessed. For swab sampling the surface (sampling area-25 cm^2) was successively wiped with one micro polyester swab (3×2.5×10 mm) moistened with diluent methanol. The influence of swab material on quantitative determination of alprazolam was checked as well. The method for quantitative determination of alprazolam residues was developed using LC system Ag 1260 Infinity and Prodigy C8(2) 250×4.0 mm, 5 µm column with a mobile phase: a mixture of methanol, phosphate buffer pH 3.0 and acetonitrile (10:45:45 v/v); the flow rate-1.4 mL/min; the detector wavelength-220 nm; the injection volume-20 µL; the column temperature-300 °C. The method was validated with respect to robustness, system suitability test, specificity, linearity-range, accuracy, precision (intra-day and inter day), limit of detection (LOD) and quantitation (LOQ). The stability of alprazolam sample solutions and 0.45 µm membrane filter compatibility were studied as well. These studies were performed in accordance with established ICH Q2 guideline and USP requirements. The calibration curve is linear (r^2 =1.00000) over a wide concentration range of 0.0075-10 µg/mL; LOQ-0.0075 µg/mL and LOD-0.005 µg/mL. The method can be applied to determine quantitatively alprazolam residues in test solutions with very low concentrations below the acceptable concentration of the cross-contamination limit.

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ASYMMETRIC ORGANOBORANE CONVERSIONS VIA THE AMAZING 9-BORABICYCLO[3.3.2]DECANES

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The stereoselective addition of reagents containing the chiral 10-substituted-9-borabicyclo[3.3.2]decane (BBD) moiety to aldehydes, ketones, aldimines and ketimines will be described. The rigid and robust nature of these systems permits a wide variety of organoborane conversions to not only be conducted in a highly enantioselective manner, but also, it facilitates the recovery of the chiral borane by-product which can be recycled through simple operations. Moreover, numerous chemical conversions can be performed on these organoboranes providing remarkable new reagents for organic synthesis. The origin of the observed selectivities will be presented and discussed in terms of the compact chiral reaction centers provided by the BBD systems.

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ANTIBACTERIAL NAPHTHALENE-BASED AGENTS

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Although naphthalene can be considered as the simplest compound from the group of arenes, it is one of the most interesting arenes. Naphthalene-based drugs include not only clinically used anti-infective chemotherapeutics, but also other agents with significant antimicrobial properties. The naphthalene scaffold can be found in several other therapeutic classes such as antidepressants, nonsteroidal anti-inflammatory drugs, α1-adrenomimetrics, α1-adrenolytics, β1-adrenolytics and peroral anti-diabetics. Thus, it can be stated that this scaffold can be considered as a privileged structure. The naphthalene scaffold can be easily and rapidly functionalized, which provides a possibility of a great number of targeted modifications as well as modification/optimization of physicochemical properties. This contribution is focused especially on the investigation of ring-substituted hydroxyl naphthalene carboxamide derivatives that expressed promising biological activities as antibacterial agents against a number of human pathogens. Structure-activity relationships and the supposed mechanism of action are discussed.

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CANDLELIGHTSTYLE ORGANIC LIGHT-EMITTING DIODE ENABLING BLUE HAZARD FREE LIGHTING

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Intense white light consisting of blue or violet emission might cause damage to human eyes, suppress melatonin-secretion, disrupt circadian rhythm and ecosystems, discolour artifacts, and pollute the night skies. Developing a blue hazard free lighting with high lightquality and energysaving character is highly demanding and challenging. So far, organic light-emitting diodes (OLEDs) have proven to be a great lighting measure that is friendly to human, environments and ecologies with energy-efficient and high-quality character besides being mercuryfree and having extremely high spectrum tailoring capability. In this study, the developed candlelight-style OLED consisting of multiple blackbody-radiation complementary organic emitters, namely sky-blue, green, yellow, and deep-red and provide a very-high spectrum resemblance index with respect to natural light, i.e. >90. Specifically, the resultant OLED showed a low colour temperature (<1,900 K), whose melatonin suppression sensitivity is only 3% relative to that of a 480 nm blue light. Its maximum retina permissible exposure limit is 3,454 seconds at 100 lx, 11, 10 and 6 times longer and safer than the counterparts of a compact fluorescent lamp (5,920 K), light emitting diode (5,500 K) and OLED (5,000 K). Additionally, its high device efficacy and long operation lifetime enable commercialization feasibility. The fabricated candlelight-style OLED can be an ideal lighting measure for indoor as well as outdoor illumination purpose due to its friendly nature to human and ecosystems.

