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Posters

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Inclusion complexes of propiconazole nitrate with substituted β-cyclodextrins II: In vitro assessment of antifungal properties

Irina Roşca¹, Bogdan Minea¹, Dragoș Peptanariu¹, Narcisa Marangoci¹, Adrian Fifere¹ and Mihai Mareș²
¹Petru Poni Institute of Macromolecular Chemistry, Romania
²Ion Ionescu de la Brad University, Romania

Candida albicans infections are an important health issue fuelled, paradoxically, by the advancements in medical care. The prophylactic administration of antifungals generates antifungal resistance and this underlines the need for new antifungal agents. Inclusion complexes of protonated propiconazole nitrate (PCZH-NO₃) with three substituted Cyclodextrin (CD) derivatives, namely sulfobutylether β CD (SBE7 β CD), sulfated β CD (β CD SNa) and monochlorotriazinyl β CD (MCT β CD) were investigated as new antifungal systems. The antifungal activity of the inclusion complexes was assessed on 20 Candida spp. clinical isolates. The in vitro susceptibility testing was performed following the EUCAST EDef 7.2 guideline. To assess the cytotoxicity, the CellTiter 96 aqueous one solution cell proliferation assay was performed on Normal Human Dermal Fibroblasts (NHDF). All complexes showed antifungal activity at low concentrations. The IC₅₀ values were two to three orders of magnitude higher than the concentrations required for antifungal activity. The 95% CIs indicate a significantly higher cytotoxicity for the complex with the parental β CD compared to those with the other three CD derivatives. The much lower concentrations required for the antifungal effect, compared to the IC₅₀ cytotoxicity values, prove a high selectivity of the active compound for the fungal cells. The lack of significant differences in the antifungal susceptibility tests and the differences in cytotoxicity between the β-CD complex and the other three suggest that the type of cyclodextrin may be more important for the interaction with the human organism than it is for the actual antifungal activity.

Biography

Irina Roşca has completed her PhD in Biology at Faculty of Biology from Al I Cuza University, Iasi, Romania and is a Scientific Researcher at Centre of Advanced Research in Bionanconjugates and Biopolymers from Petru Poni Institute of Macromolecular Chemistry. She has published more than 10 papers, she was Principal Investigator in 1 project and worked in another 8 projects related to biotechnology, microbiology and ecology.

Notes:
Inclusion complexes of propiconazole nitrate with substituted β-cyclodextrins: Synthesis, characterization and in silico assessment

Narcisa Laura Marangoci, Bogdan Minea, Alina Nicolescu, Andrei Neamtu, Cristian-Dragos Varganici and Irina Rosca
Petru Poni Institute of Macromolecular Chemistry, Romania

Propiconazole is a triazole developed and marketed by Janssen Pharmaceutics (Belgium) as an antifungal pesticide. Protonated propiconazole nitrate (PCZH NO3), a derivative of propiconazole, was proved to have a better antifungal activity and lower acute toxicity, comparable to those of commercial azole drugs, which makes it a good candidate for clinical use. As most clinical azoles, PCZH NO3 has the major inconvenient of being hydrophobic, which severely reduces its bioavailability. To address this issue, the formation of a host guest inclusion complex with β Cyclodextrin (β CD) as a host carrier molecule was investigated, with good results. The main purpose of this study is to report the synthesis and characterization of the inclusion complexes formed by PCZH-NO3 with three substituted cycloextrin (CD) derivatives, namely namely sulfobutylether β CD (SBE7 β CD), sulfated β CD (β CD SNa) and monochlorotriazinyl β CD (MCT β CD) and to to investigate them as new antifungal systems. The inclusion complexes were prepared using the freeze-drying method. The structures were confirmed by Nuclear Magnetic Resonance spectroscopy (NMR), Differential Scanning Calorimetry (DSC) and in silico docking and molecular dynamics simulations. This study demonstrates the coexistence of two types of PCZH-NO3 inclusion into the CD cavity. The complexes with SBE7 β CD had the lowest dissociation constant values. Inclusion efficiency was close to 100%. Comparative in silico docking and molecular dynamics simulations were performed. The antifungal activity was assessed on Candida spp. and the cytotoxicity was assessed on Normal Human Dermal Fibroblasts (NHDF).

Biography

Narcisa Laura Marangoci has completed her PhD in Chemistry at the Romanian Academy, and, since 2005, has been a Scientific Researcher at Centre of Advanced Research in Bionanocongjugates and Biopolymers at Petru Poni Institute of Macromolecular Chemistry from Iasi. Her professional experience includs synthesis, characterization and applications of functional polymers, supramolecular compounds, "host-guest" inclusion complexes (25 ISI scientific papers) and also design and implementation of national and international projects.

nmarrangoci@icmpp.ro

Notes:
Silver nanoclusters doped in mordenite zeolite as photocatalysts toward pesticides

Imad A Abu-Yousef and Sofian M Kanan
American University of Sharjah, UAE

Silver-based nanoclusters incorporated into mordenite zeolite were prepared and analyzed using various spectroscopic techniques. In the zeolite hosts, both theoretical and experimental results show the presence of silver nanoclusters with various sizes and environments. Upon increasing the excitation wavelength from 250 to 300 nm, the study indicates that the high energy mode (at 415 nm) was deactivated and the low energy emission mode (at 520 nm) was gradually activated. The catalyzed system increases the photodecomposition of phosmet in comparison with the uncatalyzed system upon irradiation with different UV wavelengths. In addition, the largest catalytic activity was observed upon the irradiation of the catalyzed solution at 302 nm, in which an increase in the decomposition rate by 40 folds was observed. We discovered that the photodecomposition products are similar for all systems but variations in the relative amount of these products were observed at different conditions in which phosphorothionic acid was formed as a major product in both catalyzed systems.

Biography

Imad A Abu-Yousef earned his PhD in Organo-Sulfur Chemistry in 1995 from McGill University (Montreal, Canada). Subsequently, he pursued a Post-doctoral fellowship in Polymer Chemistry at McGill University. His research work was recognized by prestigious institutions that have bestowed awards on him, including the Jordan Higher Education Natural Sciences Award (Jordan, 2010), the National Bank of Sharjah Excellence in Research and Scholarship Award (United Arab Emirates, 2002) and Abdul Hameed Shoman Award for Outstanding Young Chemist Researcher in the Middle East (Jordan, 2000). He published more than 50 papers in reputed international journals and has been serving as an Editorial Board Member of the Journal of Saudi Chemical Society, an Elsevier Published Journal.

iabuyousef@aus.edu

Notes:
Improving PLA properties through the incorporation of electrospun nanofibers based on PVA and cellulose nanowhiskers

Carol López de Dicastillo, Luan Garrido Ayala, Abel Guarda and Maria Jose Galotto
Universidad de Santiago de Chile, Chile

Driven by a growing consciousness for the environment and the need to diminish plastic waste, there is a great interest to develop sustainable and ecofriendly materials with enhanced properties. Among biodegradable polymers, poly (lactic acid), PLA, has attracted the most interest in recent years because it is being produced industrially and it comes from a renewable source. However, in order to be massively used in the food industry, some characteristics must be improved, such as mechanical and barrier properties. Some works have aimed the improvement of these characteristics based on the incorporation of different additives and during last years, the most innovative solution is the reinforcement through nanotechnology, such as the incorporation of organic clay or cellulose nanoparticles (CNW) in its formulation. Regarding the latter technique, the biggest inconvenient is the incorporation of the reinforcing material to the polymeric matrix homogeneously, preventing agglomerations to maximize results. Therefore, the objective of this work was to create a biocomposite based on PLA nanoreinforced with CNW nanoencapsulated with poly (vinyl alcohol), PVOH, through electrospinning technique. First, the optimizations of the electrospinning parameters were studied owing to obtain nanofibers with good appearance, measured by SEM microscopy, high concentration of CNW and minimum amount of PVOH. Thus, it is intended to incorporate homogeneously the CNW in the PLA preventing agglomerations, obtaining a material with better mechanical and barrier properties without altering the advantageous characteristics such as optical properties and biodegradability. Materials were obtained through extrusion and were thermally, morphologically and mechanically characterized.