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ALL SOLID THIN FILM BATTERIES

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Li ion batteries (LIB) are extensively used in wide range of electrical and electronic devices such as laptops, desktop computers and mobile phones to most of the electrical vehicles. All solid batteries composed of cathode, anode and electrolyte in solid form and has several advantages such as improved safety, absence of leakage related issues, high energy and power density compared to the conventional Li ion batteries having liquid electrolytes. In the present case, feasibility of making epitaxial cathode material thin films (Ex: $LiCoO_2$, Li_2MnO_3 etc…) of different orientations and utilization of the $SrRuO_3$ layer as a bottom electrode for measuring electrochemical properties of cathode films will be presented. In addition to that, growth and evaluation of dielectric properties of Li ionic conducting (Ex: $LiLaTiO_3$) thin films on STO (100) and (111) substrates at different oxygen partial pressures will be demonstrated. Growth and characterization of anode materials for the thin film based all solid batteries started with Li based oxide materials such as $Li_4Ti_5O_{12}$ and $LiTi_2O_4$ will be presented. Possibilities of fabrication of complete all solid thin film battery device will be discussed at the end.

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CLAY BASED COMPOSITE POLYMER COATINGS: FABRICATION, CHARACTERIZATION AND APPLICATION

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Extending the life of any material and preventing the material from deterioration is of primary importance as this is associated with efficiency and economy of product. Protection from damage can be provided by coating the surface of the material. Coatings not only ensure protection but also offers decorative look to the material and endows it with advanced features. Coatings available today are quite expensive and each coating serves a specific purpose that is deemed to be a limitation in field of coating. To overcome this, the authors developed clay based polymer coatings which display exciting features at an economical way and are perfectly environmental friendly. The clay mineral used for the study is halloysite nanotubes (HNTs) which are naturally available and display unique and attractive features. HNTs possess a hollow tubular structure with 1000 nm, longitude length, outer diameter of 50 nm and 15 nm lumen spaces. HNT based polymer coatings are fabricated by ultrasound assisted processes which is a cleaner, greener and efficient method and can be applied to the substrate by simple dip coating method. These coatings were characterized by various techniques to determine its performance. They demonstrated extraordinary mechanical, thermal, hydrophobic, scratch resistance properties, additionally they enhanced solar material protection factor (SMPF) and solar skin protection factor (SSPF). These coatings can be applied to metals to protect them from corrosion, creep, fatigue, wear and tear.

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NOVEL METHODS OF DETECTING OXYGEN AND NITROGEN REACTIVE SPECIES

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Nitric oxide (NO) has been implicated recently in a number of diverse physiological processes, including smooth muscle relaxation, inhibition of platelet adhesion and neurotransmission. Besides these beneficial functions, NO exhibits cytotoxic affect such as inactivating biologically important mitochondrial respiratory enzymes and neutrophil NADPH oxidase. To understand the mechanism by which NO is synthesized by nitric oxide synthase (NOS) in tissues and how NO mediates various physiological responses, it is useful to be able to observe real time NO generation at the site of production. We have shown direct, real-time, in-vivo measurement of nitric oxide (NO) in mice using the water soluble metal chelator complex, N-methyl-D-glucamine dithiocarbamate (MGD), and Fe(II) and the lipophilic reagent, N, N-diethyl-dithiocarbamate (DETC), as monitored by electron paramagnetic resonance (EPR) at L-band. The EPR spectrum from the product [(MGD)2-Fe (II)-NO] or [(DETC)-Fe(II)-NO] was observed noninvasively in lipopolysaccharide (LPS)-treated mice. In-vivo EPR measurements of [(MGD)2-Fe(II)-NO] at several regions in the body (from the head to the tail) indicated that the NO was generated mostly in the upper abdomen near the liver. This was confirmed by ex-vivo EPR measurements on isolated organs where the higher NO levels were detected in the liver and kidney. In the case of [(DETC)-Fe(II)-NO], we were successful in observing relatively high concentrations of NO trapped in excised brain tissue. The spectroscopic results also showed that both the DETC and Fe(II) independently cross the blood brain barrier and combine with NO in the lipid regions of certain parts of the brain. Lastly, the NO-adduct detected in LPS-treated mice brains was not inducible NOS, but probably rather constitutive NOS, since it was not suppressed by the administration, prior to LPS injection, of phenyl N-tert-butyl nitrone (PBN), an inhibitor of the expression of induced nitric oxide synthase (iNOS).