Biography
Carol Lopez de Dicastillo is currently working as Associate Researcher in the Food Packaging Laboratory, in the Department of Food Technology from the University of Santiago de Chile. Her undergraduate background is on chemistry, and she has focused her PhD and post doctorate on Food Technology and Materials Science. Her PhD was carried out in the Institute of Agrochemistry and Food Technology (IATA-CSIC) in Valencia and it was based in the development of hydrophilic active materials, mainly focused on antioxidant releasing systems. Nowadays, new topics have joined her work, such as biodegradable polymers, nanotechnology, electrospinning and search for natural compounds from plant extracts.

analopez.dediscastillo@usach.cl
Antimicrobial supercritical impregnation of nanocomposites for food packaging

Maria Jose Galotto, Martinez F, Rojas A, Torres A, Romero J and Guarda A
Santiago de Chile University, Chile

Antimicrobial Active Packaging is one of the most innovative field on food packaging. It involves the incorporation of an active antimicrobial component in the polymer matrix that should be release during the period of time that food is in direct contact with plastic material. Essential oils are one of the most common antimicrobial active components that are included in polymer matrix but as they are volatile extrusion process is a great disadvantage. In the present work, the study of the supercritical operation condition (pressurization and depressurization rate was carried out in order to determine the amount of active compound impregnated and the kinetic release of the active component from the polymer matrix., comparing polymer matrix and nanocomposites. Nanocomposites of LDPE and Cloisite C20A (modified montmorillonite) 2.5 and 5% were extruded and supercritical fluid impregnation was done at different conditions pressure: 12Mpa, impregnation time: 30 and 60 min, depressurization rate: 10 and 1 MPA/min, temperature 40°C. Physico-chemical characterization of impregnated films were analyzed, and the kinetic release of the active component from the polymer matrix comparing traditional polymer matrix and nanocomposites, were analyzed.

Biography
Maria Jose Galotto is a Full Professor and Head of the Food Packaging Laboratory, in the department of Food Technology from the University of Santiago de Chile. Her undergraduate background is on chemistry and food science and technology, and she has focused on food packaging materials. Nowadays she is working on the development of active food packaging materials and nanotechnology.

maria.galotto@usach.cl
Preparation and characterization of chitosan-co-hyaluronic acid cryogels

Tugce Kutlusoy and Nilhan Kayaman Apohan
Marmara University, Turkey

Hydrogels comprised of cross-linked polymer networks that have hydrophilic homopolymer or copolymer and these networks have a high affinity for water because of having hydrophilic groups. Hydrogels can be derived from synthetic and natural polymer. Cryogel is one of the new types of polymeric gel that has a significant potential in biotechnology. Cryogel that have elastic structure is used in tissue engineering applications. Cryogel formation occurs below the freezing point of the solvent; thus, a major portion of the solvent freezes creating interconnected ice crystals, the polymer precursors that have been in liquid unfrozen form are polymerized to have network around the ice crystals. Frozen crystals solvent acts as pore-forming agent. After the polymerization, when frozen reaction mixture is cooled to room temperature, ice crystals melt and obtained network structure that have macroporous polymers. In this project, cryogels of chitosan-hyaluronic acid’s efficiency in tissue engineering applications as scaffold has investigated. Therefore, firstly homopolymers of chitosan and hyaluronic acid cryogels have synthesized separately, then copolymer of chitosan and hyaluronic acid cryogels were prepared to improve mechanical and biomaterial properties, to use as scaffold for tissue engineering and to examine cell compatibility.

Biography
Tugce Kutlusoy has completed her Bachelor’s and Master’s degree from Marmara University. She is a graduate student of Marmara University.
tugce_kutlusoy@hotmail.com

Notes:
Synthesis and characterization of high performance polyimide nanofibers and application on lithium-ion batteries

Emre Aytan, Nilhan Kayaman Apohan and Mustafa Hulusi Ugur
Marmara University Institute of Science, Turkey

Synthesis and characterization of high performance polyimide nanofibers and application on lithium-ion batteries: Polyimide (PI), as one of high-performance engineering polymers, has been widely applied in many advanced technology fields due to their great thermal stability, remarkable mechanical properties, low dielectric constants and inertness to solvent and radiation resistance. Therefore, electrospun PI nanofiber membranes with diverse molecular structures, controllable fiber diameters and membrane thicknesses have been intensively investigated to obtain high-performance and multifunctional composite fiber membranes. Additionally, it shows good affinity with gel electrolytes which contain plasticizing solvents like ethylene and ethyl methyl carbonate. Thus, these solvents can be strongly combined within the polymer chains in network that can largely enhance the electrolyte retention of PI-based battery electrolytes. In this work; a new highly ion conductive plasticized PI-reinforced UV-cured electrolyte membrane has been synthesized. Oxi-4,4'-dianiline (ODA) and 3,3',4,4'-benzophenonetetracarboxylic dianhydride (BTDA) based polyimide fibers were fabricated via electrospinning method and then UV cured with Bisphenol A Ethoxylate Dimethacrylate (BEMA), poly (ethylene glycol) methyl ether methacrylate (PEGMA) and 3-(methacryloyloxy) propyltrimethoxysilane (MEMO) containing formulations. In order to measure electrochemical stability and ionic conductivity for Li batteries, UV cured films doped with lithium hexafluorophosphate (LiPF6). The structural and electrochemical properties of the electrolytes thus obtained were systematically examined by a variety of methods including FTIR, TGA, DSC, EIS, LSV and SEM measurements.

Biography

Emre Aytan has completed his Bachelor's degree from Marmara University and is an MSc student at Marmara University Institute of Science. His thesis is on developing a polyimide fiber electrolyte via electrospining with cooperation of PhD student M H Ugur and his advisor N K Apohan.

emreaytan@hotmail.com
Molecularly imprinted polymer (MIPs) is investigated by different research groups in a varied time. MIPs are preferred because of its resist on a high temperature, extreme pH values and organic solvent. MIPs are prepared by the polymerization of a functional monomer and crosslinker in the presence of target molecule. It is a process which prepared by replicate the target molecules high affinity receptor regions on polymers. After the polymerization, the templates are removed from the polymer, leaving specific recognition sites complementary in size and shape to the template molecule. Thus it can be used as a plastic antibodies which have been produced by molecular imprinting technique and mimics antibodies functions. For this purpose Diphtheria toxin has been chosen as a target molecule. MIP is performed by using classical two phase mini emulsion polymerization technique. After the polymerization, obtained nanoparticles is removed from the target molecule by dialysis membranes. The morphology and size control of the nanoparticles were characterized by Scanning electron microscopy (SEM) and Dynamic Light Scattering (DLS). The nanoparticles have highly monodisperse and regularly spherical shaped, which have an average diameter of about 200-300 nm.

Biography

Merve Yaşar has graduated at Chemistry Department from Marmara University in 2014. She is currently pursuing her Master degree. At the same time, she is pursuing Tubitak project which is 115S224.

merveyasar.my@gmail.com

Notes:
Novel macroporous poly-pickering-HIPE composites for heterogeneous photocatalysis

Elif Yüce¹, Fatma Nur Pınar¹, E Hilal Mert¹, Funda Çira¹ and Peter Krajnc²

¹Yalova University, Turkey
²University of Maribor, Slovenia

In recent years, highly porous polymer composites are attracting considerable interest due to their large surface area, high chemical resistance, permeability properties, and low densities. These materials have numerous applications such as catalysis, filtration, energy exchange, sensors, etc. For this reason, preparation of such materials with different processes is frequently in focus of research. In this study we report novel macroporous composites for heterogeneous photocatalysis applications. With this aim, Pickering-high internal phase emulsions (Pickering-HIPEs) have been used as templates to build hierarchical open porous polymer networks. HIPEs are concentrated emulsions consisting of a high ratio of internal or dispersed phase. In case of, either one or both phases of a HIPE contain monomers, polyHIPEs can be produced. HIPEs are usually stabilised by using relatively high amounts of emulsifying agents against coalescence. However, it is also possible to stabilise a HIPE with the use of nanoparticles. In this case, the resulting emulsion and the final material are classified as Pickering-HIPE and poly-Pickering-HIPE, respectively. Herein, poly-Pickering-HIPEs were prepared using poly(ethylene glycol-co-propylene glycol-co-ethylene glycol) surface modified TiO₂ nanoparticles (TiNPs). For this purpose, TiNPs were synthesised via sol-gel method and the resulting nanoparticles were introduced into the continuous phase consisting of monomers. The structural properties of TiNPs were characterised by using FTIR and XRD. Morphological properties of the resulting poly-Pickering-HIPE composite, on the other hand, were characterized by Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM). Moreover, mechanical properties of the poly-Pickering-HIPE were measured by performing uniaxial compression experiment. The specific surface areas of the TiNPs and poly-Pickering-HIPE were determined from the adsorption/desorption isotherms and calculated by the Brunauer-Emmett-Teller (BET) equation.