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SULFATED POLYBORATE: A HOMOGENOUS CATALYST FOR VARIES ORGANIC TRANSFORMATION

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The present study describes the application of sulfated polyborate. The development of the green, practical, and convenient catalytic methods for the commercial process of current interest and organic synthesis is valuable. Hence, the sulfated polyborate was prepared from readily available boric acid, as an economic and non-toxic starting material, characterized and effectively applied for various organic transformations. Herein, we report its applicability in the promotion of clean, efficient, environmentally benign, and high yielding rapid reaction procedure using cost-effective and recyclable catalyst is very much desirable for of 3-methyl 4-(hetero)arylisoxazol-5(4H)-ones, 4-substituted-1,5-benzodiazepines, 2,3-dihydroquinazolin -4(1H)-ones and xanthenes and its derivatives. We have developed a rapid, simple, efficient, and environmentally benign one-pot three-component protocol for the synthesis of above reaction with good to excellent yields. The new homogeneous catalyst, sulfated polyborate is simple, highly efficient and recyclable in this protocol. The main advantages of this approach are of solvent free conditions, cheap raw materials, easy workup, non-hazardous and environment-friendly reaction conditions, recyclable catalyst, excellent yields, and short reaction time.

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NUMERICAL EVALUATION OF THE EFFECT OF THE ACTIVATION METHOD AND THE USED ACTIVATOR ON THE DEVELOPMENT OF THE POROUS STRUCTURE OF THE CARBONACEOUS MATERIALS

Mirosław Kwiatkowski and Jagoda Worek
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The work presents numerical evaluation of the effect of the chemical activation method and the used activator on the development of the porous structure of the carbonaceous materials. The computer calculations were carried out based on of the adsorption isotherms of nitrogen. On the basis of the research and analyses, a significant effect of the type of the activating agent used and activation method applied on the formation of the porous structure on the adsorptive properties of the produced adsorbate was observed consequently. The new adsorption models with the unique numerical procedure of the fast multivariate fitting of theoretical models to adsorption isotherms applied in this work prove highly advantageous when compared with popular methods of porous structure description by providing a wider range of information on the analysed porous structure and offering unique possibilities of evaluating reliability of the obtained information on the analysed porous structure.

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POLYMER BLEND ELECTROLYTES FOR EDLC APPLICATIONS

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Polymer blend electrolytes are prepared using two different polymers and an inorganic salt by solution casting technique. The complexation between polymers and salt is confirmed by XRD and FTIR studies. The ionic conductivity increases with respect to salt concentration. The highest ionic conductivity is 4.2x10^{-3} S/cm. Electrical double layer capacitors (EDLCs) are fabricated using the most conducting polymer electrolyte and carbon-based electrodes. The electrochemical performances of fabricated EDLCs are studied through cyclic voltammetry (CV) and galvanostatic charge-discharge studies. EDLC comprising polymer electrolyte shows the specific capacitance of 20.1 F/g with excellent electrochemical stability.

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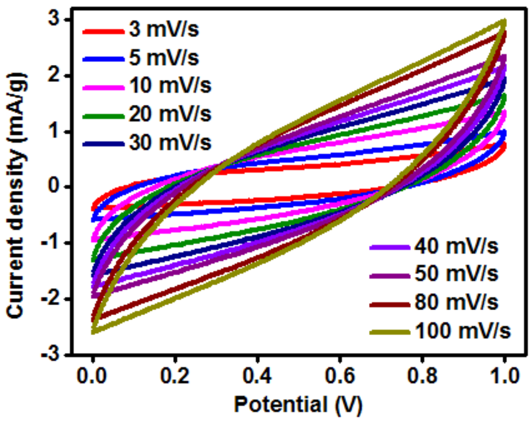

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MULTISCALE POROUS CARBONS: FROM DESIGN TO APPLICATION

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Porous materials displaying a multiscale and interconnected porosity are of critical interest for a wide range of applications involving mass transfer such as heterogeneous catalysis, supported catalysis, adsorption and energy storage. In the last decades, much effort has been given to prepare such materials with porosity on different length scales, so-called hierarchical porous materials, that combine the structural advantages of macropores (i.e. pore diameter ø>50 nm), mesopores (i.e. 2<ø<50 nm) and micropores (i.e. ø<2 nm). While macropores can improve mass transport and accessibility through the whole pore network, micro- and mesopores provide high specific surface area. In our group, we develop various innovative approaches (e.g. emulsion, spinodal decomposition, gelation/drying, solvothermal treatment, silica-based sacrificial template) to synthesize hierarchical porous carbons and composites from lignocellulosic biomass (e.g. saccharides, polysaccharides, lignocellulosic agrowastes). Those approaches allow a fine control over textural and morphological properties and yield porous functional carbons with promising properties as adsorbents, (bio) catalytic supports, electrocatalysts or additives for lithium-ion battery electrodes. Besides textural and morphological control, we are interested in the preparation of monolithic porous carbons. Those monolithic carbons display tuneable macroporosity (from 3 to 40 µm), bimodal mesoporosity and high specific surface area (>1000 m2g-1). They can be integrated in flow through devices for catalysis and adsorption. In particular, flow through biocatalytic reactors were recently developed for the production of formate from carbon dioxide via the co-immobilization of two enzymes within those hierarchical porous carbon monoliths. We could produce four mmol formate per mg of enzyme during three days, which is the highest formate productivity reported to date regarding biocatalytic processes.

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STUDY OF CHARGE CARRIER DYNAMICS IN ANATASE AND RUTILE TIO2: IMPLICATIONS ON PHOTOCATALYTIC WATER SPLITTING

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Understanding of the fundamentals behind charge carrier dynamics of photocatalytic materials is still illusive, hindering progress in our quest for renewable energy. TiO_2 anatase and rutile are the most understood phases in photocatalysis and serve as the best model systems for fundamental studies. The ultrafast charge carrier dynamics, especially on TiO_2 anatase single crystals (the most active phase), are unresolved. The femtosecond time-resolved spectroscopy was carried out to explore the dynamics of photoexcited charge carriers' recombination in the anatase single crystal, for the first time using pump fluence effects, and we compared it to that in the rutile single crystal. A significant difference in charge carrier recombination rates between both crystals is recorded. More specifically, we found that the time constants for carrier recombination are two orders of magnitude slower for anatase (101) when compared to those of rutile (110). Moreover, bulk defects introduced by reduction of the samples via annealing in ultrahigh vacuum resulted in faster recombination rates for both polymorphs. Both states (fresh and reduced) probed by pump fluence dependence measurements revealed that the major recombination channel in fresh and reduced anatase and reduced rutile is first-order Shockley–Read–Hall-mediated. However, for fresh rutile, third-body Auger recombination was observed and attributed to the presence of higher density of intrinsic charge carriers. At all excitation wavelengths and fluence investigated, the anatase (101) single crystal shows longer charge carrier lifetimes when compared to the rutile (110) single crystal. This may explain the superiority of the anatase phase than the rutile phase in M/TiO_2 catalysts for molecular hydrogen production.