Biography
Elif Yüce has completed her Bachelor’s degree from Yalova University Yalova University, Polymer Engineering Department. She is a MSc student at the same Department and is working as a project researcher.

Notes:
Poly-pickering-HIPEs as heterogeneous photocatalysts

Fatma Nur Parın1, Elif Yüce1, E Hilal Mert1, Peter Krajnc2, Nevim San1 and Dila Kaya3

1Yalova University, Turkey
2University of Maribor, Slovenia
3Yildiz Technical University, Turkey

In recent years, the field of heterogeneous photocatalysis has been growing rapidly, as a result of the various developments especially in relation to energy and the environment. In this context, the large band-gap semiconductors are attracting considerable interest in many practical applications such as catalysts, solar cells, dyes, and commercial products ranging from drugs to foods. For industrial applications, high activity, resistance to poisoning and stability for prolonged use at elevated temperatures, mechanical and chemical stability in various conditions are needed. In this respect, TiO2 has been the most preferred material in many fields due to its long-term photo-stability, relative low toxicity, semiconducting and catalytic properties. In this study, we prepared a new kind of macroporous composite having photocatalytic activity, via emulsion templating. With this aim, Pickering-high internal phase emulsions (Pickering-HIPEs) stabilised with surface modified TiO2 nanoparticles (TiNPs) were used as templates. TiNPs were synthesised via sol-gel method by using poly(ethylene glycol-co-propylene glycol-co-ethylene glycol) triblock copolymer. By the polymerisation of the Pickering-emulsion templates poly-Pickering-HIPE/TiO2 composites, having relatively good mechanical properties and thermal stability, were obtained. The photocatalytic activity of poly-Pickering-HIPE/TiO2 composites were determined by investigating the kinetics of the photocatalytic degradation of 4-nitrophenol (4-NP), an environmentally important pollutant, in a constant temperature batch-type photoreactor. The effects of initial pollutant concentration, catalyst concentration and pH value of suspension on the degradation rates of 4-NP have been studied. A kinetic expression, which can be used in the development of large-scale photocatalytic reactor and optimization of experimental conditions, has been obtained.

Biography

Fatma Nur Parın has completed her Bachelor’s degree as high honor student from Yalova University, Polymer Engineering Department. She is a MSc student at the same Department and is working as a project researcher.

nurparin@hotmail.com

Notes:
e-Posters
Simultaneous use of dopant combination during synthesis of polyaniline: An approach towards synergistic improvement in different properties

Subhendu Bhandari\textsuperscript{1,2} and Dipak Khastgir\textsuperscript{2}
\textsuperscript{1}Maharashtra Institute of Technology, India
\textsuperscript{2}Indian Institute of Technology Kharagpur, India

Polyaniline (PAni) is one of the most widely explored intrinsically conducting polymers which is conducting in nature in its partially doped form. The present investigation reveals the synergistic effect of simultaneous use of dopant combinations during synthesis of PAni on its different properties. Individually and dual doped PAni were synthesized via electrochemical and solid state route. Electrochemical synthesis was carried out in polar protic (aqueous) as well as aprotic (dimethyl formamide) solvent using sulfuric acid (H\textsubscript{2}SO\textsubscript{4}) and p-tuluenesulfonic acid (PTSA) as dopants. Solvent-free solid state synthesis of PAni involved the dopants citric acid monohydrate (CA) and camphorsulfonic acid (CSA). For all cases total dopant concentration was maintained at 1M and relative proportion of the dopant concentrations was varied at 1:3, 2:2 and 3:1. Simultaneously dual doped PAni exhibited synergistic improvement in electrical conductivity for all cases. Dopant ratios of [H\textsubscript{2}SO\textsubscript{4}]:[PTSA]=3:1 and [CA]:[CSA]=3:1 resulted in highest extent of synergy for respective synthesis processes. Dopant combination of H\textsubscript{2}SO\textsubscript{4} and PTSA in protic and aprotic polar medium of synthesis exhibited maximum improvement of conductivity by 1.5 and 2.6 fold increase. However, the combination of CA and CSA in solid state synthesis exhibited a maximum of 8 fold increase of conductivity compared to individually doped samples which is even higher in comparison with 4\% (w/w) addition of multiwalled carbon nanotube in CA doped PAni. Synergistic improvement was also observed for different dual doped PAni in supercapacitive behaviour as well as thermal degradation characteristics within certain range of temperature.

Biography

Subhendu Bhandari has completed his PhD from Indian Institute of Technology Kharagpur, India. At present, he is an Assistant Professor in Plastics and Polymer Engineering Department, Maharashtra Institute of Technology, Aurangabad. He has published 9 papers in reputed journals and filed 1 patent.

subhenduonly@gmail.com

Notes:
Cytotoxicity evaluation of a hydroxyapatite-reinforced polymeric resin using human peripheral blood mononuclear cells

Nayeli Camacho1,2, R G Casañas-Pimentel1, E San Martín-Martínez1, J B Rojas-Trigos1, J A Beltrán Fernández2 and G M Urriolagoitia-Calderón2

1Center for Engineering and Industrial Development, Mexico
2National Polytechnic Institute, Mexico

The use of hydroxyapatite-reinforced composite materials in the medical field has considerably increased in recent years because of the high biocompatibility and bioactive properties of this material, especially when it is used in bone replacement applications. It is imperative that new materials are thoroughly analyzed to ensure bio-functionality. This study describes the response of human peripheral blood mononuclear cells (PBMCs), separated from leukocyte packages obtained from healthy donors, in contact with a 90-10 weight % composite manufactured from an isophthalic polyester resin and reinforced with HAp and calcium triphosphate particles. The viability of PBMCs in the presence of this novel composite was evaluated every 24 hours for 5 days using commercial luminescent cell viability assay (Premix WST-1 Cell Proliferation Assay), positive and negative controls were used. PBMCs are part of the immune system and are usually stimulated by antigens and mitogens. Although the viability assessment demonstrated that HAp-reinforced resin does not have a cytotoxic effect on the PBMCs, the high cell proliferation values obtained via ELISA could be due to a mitogenic or antigenic effect of the composite. Because of the elevated cell proliferation, it was needed to confirm that the material was not acting as a mitogen. To do this, yellow tetrazolium MTT (3-(4, 5-dimethylthiazolyl-2)-2, 5-diphenyltetrazolium bromide) assay with the cell line 231 (breast cancer cells) was performed. The viability of this 231 cell line was not affected by the presence of the composite. Based on the results, a pro-inflammatory mediator production assessment should be performed.

Biography

Nayeli Camacho completed her PhD from the University of Texas at El Paso in the USA and Post-doctoral studies from the National Polytechnic Institute, Engineering Department, Mexico City, Mexico. She is a CONACYT Research Fellow working at the Center for Engineering and Industrial Development which is part of a system of research centers managed by the National Council of Science and Technology, CONACYT.

ncamacho@miners.utep.edu

Notes:
Use of organic ionic plastic crystal (OIPC) membranes for selective permeation of CO$_2$ over nitrogen

Jonathan Lane McDonald
Deakin University, Australia

CO$_2$ is a major contributor to anthropogenic climate change. Because it will take decades to replace existing coal-fired power generation infrastructure, post-combustion capture is important to reduce carbon emissions while the transition to more sustainable power generation is underway. At Deakin University, I use organic ionic plastic crystal (OIPC) membranes to separate CO$_2$ from nitrogen. A plastic crystal has multiple solid phases, including a "normal", highly regular crystalline phase. As a plastic crystal is heated, the associated volumetric expansion allows varying degrees of motion or rotation of lattice constituents and functional groups. While this motion is taking place, the long range order of the crystal is preserved. These properties confer high diffusion rates even in solid phases. An OIPC has the same properties, but consists entirely of ions. This makes them non-volatile, more thermally stable, and highly tunable as appropriate ion selection can ideally be done on an application-specific basis. The high diffusion rates and correlation between diffusion rates and the degree of rotation/mobility of the OIPC lattice has been well studied in the context of lithium diffusion through OIPC solid-state electrolytes. In this work, the OIPCs P1224PF$_6$ and C$_2$mpyrBF$_4$ were supported in nanofibrous PVDF and the ideal selectivities for the CO$_2$/N$_2$ gas pair were measured at 35°C. The results were separation factors of 29 and 33, respectively, which are competitive with conventional polymers and supported ionic liquid membranes.

Biography

Jonathan Lane McDonald completed a Bachelor of Science in Chemistry at the University of South Alabama. He then graduated with a Master of Science in Environmental Toxicology from the same school before beginning his PhD in Materials Engineering at Deakin University in Melbourne Australia.

jlmcdona@deakin.edu.au
Accepted Abstracts
Localized electrochemical generation of Cu and Au metallic microstructure on doped-silica surface by SECM
Ahmed Kandory
Université de Franche-Comté, France

Composite materials formed by copper and gold ion nanoclusters embedded in glasses were prepared via the Sol-gel method. A simple and rapid electrochemical preparation of copper and gold metallic particles is proposed using scanning electrochemical microscope (SECM). This method is not expensive and can be performed at mild conditions. The localized generation of copper and gold metallic structures on coating silica matrix has been performed by localized electro reduction of methyl viologen and p-benzoquinon which generate reducing species which in turn diffuse towards the silica matrix and reduced the metal ions. The diameter of working electrode and electrolysis period were the main parameters and which were studied to show the effect on the size of generated dotted metallic micro patterns. The composition of the modified silica films were characterized with X-ray diffraction, SEM, optical microscope and XPS.

ahmed.kandory@univ-fcomte.fr

Metal organic frameworks as reusable materials for organic transformations
Amarajothi Dhakshinamoorthy
Madurai Kamaraj University, India

Metal organic frameworks (MOFs) also called as porous coordination polymers are porous crystalline materials constituted by nodes of metal ions or metal clusters held in place with rigid bi- or polypodal organic linkers, typically aromatic polycarboxylates. MOFs have received considerable attention in recent years as a new class of porous materials with high specific surface area and pore volume. These properties allow them to be one of the promising materials in gas storage for energy applications, as well as in heterogeneous catalysis. One of the additional advantages in MOFs is the ability to control the specific surface area and pore volume by adjusting the size of the ligands during synthesis. As a consequence, these materials have found many interesting applications in heterogeneous catalysis. MOFs also have the qualification of being in the porous solid family as they can be readily recovered and reused without much loss in the catalytic activity depending on the reaction conditions employed. The presentation will begin with a brief introduction of MOFs’ structural characteristics, the role of ligands and various active sites responsible for catalytic reactions. The present lecture will be focussed on the results achieved using MOFs as heterogeneous catalysts in Lewis acid catalysis, aerobic oxidation and others. Further, the results attained with MOFs will be compared with other heterogeneous catalysts like zeolites and homogeneous counterparts. The selected examples will explain how one can conveniently use MOFs as heterogeneous green catalysts in achieving high conversion and selectivity by maintaining their stability. The beneficial advantages of MOFs over other heterogeneous catalysts will also be highlighted.

admguru@gmail.com
Development of an efficient capture resin for sphingolipids by using a chemoselective reaction and a stereochemical analysis method

Ananda Kumar C 1, Siddabasave Gowda B1, Keiko Yamane2, Okamoto Saori2, Atsufumi Nakahashi1, Mostafa A S Hammam2, Tohru Taniguchi2 and Kenji Monde2

1 Visvesvaraya Technological University, India
2 Frontier Research Center for Post-Genome Science and Technology, Japan
3 Hokkaido University, Japan

Sphingolipids comprise a complex range of lipids in which fatty acids are linked via amide bonds to a long-chain base or sphingoid-base backbone. Sphingolipids exist mostly in membranes and involved in a number of cell signaling systems. Sphingosines are a related class of long chain aliphatic compounds possessing two chiral centers which produce four stereoisomers and they are the backbone of more complex sphingolipids, including ceramide, sphingomyelin, cerebrosides and glycosphingolipids. These compounds are expressed on the surface of cell membranes and play an important role in cell-cell interactions, in signal transduction and in anchoring of proteins and also sphingosines are the inhibitors of protein kinase C. Due to their stereochemical interest and biological importance, the analysis methods for sphingosine and sphingolipids are therefore extremely important in drug discovery and as well is in life science. However conventional extraction methods of sphingolipids have been complicated with multistep protocols and no efficient stereochemical analysis method for biological samples has been established. Herein, we presenting an efficient extraction methodology by introducing a new concept called selective capture with catch and release process by chemoselective reaction utilizing glutaraldehyde resin and stereochemical analysis method using chiral HPLC technique.

csanandakumar@gmail.com

Thermal and mechanical properties of porous ceramics

Chaouki Sadik
Hassan II University, Morocco

Production of porous silica-alumina refractory insulating firebricks from mixtures of silica sand and recycled alumina was investigated. Expanded perlite and saw-dust were added to create the pores. Adding of expanded perlite gives more mechanically stronger refractory (FS:36.7 MPa) but less porosity (p:35.8%) compared to the refractory containing sawdust (FS:29.7 MPa; p:45.8%). The latters are characterized by their lower thermal conductivities (0.53 W/mK). Ultrasonic pulse velocity testing was used for non-destructive quantification of thermal shock damage in refractory samples. The formation of cracks decreases the velocity of ultrasonic pulses travelling in the refractory because it depends on the density and elastic properties of the material. The thermal shock resistance shows the ability of the samples to withstand rapid changes in temperature. Various properties, such as nitrogen adsorption and surface area were also examined.

schawki37@gmail.com

Notes:
Application of clay nanoparticles in removal of lead and cadmium from water

David Mutegi Marikah1, Wanyika Harrison1 and Erastus Gatebe2
1Jomo Kenyatta University of Agriculture and Technology, Kenya
2Kenya Industrial Research and Development Institute, Kenya

The importance of water purification especially removal of heavy metals has been emphasized again and again, hence the need to develop water purification materials that are cheap, easily available and efficient. This study involves removal of Lead and Cadmium from water using clay nanoparticles (CNP) through batch process. Clay was acquired locally, purified by treating with H2O2 and NaOH and CNP isolated by sedimentation and centrifugation. The CNP were characterized using FTIR, UV/VIS and XRD where the crystal size was 40.1 nm. CNP had a Lead removal efficiency of 88% at initial concentration of 80 ppm and 94% for Cadmium at initial concentration of 50 ppm. Lead adsorption study data fitted well in Freundlich isotherm with a R2 of 0.9718 while Cadmium data fitted well in Langmuir isotherm with a R2 of 0.9921 and qm (maximum adsorbed capacity) of 400 mg/g. Both data were fitted in Elovich isotherm where Lead had a R2 of 0.9172 and 0.0238 for Cadmium. The free energy of adsorption was calculated using BD, a constant related to free energy and derived from Dubinin –Radushkevish isotherm, where -3.107 kJ/mol for Cadmium and -5.345 kJ/mol for Lead. Finally the data was fitted in Florry-Huggins isotherm to determine surface coverage, where the number of Cadmium ions on the surface of CNP was 2.30 and 0.2 Lead ions on CNP surface. Clay being locally available in large quantities in deposits, can provide a cheap material for removal of Lead and Cadmium in water and isolation of CNP , increases its efficiency as evident by the 88% removal efficiency for Lead and 94% for Cadmium hence would highly recommend use of CNP for Lead and Cadmium removal both at household and large-scale levels.