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G-C3N4 BASED PHOTO-CATALYSIS FOR SUSTAINABLE FUTURE ENERGY CONSERVATION IN CHEMICAL TRANSFORMATIONS UNDER VISIBLE LIGHT

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Solar energy has been proposed as the most attractive alternative energy source for the development of clean and renewable energy. Heterogeneous photo catalysis offers the capability to directly harvest, convert, and store solar energy in the form of sustainable organic fuels and platform chemicals. In such context, semiconductor photo catalysis has recently emerged as a promising technology for the generation of clean energy and for the application of solar energy in catalysis. Recently g-C_3N_4 is a polymer n-type semiconductor possessing unique electronic, optical, and physiochemical properties, which underpin its use in electronics, catalysis, and energy production/storage. Carbon nitride has attracted the attention of researchers because of its unique and interesting physicochemical properties viz., efficiency of operation under visible light, semiconductor properties (band gap of ~2.7 eV), high stability, nontoxicity, metal free organo catalyst, environmentally benign photo catalysts and simple fabrication from cheap raw materials without any additive. Recently, Prof Yoel Sasson; our research group demonstrated g-C_3N_4 based photo catalysis with enormous possibilities. Few of them are; we describe for the first time a pressure free, mild photochemical protocol for selective reduction of olefin and nitro compounds using a non-hazardous, abundant, and eco-friendly H_2O–Mg pair as a H_2 donor in the presence of a Pd-g-C_3N_4 photo catalyst at RT. The new reaction system is a more expedient and greener protocol compared to earlier studies. In another approach, a novel heterogeneous photoactive catalyst is developed by incorporating ruthenium over a new photoactive g-C_3N_4 support for efficient photocatalytic transfer hydrogenation with significant features of the photoactive catalyst Ru-g-C_3N_4 are viz., it is easy to handle in visible light (LED lamp), does not require an external base, solvent free, non-toxic, environmentally friendly and proceeds under very mild reaction conditions. In my present postdoc (RCPTM), we are exploring the single atom based g-C_3N_4 heterogeneous catalysis.

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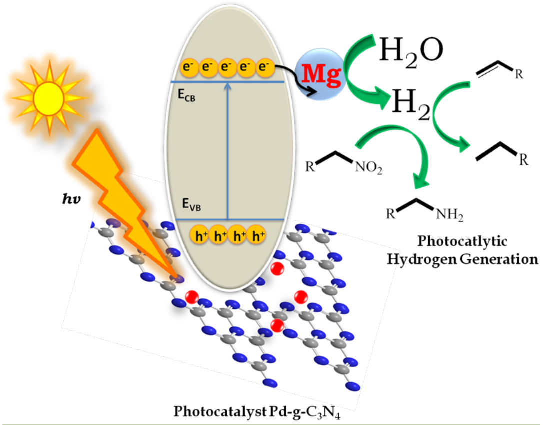

Figure 1: Pd-g-C3N4 photo catalyst for Hydrogen generation

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REDDISH ORANGE LIGHT EMITTING AND THERMAL STABILITY OF THE SM$_2$O$_2$S/SM$_2$O$_2$SO$_4$ PHOSPHORS

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A spectroscopy study of Sm^{3+} phosphors was performed through photoluminescence spectra measurements. The phosphors were prepared from the thermal decomposition of hydrated samarium sulfate to obtain samarium oxysulfide (Sm$_2$O$_2$S) and oxysulfate (Sm$_2$O$_2$SO$_4$). Reddish-orange color emission was monitored from that of oxysulfide phosphor under ultraviolet (UV) excitation at 6H$_{5/2}$—>4I$_{13/2}$ (466 nm) and the photoluminescence emission properties were characterized. The Sm^{3+} oxysulfide/oxysulfate phosphors can be efficiently excited by UV and blue light, and their emission spectrum consists of three important narrow lines: 4G$_{5/2}$—>6H$_{5/2}$ (575 nm), 4G$_{5/2}$—>6H$_{7/2}$ (613 nm), and 4G$_{5/2}$—>6H$_{9/2}$ (658 nm) intraconfigurational transitions respectively. The final thermal stability of oxysulfide/oxysulfate phosphors was investigated systematically by TG/DTG measures. Based on the results, the as prepared Sm$_2$O$_2$S/Sm$_2$O$_2$SO$_4$ materials are promising reddish-orange-emitting phosphors for UV based white light-emitting diodes.