davidmarikah@gmail.com

Studies on flexible bionanocomposite films composed of carboxymethyl cellulose and nanocellulose for packaging

Debabrata Chakrabarty
University of Calcutta, India

Moderately flexible nanocellulose/carboxymethyl cellulose (CMC) bionanocomposite films were prepared from CMC solution (30 wt.%) containing nanocellulose (NC) (70 wt.%) which was in the form of dispersion by using solvent casting method. Samples of composites where CMC was crosslinked were also investigated. The mechanical properties, thermal stability & barrier properties of the nanocomposite films were studied by tensile testing, TGA, DSC & MVTR characteristics. The crystallinity & morphologies of composites were analyzed with XRD & scanning electron microscopy (SEM). The addition of CMC (minimum quantity of 30 wt.%) to the NC films increased tensile strength and reduced elongation at break of the composite films. The CMC crosslinked with GTMA produced composite films with improved thermal stability as was revealed from DSC & TGA thermograms of linear and crosslinked CMC/NC blends at an identical concentration of NC. The barrier properties of such transparent composite films were improved in terms of MVTR values with respect to CMC in the presence of NC.

chakrabarty_deb@yahoo.com

Notes:
Impact toughness of notched composite material jute/polyester

Djeghader Djamel¹² and Redjel Bachir¹
¹University of Badji Mokhtar, Algeria
²University of Mes Sadiik Ben Yahia, Algeria

In recent years, the use of composite materials reinforced with natural fibers has been the subject of several studies to provide a possible replacement of ceramic reinforced in composite material. They are renewed, recyclable, less abrasive and lightweight. In this study, Impact Charpy tests were carried out on prismatic samples with lateral notches of different depths of a polyester matrix composite material, reinforced with three layers of bidirectional jute fibers corresponding to a rate of 40%. Three distances between supports were tested: 40 mm, 60 mm and 70 mm. The tests were performed in 3 points bending with an impact velocity of 3.85 m/s and a pendulum of 7.5 joules. The Williams method based on the principles of linear elastic fracture mechanics was used to interpret these results and yielded an estimate of the fracture energy and toughness GIC intrinsic parameter of this material from the total energy $U$ dissipated during impact. The impact energy $U$ measurement results according to BDφ for all notched specimens tested for the three distances between support 3 used are characterized by a high dispersion of data points around the linear regression line. This dispersion characteristic of composite materials is a consequence mainly of the heterogeneity of the material in the path of the cracking and of the dispersion of the mechanical test itself. The impact toughness GIC decreases with increasing distance between supports.

djameldjghader@yahoo.fr

Phenomenon of destabilization of the cementite in pearlitic steels and their influence on the development of high levels of mechanical strength

Elena Brandaleze and Mykhaylo Romanyuka
National Technological University, Argentina

In this paper the deformation mechanisms in steels with high carbon content (> 0.8% C) cold drawn studied. Plastic deformation phenomena promote dissolution of cementite in pearlite, achieving high strength and ductility. For this reason, these steels are used in critical applications such as cranes or support cables of suspension bridges. With the aim of studying the stability of iron carbides that impact in increasing the mechanical properties are tested to breaking twist, two wire samples processed under the same conditions. These have different behavior, one suffered fracture flat (normal) and another delaminated fracture. To this end, studies of optical and scanning electron microscopy (SEM) are made. In addition, assays differential thermal analysis (DTA/DSC) and applying thermodynamic simulation FactSage to evaluate the stability of carbides are made. The results show heterogeneity between the central and peripheral zone of both wires and the presence of the phenomenon of curling (curling). Both phenomena are more pronounced in the normal wire, for its greater plasticity. The phenomenon of precipitation of carbides epsilon carbon diffusion-perlite ferrite, interface justifying increased mechanical strength is identified.

mromanyuk@frsn.utn.edu.ar
ebrandaleze@frsn.utn.edu.ar

Notes:
Evaluation of nanocomposites usage for efficiency enhancement in active layer organic light emitting diodes

Hossein Fetanat
University of Tabriz, Iran

Since years, conjugated polymers have received attention as low cost materials in active layer light emitting diodes but low efficiency of these materials made it a problem which should be considered. Recently, metal nanoparticles are used in display device's active layer to increase the efficiency of materials. Metal nanoparticles enhance coupling between the Localized Surface Plasmon Resonance (LSPR) and excitation in emitting material. In this work, we use SILVACO and MATLAB simulators to examine silver nanoparticles. With the control of Surface Plasmon (SP) and the emission wavelength we can find the best absorbance peak location which maximized photoluminescence (PL) intensity, depending on various Ag, Au and Al dot condition. These metal nanoparticles are used in Solar cells and Polymer LEDs for maximizing the coupling between the LSPR.

Influence of the pyrolysis temperature on activated carbon properties and CO2 adsorption

Jacek Mlodzik, U Narkiewicz, A W Morawski, R J Wrobel and B Michalkiewicz
West Pomeranian University of Technology, Poland

Activated Carbons (ACs) are one of the most promising sorbents. Their properties are widely depending on source material. It allows obtaining ACs with high surface area and well developed porous structure. The pyrolysis temperature influence on specific surface area, micropore volume and CO2 adsorption was investigated in this study. The ACs was obtained by technology patented by our team. Liquid molasses was mixed with dry KOH in dry mass ratio 1:1. The mixture was dried at 200°C and then it was grounded, pyrolyzed at 650-850 °C, 1 hour, nitrogen atmosphere) and grounded again. Obtained powder was washed with deionized water, soaked in HCl (5 mol/dm³) and washed again, till filtrate was neutral. Adsorption and desorption of nitrogen at -196oC was provided with Quantochrome apparatus, so as CO2 adsorption at 25°C. Specific surface area was calculated using BET equation (SBET), micropore volume was calculated using DFT method. The highest SBET was obtained in AC pyrolyzed at 800°C (2480 m²/g). Micropore volume percentage in total pore volume was calculated. The highest value (72.5%) was obtained in the case of AC pyrolyzed at 700°C. Micropore volume of AC pyrolyzed at 700°C was 0.609 cm³/g. CO2 adsorption value ranged 1.62-3.39 mmol/g. Those properties confirmed that molasses based ACs are potentially very promising sorbents of CO2.

jacek.mlodzik@zut.edu.pl

Notes:
Effects of $\text{K}_2\text{CO}_3$ modification on development of microporous commercial activated carbon WG12 for $\text{CO}_2$ adsorption

Joanna Srenscek-Nazzal¹, Umut Mutlu¹, Urszula Narkiewicz¹, Antoni W Morawski¹, Rafał Wrobel¹ and Beata Michalkiewicz¹

¹West Pomeranian University of Technology, Poland

Rapidly increasing concentration of $\text{CO}_2$ in the atmosphere has drawn more and more attention in recent years. The adsorption has been considered as an effective technology for $\text{CO}_2$ capture. Activated carbons (ACs) are an outstanding adsorbent and commonly used for adsorption of $\text{CO}_2$. The main purpose of this work was to prepare various ACs from the same precursor at various activation temperatures, investigate both porosity development (surface area, pore volume, micropore volume) and $\text{CO}_2$ adsorption. A commercial AC WG12 (Gryfiskand Sp. z o. o. Poland) was chemically activated with $\text{K}_2\text{CO}_3$ at temperatures ranging from 600 to 850 °C, with a constant mass ratio WG12:$\text{K}_2\text{CO}_3$=1. The micropore volume (and specific surface area) of the resulting ACs varied from 0.42 cm$^3$/g (1128 m$^2$/g) to 0.48 cm$^3$/g (1247 m$^2$/g) depending on the temperature used in the activation process. The AC obtained at temperature of 850°C exhibited the highest specific surface area and micropore volume. The $\text{CO}_2$ adsorption increased with increasing the temperature. The highest adsorption of $\text{CO}_2$ (2.6 mmol g$^{-1}$) was obtained on the AC prepared at the temperature of 850°C.

One-pot synthesis of NiO nanorods- like hierarchical microspheres as electrode material for electrochemical performance

K Kaviyarasu¹, E Manikandan¹², J Kennedy¹³, M Jayachandran⁵, R Lachumananandesiivam⁶, U Umbelino De Gomes⁷ and M Maaza¹²

¹iThemba LABS-National Research Foundation, South Africa
²University of South Africa, South Africa
³Bharath University, India
⁴National Isotope Centre, New Zealand
⁵CSIR-Central Electrochemical Research Institute, India
⁶Federal University of the State of Rio Grande do Norte, Brazil
⁷Universidade Federal do Rio Grande do Norte, Brazil

We report the effect of calcination on the structural and optical properties of nanocrystalline NiO nanoparticles. A novel sol-gel technique was used to prepare the NiO nanorods at room temperature (RT). These were successfully synthesized by virtue of a single source precursor method at mild reaction conditions between nickel nitrate and sodium hydroxide. Composition, structure and morphology of the products were analyzed and characterized by X-ray powder diffraction (XRD). The ultra-violet visible (UV-vis) absorption peaks of NiO exhibited a large blue shift and the luminescent spectra had a strong and broad emission band centered at 328 nm. The intense band gap was also observed, with some spectral tuning, to give a range of absorption energies from 2.60 to 3.41 eV. The various functional groups present in the NiO nanorods were identified by FTIR analysis. High resolution transmission electron microscopy (HRTEM) and the chemical composition of the samples the valence states of elements were determined by X-ray photoelectron spectroscopy (XPS) in detail. The electrochemical response of NiO proved that the nano-nickel has a high level of functionality due to its small size and higher electrochemical activity without any modifications. The above studies demonstrate the potential for the utilization of NiO nanoparticles as a promising material for opto-electronics applications.
Synthesis and characterization of yittrium doped Co nano ferrite for biomedical applications

Ketaki K Patankar
Rajaram College, India

Yittrium doped Co nano ferrites, CoFe$_{2-x}$O$_4$, where $x$ varies as 0.05, 0.1, 0.15 and 0.2 were successfully synthesized using solution combustion route. X-ray diffractogram confirm the Spinel structure formation and neutron diffraction analysis reveals the magnetic structure. The magnetic parameters obtained from VSM, namely coercivity and residual magnetisation were discussed in the light of results obtained from structure analysis. The electrical resistivity measurements confirmed polaron conduction mechanism in these ferrites. The dielectric measurements, and the impedance analysis have shown interesting results and are explained using Koop's theory. Some peculiar results pertaining to loss tangent are explained proposing new models.

Development of air plasma thermal spray coating for thermal barrier coating and oxidation resistance applications on Ni-base super alloys

Khalid Fared Ahmed
Buraydah Colleges, Saudi Arabia

Aerospace gas turbine engines are now designed such that the heat resistant super alloys operate at temperature very close to their melting, so current strategies for performance improvement are centered on thermal barrier coatings. Lower thermal conductivities lead to temperature reductions at the substrate/bond coat interface which slows the rate of the thermally induced failure mechanisms. Alternatively, lower thermal conductivity TBC layers might allow designers to reduce the TBC thickness thereby decreasing the significant centrifugal load that the mass of the TBC imposes on the rotating turbine engine components. One approach to improve TBC system is to optimize the pore morphologies in order to reduce the thermal conductivity while still retaining high in-plane compliance. The second approach to improve TBC system performance is to optimize the surface microstructure, surface densification, phase structures mechanical characteristic, chemical structure, and thermo-physical properties. The main focus of this work is to study the influence of AlPO$_4$ (and laser)-sealed ZrO$_2$-MgO coatings on thermal barrier coating system comprised of zirconia stabilized with magnesia top coat to predict the best improvement of TBC system and to optimize the surface microstructure, surface densification, phase structures, mechanical characteristic, chemical structure, and thermo-physical properties as well as their properties with those obtained using reference techniques. Thermal expansion studies were used to study the high temperature stability of the different coatings (reference and modified coatings) structures. As low thermal conductivity is one of the most important features of TBC, thermal diffusivity and specific heat measurements were carried out. Also the mechanical measurements (e.g., micro-hardness, tensile bond strength, young's modulus), phase analyses using XRD and chemical analysis using Electron Dispersive X-ray (EDX) for elemental analysis in scanning microscopy studies.

Notes:
TEM, EPR, Mossbauer studies on nano (CuxBa1-x)(AlxFe12-x)O19

S Lakshmi Reddy1, T Ravindra Reddy1 and Tamio Endo2
1S V D College, India
2Mie University, Japan

We report the influence of Cu2+/Al3+ substitution and magnetic properties in the nano particles of ferrite of basic composition CuxBa1-x.(AlxFe12-x)O19 (0.0 ≤ x ≤ 1.0) synthesized by solid-state reaction route method. X-ray diffraction (XRD), transmission electron microscopy (TEM), electron paramagnetic resonance (EPR), Mossbauer, VSM, Fourier transformation infrared (FTIR) spectroscopy techniques, and magnetic measurement are used to investigate the structural and magnetic properties of the synthesized nano particles. XRD results confirm that all the samples are single-phase hexagonal in structure. The unit cell parameters “a” and “c” are calculated as from 6.276 to 5.777 Å and 23.195 to 23.00 Å respectively with variation of composition from x= 0.00 to 1.00. The average crystallite size of the synthesized nano particles was calculated through Scherrer formula and confirmed by TEM and was found to be 100 nm. FTIR results show the presence of two vibrational bands corresponding to tetrahedral and octahedral sites. EPR spectra are compositional dependent at lower Al/Cu concentration. EPR spectra are due to Fe³⁺ with x=0 composition and x=1.0 is due to both Fe³⁺ and Cu²⁺. EPR results at room temperature reveals that it is ferromagnetic with composition x=0.0 and with x=1.0 it is paramagnetic. Copper is placed in the tetragonal elongation site with magnetically non-equivalent ions in the unit cell. These do not have strong exchange coupling between them. Nonlinear optical properties of the samples indicate that these ferrites are potential candidates for optical limiting applications. Mossbauer studies are suggesting that the sample is ferromagnetic with composition x=0.0 and with x=1.0 super paramagnetic. These results are supported by ESR and VSM studies. Magnetic properties are characterized by vibration sample magnetometer (VSM). All the magnetic properties are found to decrease with the increase in Al–Cu content, which is due to the occupation of the doped cations at the octahedral sites (12k and 2a) having spin of electrons in upward direction. In addition, the effects of the substituent agents on these properties of the barium ferrite powders are investigated.

drreddy_in@yahoo.com

Effect of oil shale additions on high belite raw mix and clinker

M M Radwan, Laila M Farag and H K Abd El-Hamid
National Research Centre, Egypt

Raw mixes for high belite cement clinker (HBCC) have been designed on basis of chemical analyses of Egyptian raw materials with and without the additions of Egyptian oil shale obtained from Younis Gharb mine located at the Red Sea Coast in the Eastern desert of Egypt (calorific value ~2500 kcal/kg shale). LSF of the mix was maintained at 80%, silica modulus at 2.25 and C3A in the clinker not exceeding 4%. From raw mix design it was found that, with increase of % shale additions the limestone % in the raw mix decreases whereas % secondary compounds, SO3 and P2O5, increase in the clinker. Two raw mixes: One with about 11 wt% oil shale and one without shale as blank were selected for preparation of HBCC in the laboratory. The investigated firing temperatures were 1300 and 1350 oC. Characteristics of the produced high belite clinker, such as chemical composition, X-ray diffraction analysis, scanning electron microscopy besides physico-mechanical properties of its hydrated pastes have been determined and compared with the corresponding values of commercial ordinary Portland cement. It was found that, the most appropriate temperature for firing HBCC raw mixes is 1350oC. Generally, shale additions had slight effect on the physico-mechanical properties of the produced high belite clinker.

mmahmoudradwan@yahoo.com
The use of polymers and biopolymers to make arid and semi-arid land suitable for agriculture