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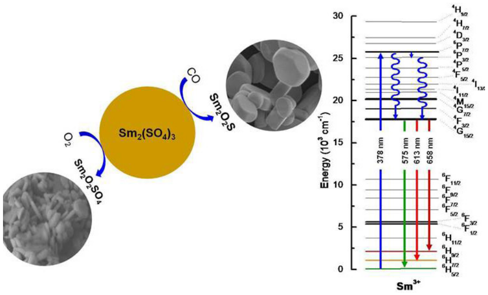

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CIRCULAR ECONOMY BY DESIGN: NIAGA®, AN ABSOLUTE BREAKTHROUGH IN CARPET PRODUCTION AND RECYCLING

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For more than 60 years much of the commercial carpeting has been made the same way. They are composed of a complex array of chemicals, including Latex and PVC, rendering the carpet materials unrecoverable at the end of the products use. Traditionally, when a carpet reaches the end of its life there are two stark choices: bury it or burn it. The consequence is that a large amount of valuable material is lost. The alternative to burying old carpet is to burn it. Most industrial incinerators operate at temperatures of 850° C or higher. Aside from causing huge carbon emissions they can release potentially harmful dioxins, while requiring intensive management and safety procedures. The DSM-Niaga concept involves a rethought of the way we make the products by only using clean materials. The Niaga® Technology for carpet production is based on using a simple set of clean materials enabling 100% recycling in new carpets after use. The glue that holds the whole concept together comes from DSM in the form of an engineered adhesive. It binds the fiber (top) of the carpet and the backing together, replacing latex, which is heavy, takes a lot of energy to cross-link (join with other materials), and makes the carpet prone to stains and burning. The benefits of this new technology comprise full recyclability; reduces water and energy consumption in production; eliminates volatile organic compound (VOC) emissions and improves indoor air quality. Although Niaga® is initially focused on the carpet industry, the technology has intriguing potential. In fact, virtually any product manufactured from man-made materials like polyesters and polyamides from diapers to car mats could employ Niaga Technology. US based company Mohawk, the world's second largest carpet company, is launching the first product based on this technology on the market under the name Airo.

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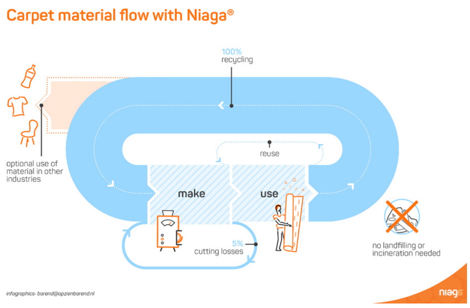

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SYNTHESIS OF ORGANIC MOLECULES AND THE BUILDING BLOCKS FOR LIFE BY LOW ENERGY ELECTRON IRRADIATION OF ASTROPHYSICAL ICES

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Molecular seeds for life on earth were provided *via* meteorite or cometary impacts. Given the fact that both ionizing radiation and matter exist throughout the universe, the existence of this panoply of bio/organic molecules in space suggests that life's building blocks can be synthesized via space-radiation processing of molecular ices in cold regions of the interstellar medium, or on solar system bodies. This radiation processing, or synthesis, can be studied in the laboratory, but to date, most efforts focus on stellar UV radiation, or high energy particles (stellar wind, cosmic rays, etc.). The latter produce abundant low energy electrons (LEEs) below 100 eV in matter, however the role of LEEs in the synthesis of life's building blocks in space has, until recently, been rather assumed than studied. In this thesis, I describe an extended and detailed investigation in which bio-organic molecules, including amino acids, may be formed by LEE in simulated space environments: thin films of differing molecular composition (e.g., O¬$_2$, CH_4, NH_3, and mixtures thereof) are condensed under ultra-high vacuum upon a metallic substrate at ~20 K, and exposed to low energy (0-100 eV) electron irradiation. Multiple in situ surface-analysis methods, namely electron stimulated desorption (ESD) of ions, X-ray photoelectron spectroscopy (XPS), and temperature programmed desorption (TPD), have been employed to investigate the LEE-driven chemistry and to observe the formation of new complex chemical species. Among these, we identify acetylene (C_2H_2), ethane (C_2H_6), propylene (C_3H_6), and ethanol (C_2H_5OH), as well as glycine (NH_2CH_2COOH), the simplest building block of proteins, formed in CH4:CO2:NH3 ices by LEEs down to 9.5eV; still unidentified are molecules containing C_2O_2, C_2O_3, N2, and NO moieties, or CN and HCN subunits, the basic building blocks of adenine. LEEs induce the production of new chemical species containing both C-O and C=O, as well as O-C=O, N-O, N=O, and multiple C-C bonds.

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CONTROLLED SYNTHESIS AND LAYER-NUMBER-DEPENDENT CATALYTIC PROPERTIES OF FEW-LAYERED MOS_2/CDS VAN DER WAALS HETEROSTRUCTURES FOR EFFICIENT PHOTOCATALYTIC H_2 EVOLUTION

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In a typical photocatalytic reaction, efficient solar light harvesting and charge generation, as well as effective charge transport, are key factors that determine the efficiency of the photocatalytic system for H2 production. Atomically layered heterostructures have attracted significant research interest due to their unique layer-dependent catalysis and electronic properties. Previous studies have reported that the catalytic properties of MoS2 layered materials are highly dependent on the number of layers, and the difficulty of controlling the number of layers over a substrate has been a bottleneck for widespread use. Therefore, developing a simple, facile and environmentally friendly method to fabricate van der Waals heterostructures (vdWHs) with precisely controlled MoS2 layers for achieving highly efficient H2 generation is still a challenge. Here, we report for the first time that the H2 bubbles generated by photocatalytic water splitting are effective in the layer-by-layer exfoliation of MoS2 nanocrystals (NCs) into few layers (Figure 1). The as obtained few layers can be *in situ* assembled with CdS nanosheets (NSs) into vdWHs of few-layered MoS2/CdS NSs which, in turn, are effective in charge separation and transfer, leading to enhanced photocatalytic H2 production activity. The few-layered MoS2/CdS vdWHs exhibited a H2 evolution rate of 140 mmol g(CdS)-1 h-1 and achieved an apparent quantum yield of 66% at 420 nm. This study provides a new strategy for the design of noble-metal-free few-layered MoS2/CdS vdWH systems for photocatalytic H2 generation. We believe that this bubble exfoliation strategy can be extended to a range of other layered transition metal dichalcogenide compounds

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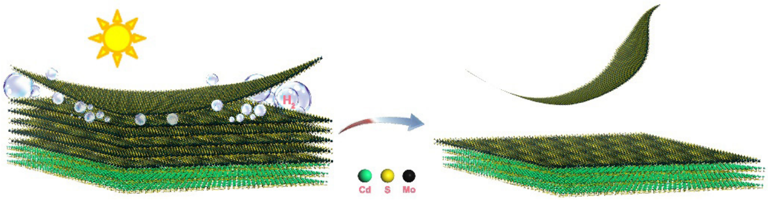

Figure 1: Schematic illustration of the exfoliation of MoS2 nanocrystals and the fabrication of vdWHs of few-layered MoS2/CdS nanosheets by bubble exfoliation

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ELECTROCATALYTIC WATER OXIDATION BY COBALT-CARBONATE

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Water oxidation ($2H_2O \rightarrow O_2+4H^++4e^-$) is a key step in artificial photosynthesis. It has significant importance in biological processes, solar energy conversion and water electrolysis. Herein we present the homogeneous electro-catalytic water oxidation by cobalt-carbonate (Co-C) system. It is shown that cobalt-carbonate acts as an efficient water oxidation catalyst with onset potential of 1.22 V and peak/plateau of 1.36 V vs. Ag/AgCl with a current density of 10.5 mA cm^{-2} at an overpotential of 680 mV. Before catalysis, there appears a $Co^{III/II}$ peak with Epa at around 0.72 V. This peak is electrochemically irreversible and dependent on bicarbonate, carbonate, and metal salt concentrations as well as pH. It follows a proton-coupled electron transfer (PCET) where the CoII is stabilized by mono-dentate bicarbonate and water whereas the CoIII is coordinated to bidentate carbonate ligands. The peak shifts cathodically with increasing metal salt concentration, which means that a dimer is formed after oxidation. The catalyst further undergoes oxidation to form a CoIV=O species which then forms peroxo/percarbonate intermediates followed by the release of oxygen and goes back to its initial state. The catalytic current depends linearly with the metal salt concentration. The Tafel slope is calculated to be 195 mV dec^{-1}. After chronoamperometry at 1.3 V for 3.5 hours, a green solution is formed with a green deposit on the electrode surface. From the absorption spectra (peak at 258 nm), the green compound is found to be $Na3[CoIII(CO_3)_3]$. The same peak is also observed after pulse radiolysis of CoSO4 in NaHCO3. The anodic peak current (id) of CoIII/II peak follows the Randles-Sevcik equation and thus the process is homogeneous and the rate constant (kcat) of catalysis is 100.5 s^{-1}. The rate constant (k0) of the electron transfer for the $Co^{III/II}$ peak is 0.85 x 10-3 cm s^{-1}.