Maghchiche Abdelhak
Batna university, Algeria

The use of polymers as a soil-stabilizer additive has expanded significantly in agricultural use to control soil degradation and desertification and also to improve arid and semi-arid soils. This research was conducted to determine the effects of different synthetic polymers and biopolymers at low concentration (0.03%–1%) at arid and semi-arid soil of North Africa. Polystyrene, polyacrylamide; cellulose and the mixture of polyacrylamide with other polymers were characterized by viscosity, infrared spectroscopy, X-ray Diffraclometry, Thermal Analysis (TG and DSC) and Scanning Electron Micrographs (SEM). The results showed that the polymer composites (10 mg/L polyacrylamide and 0.5 g/L cellulose) in soil could improve better soil physical properties and augment 60% water retention at arid soils compared with application of any other polymer at the same concentration. This work can help to improve the productivity of arid and semi arid soils by using low concentration of biopolymers from plant fibers and polymers from synthetic plastics compounds or wastes plastic industry to augment water holding capacity improve the physical properties of soils by binding soils particles together reducing the losses of water by evaporation and deep percoloration, and to make valuable products of plastic industry and renewable organic fibers to protect environment.

amaghchiche@yahoo.fr

Exploration and development of Perylenebisimides (PBIs) as potential memory units with magnetic signalling

Masood Ayoub Kaloo, Ruchika Mishra and Jeyaraman Sankar
Indian Institute of Science Education and Research, India

Perylenebisimides (PBIs) are highly robust, extensively conjugated organic materials with unique optical and redox properties. Presence of imide functionalities impart PBI a highly electron-deficient nature and hence n-type semiconductivity. The dyes can be reduced to corresponding radical anions, hence potential to store electrical energy. For the first time, we attempted to reduce this dye via interface with anions in organic media (THF, DMSO). A drastic modulation of their absorption and emission properties was noticed in solution (panchromatic UV-Vis-NIR and Quenching). The reduction processes was proposed to be a Single Electron Tranfer (SET) from anion to PBI. SET phenomenon was further facilitated by incorporation of electron-with drawing substituents in bay region. The reduced PBIs were regenerated through specific chemical inputs with high redox-potential like (Zr4+, Fe3+, etc.). The anion/cation executed switching behaviour was fully established through EPR, apart from electrochemistry and spectroscopy (absorption and emission). The stability of EPR active radical state in TLC or colun chromatography, was explored for molecular memory. The reversible and reconfigurable magnetic sequences were visualized in the form of a feedback loop, with EPR active outputs (μα), demonstrating a data storage feature with the “write–read–erase” function. The phenomenon of bi-stable behaviour “magnetic to non magnetic” presented in this study signify a promising asset for futuristic non-volatile memory. In this presentation, design, development, exploration of PBIs as materilas of choice with promising information storage capability will be discussed. In addition to this, their structural tuning and interation with anions will be throughly presented.

masood@iiserb.ac.in
Traffic anomaly detection and DDOS attack recognition using diffusion map technologies

Michael Zheludev and Evgeny Nagradov
Qrator Labs, Russia

Network attacks is becoming a major threat on nations, governmental institutions, critical infrastructures and business organisations. Some attacks are focused on exploiting software vulnerabilities to implement denial of service attacks, damage or steal important data, other use a large number of infected machines to implement denial-of-service attacks. In this paper we are focusing on detecting network attacks by detecting the anomalies in network traffic flow data and anomalous behaviour of the network applications. The goal is to detect the beginning of the attack in a real-time and to detect when the system is returned back to the normal state. In this paper we are not focusing on the problem of identifying the source of the attack and the attack mitigation. The input data for the analyser is statistics matrix that contains a single row for every traffic time slice. Each row contains the network-level and application-level features that come from different scales. This matrix is the input for the intrusion detection processes (both training and detection steps). Our method has two sequential steps. Study and analysis of the behaviour of networking datasets and projection of data onto a lower dimensional space - training step. This is done once and updated as the behaviour of the training set changes. During this step we can handle corrupted training sets. The output from the training step enables online detection of anomalies to which we apply automatic tools that enable real-time detection of problems. Each newly arrived datapoint is classified as normal or abnormal. The traffic analyser processes the network packets and summarises the network-level statistics. These metrics include: tcp flags usage; number of control tcp packets (packets without payload); number of data tcp packets (packets with payload); number of source (client) packets; number of source control packets; number of source data packets; number of source data bytes; number of destination (server) packets; number of destination control packets; number of destination data packets; number of destination data bytes. Challenge: How to process an “ocean” of data in order to find abnormal patterns in the data? How to fuse data from different sources (sensors) to find correlations and anomalies? How to find distances in high-dimensional data? They do not exist. How can we determine whether a point belongs to a cluster/segment or not? The goal is to identify points that deviate from normal behaviour which reside in the cluster/segment. How we treat huge high dimensional data that is dynamically and constantly changes? How can we model the high dimensional data to find deviations from normal behaviour?

qukengue@andex.ru;
mz@qrator.net
en@qrator.net

Conducting polymer electrolytes for fuel cell applications

M Muthuvinayagam
Kalasalingam University, India

The polymer electrolytes composed of poly(vinylidene fluoride) PVdF and poly(vinyl alcohol) PVA with various ratios of ammonium thiocyanate (NH4SCN) salt, have been prepared by solution casting method. The increase in amorphous nature of polymer electrolytes has been confirmed by XRD analysis. The polymers-salt interactions have been analysed by FTIR spectroscopy. The Scanning Electron Micrographs affirm the smooth morphology of the polymer electrolytes. A shift in glass transition temperature (Tg) of the electrolytes has been observed from the DSC thermograms which indicates the interaction between polymers and salt. The conductivity and dielectric measurements were carried out on these films as a function of frequency at various temperatures. From the complex impedance spectroscopy, the conductivity is found to increase in the order of 10-9 -10-3 S/cm at room temperature with the increase in salt concentration. The ionic transference number of the mobile ions has been estimated by Wagner's polarization method and the results revealed that the conducting species were predominantly due to ions.

mmuthuvinayagam@gmail.com
Preparation and evaluation of new uranyl imprinted polymerelectrode sensor for uranyl ion based on uranyl–carboxybezotriazole complex in PVC matrix membrane

Nathir A F Al-Rawashdeh
University of Science and Technology, Jordan

In this study a new uranyl selective electrochemical sensors were prepared by using uranyl ionicimprinted polymer (IIP). The IIP was prepared by thermal polymerization using acrylic acid as a monomer, ethylene glycol dimethacrylate as a cross linking and benzoyl peroxide as an initiator. Uranyl–carboxybenzotriazol (UO2–CBT) complex was used as an active material on the prepared polymer. Several uranyl electrodes were constructed by using different masses of polyvinyl chloride (PVC) matrix. Electrode parameters including slopes, working concentrations, pH, and interferences were evaluated. The electrodes exhibit a Nernstian response with slopes of 23.6 and 28.1 mV/decade for graphite uranylelectrode and liquid uranyl electrode, respectively, over a wide range of concentration from 3 × 10−6 to 6 × 10−2 M and a detection limit of 1 × 10−6 M. It can be used in the pH range of 4.3–10.5 with a responsetime of less than 60 s. The effect of ions interferences on the electrode response were evaluated. The IIP and nonimprinted polymer membranes were char-acterized by Fourier Transform Infrared Spectroscopy and Scanning Electron microscopy. The concentrations of uranyl ion in the prepared synthetic solutions determined by the standard addition method and the results were satisfactory with errors less than 7%. Finally, the prepared graphite UO2-IIP sensor was tested to determine the uranyl ions concentrations in a real environmental water sample by standard addition method. The developed electrode was found to be fast, sensitive and reliable indicated its potential use in measuring the uranyl ion concentration in the field.

nathir@just.edu.jo

Synthesis and applications of kilometers of continuous macroscopic fibres with controlled type of carbon nanotubes