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CHEMISTRY OF VOLATILE OXYGEN-BEARING COMPOUNDS FORMED BY U, NP, PU, AM AND CM

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Tracer-scale chemistry has some distinguishing characteristics which makes it differ from common (macro) chemistry. For example, the common redox and self-redox reactions 2Pu(IV)+U(IV)—>2Pu(III)+U(VI) and 2U(V)—>U(VI)+U(IV) that do not occur in extremely diluted solutions as collisions between micro components are practically excluded. Considerable differences in the chemical behaviour micro- and macro quantities of some actinides in the gaseous phase had also been observed. The initial sample contains a tracer quantity of the actinide under study that was adsorbed on the surface of quartz powder. The experiments were carried out using open quartz thermochromatographic (TC) columns (id=3 mm); oxygen served as a reagent and helium was a carrier gas; the flow rate of the gas mixture was 20 cm^3 min^{-1}; the initial sample was heated in a gas stream at 700-750 ˚C and the final temperature was –165 ˚C; the temperature gradient was –18 ˚C cm^{-1}; the duration of each experiment was 30 min. It was found that uranium formed volatile dioxide and trioxide that were adsorbed at 450±25 ˚C and 250±25 ˚C. The values of adsorption enthalpy -ΔHao for UO_2 and UO_3 on quartz were 172±6 and 126±6 kJ mol^{-1} respectively. Two plutonium radioisotopes $^{238,239}Pu$ were used in similar experiments. Contrary to the previous results, plutonium formed three oxides. The centres of their deposition zones were registered at 450±30˚C (PuO2), 250±30 ˚C (P_uO_3) and at negative temperature –105±25 ˚C (PuO_4). The values of -ΔHao for these oxides were 175±7, 122±7 and 47±6 kJ mol^{-1} respectively. Results of the TC isolation of neptunium, americium and curium oxides are also presented. In particularly, Cm formed also three oxides: CmO_2, CmO_3 and CmO_4.

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PLASTICIZATION OF CELLULOSE ACETATES AND NITRATES

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Cellulose takes the first place in abundance among all natural polymers. Various cellulose derivatives, in particular, cellulose acetates (CA) and cellulose nitrates (CN) are widely used as well. They act as raw materials in the production of smokeless powder, artificial fibres, insulating materials and films, varnishes and other products. However, the above-mentioned cellulose derivatives have high glass transition temperatures (T_g). For CA, T_g lies in the range of 370-490 K, and CN stays glassy up to a temperature of its thermal decomposition. Therefore, in order to provide CA and CN, the required set of physicochemical and mechanical properties modification by plasticization is used. However, there is a noticeable gap between the theoretical (thermodynamic) basis of the plasticization processes and practice in polymer systems production. In order to fill this gap, this review presents data on the thermodynamic characteristics (heat capacity, enthalpy, entropy, and Gibbs function) in the range from 4 to 580 K for CA and CN with various degree of OH–groups substitution of cellulose with acetyl and nitrogroups, as well as the major plasticizers for these polymers, their relaxation temperatures and phase transitions temperatures, the effect of plasticizers on CA and CN properties and the solubility of plasticizers in this polymers. Based on the obtained data, phase diagrams for CA and CN plasticizer systems were plotted and analyzed in a wide temperature range and in the entire concentration range of the components. These diagrams make it possible to determine the temperature and concentration limitations for the formation of homogeneous mixtures, i.e. true solutions of plasticizers in polymers and polymers in plasticizers, as well as two phases' gels, where one of the solutions dispersed in a matrix of another as microdroplets.

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