Bartalome Mas, V Reguero and J J Vilatela
IMDEA Materials Institute, Spain

We report on the synthesis of kilometres of continuous macroscopic fibres made up of carbon nanotubes (CNT) of controlled number of layers, ranging from singlewalled to multiwalled, tailored by the addition of sulfur as a catalyst promoter during chemical vapor deposition in the direct fiber spinning process. The progressive transition from single-walled through collapsed double-walled to multiwalled is clearly seen by an upshift in the 2D (G’) band and by other Raman spectra features. The increase in number of CNT layers and inner diameter results in a higher fibre macroscopic linear density and greater reaction yield (up to 9%). Through a combination of multiscale characterization techniques (X-ray photoelectron spectroscopy, organic elemental analysis, high resolution transmission electron microscopy, thermogravimetric analysis, and synchrotron XRD) we establish the composition of the catalyst particles and position in the isothermal section of the C–Fe–S ternary diagram at 1400°C. This helps explain the unusually low proportion of active catalyst particles in the direct spinning process (<0.1%) and the role of S in limiting C diffusion and resulting in catalyst particles not being in thermodynamic equilibrium with solid carbon, therefore producing graphitic edge growth instead of encapsulation. The increase in CNT layers is a consequence of particle coarsening and the ability of larger catalyst particles to accommodate more layers for the same composition. We further present the distribution of CNT chiralities obtained from ED, Raman spectroscopy and Emission spectra and discuss these findings in the context of the current screw dislocation growth model accepted in the field. Finally, we show the application of basic polymer fibre spinning principles to produce highly oriented CNT fibres by reducing entanglements in the gas phase through CNT dilution. The resulting fibres have tensile properties superior to those of Kevlar, high electrical conductivity and a very large surface area. The exploitation of these properties in sensors, supercapacitors and other devices is briefly demonstrated.

bartolome.mas@imdea.org
Polysaccharides are among the polymers that make up the fundamental components of life and constitute a major proportion of the Earth's biomass. Polyelectrolyte complexes (PEC) of polysaccharides (which are responsible for the steric factor of stabilization and increase in viscosity of a continuous phase) with gelatin (which provides the high rate of adsorption) are currently considered as the most perspective stabilizers of the dispersed systems in particular in food industry. A cationic polysaccharide chitosan is widely used as a "matrix" for the formation of (bio)polyelectrolyte complexes due to the attractiveness of its properties such as biocompatibility, biodegradability, low toxicity and relatively low manufacturing cost, due to the existence of rich natural sources of polysaccharide. Macromolecules of chitosan have a high density of positive charge in the acidic environment due to ionization of the free amino groups. Therefore, self-assembly of (bio)PEC occurs in acidic solutions of chitosan in the presence of the negatively charged polyelectrolyte. Gelatin is the product of collagen destruction and has been widely used as a fundamental material for microspheres, sealants, tissue adhesives and carriers for controlled delivery systems. Gelatin has also been widely used in combination with other polymers for encapsulation.

orfeo-ed-euridice@ya.ru

SWCNT glass composite- A novel material for electronic, optical and mechanical applications

Rajat Banerjee
Central Glass and Ceramic Research Institute, India

A new generation composite has been synthesized by impregnating SWCNT in oxide glass matrix using melt-quench technique. Current-Voltage relationship was studied with different temperatures and the electrical conductivity was found to increase significantly with the increase in temperatures. The activation energy of the composite was determined by Arrhenius analysis and found to be significantly low. Microstructural analysis of the composite by SEM, FESEM and TEM clearly shows the random orientations of the bundles of nanotubes throughout the glassy host. TEM micrographs show wonderful alignment of nanotube inside the bundles. The charge transport phenomena of the composite was analyzed by using variable range hopping (VRH) and fluctuation induced tunneling (FIT) model. It was found that the charge conduction through the composite was well explainable by the FIT model. Moreover an interesting optical property of this composite has been observed where one can see strong near infrared fluorescence from Single walled carbon nanotube-borosilicate glass composite around 0.84-2.03 μm with 325 nm laser excitation. Band gap fluorescence of SWCNT bundles along with defect related fluorescence from SiO2 structure were the source of the NIR emissions of the composite. Finally researchers are looking for new class of materials having high mechanical resistance, low density and microwave attenuating properties for different structural applications. All these properties are well established in this composite thereby making it one of the versatile materials for conductor-insulator interface device coupled with broadband fiber optic telecommunications, fabrication of NIR tunable lasers and high end structural application.

rajaatbanerjee@hotmail.com
Synthesis, characterization and catalytic applications of new monodentate N-alkylpyridin-4 (1H)ylidene) amines (PYE) ligands

Sabeen Zahra
University of Gujrat, Pakistan

The present study describes the synthesis, characterization and applications of protonated pyridinium amide (H-PYE) and pyridinium amide (PYE) ligands itself. H-PYE ligands [HL1-HL4] were synthesized by a solid state reaction between 4-chloro-N-methyl pyridinium triflate and corresponding amines at 220°C. PYE ligands [L1-L4] were synthesized by deprotonation of the H-PYE ligands with sodium hydride in dichloromethane solvent. Both H-PYE and PYE ligands were characterized by physical parameters, FT-IR, 1H and 13C NMR and mass spectrometry. The role of pyridinium amide ligands towards Suzuki-Miyaura and Heck-Mizoroki coupling reactions in the presence of Pd(OAc)2 was monitored and achieved remarkable results. The antioxidant activity of synthesized ligands was observed by scavenging method of DPPH radical and ligands exhibited significant activity. The biological activities of synthesized compounds were tested against four bacterial and two fungal strains and results indicated that only [HL4] displayed antibacterial activity with Chromohalobacter israelensis while both H-PYE and PYE showed minor antifungal activity with one of the strain Aspergillus niger. Enzyme inhibition activity of the ligands was performed against two enzymes i.e. acetylcholine esterase and butyrylcholin esterase. The results specified that ligands presented good inhibition. Moreover, the DNA binding studies were achieved by using UV-Visible and fluorescence emission spectroscopy which revealed hypochromic effect indicating intercalation as well as groove mode of binding.

Material selection using MERDE method: A new multiple attribute decision making method

V P Darji and R V Rao
S V National Institute of Technology, India

Manufacturing environment advancement has become extensively precise in measurement of performance using multi criteria decision making method. Material selection for the specific applications with specific properties from a large number of alternatives is a difficult task. In this paper, a new simple, rational and systematic decision making method named MERDE is proposed. The flexibility for it application is demonstrated using ten material selection problems. The mathematical procedure of MERDE method is based on arithmetic mean and consisting of a new way of normalization of the data set to make them dimensionless.
Materials chemistry in borohydride fuel cells development
Yogeshwar Sahai and Jia Ma
The Ohio State University, USA

Chemical and electrochemical reactions are important in developing new and cost effective materials for fuel cell development. A chitosan-based chemical hydrogel membrane and catalyst binder were developed by the authors and used in alkaline Direct Borohydride Fuel Cells (DBFCs). The chitosan-based borohydride fuel cell gave more than 50% higher power performance than the commercial Nafion-based one. The authors are the first to develop a chitosan membrane which resulted in much higher power density than the commercially used Nafion-based membranes. The chitosan-based catalyst binder also gave about 20% higher power density values than Nafion as catalyst binder. This chitosan-based membrane has also been successful in alkaline ethanol fuel cells. The estimated cost of chitosan-based membrane is less than 10% of the cost of Nafion. For borohydride electro-oxidation, an effective anode consisting of Ni-based composite electrocatalysts loaded on Ni foam substrate was developed and employed. The use of Ni-based catalyst reduces the cost of fuel cell without compromising its performance. Thin film electrode was prepared by electroless plating and physical vapor deposition. A nanoscale thin film anode delivered comparable power performance to an ink pasted electrode with a much higher catalyst loading. Chemical and electrochemical aspects of these materials in preparing polymeric membrane and electrode and their performance results will be presented in this paper. The effect of these materials in reducing the cost of fuel cells will be also presented in this paper.

sahai.1@osu.edu

The bimodal effect of the bulk modulus of rare-earth titanate pyrochlore
Yuhong Li, C G Liu, D Y Yang and J Wen
Lanzhou University, China

First-principles calculations have been carried out to study the bulk modulus, the lattice parameters and the bond length of RE,M₂O₇ (RE=La, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu; M=Ti, Sn) pyrochlores. The relationship of the bulk modulus and the bond length of RE₂M₂O₇ have been analyzed qualitatively. Both the bulk modulus and the <RE-O₄8f> bond present the “bimodal effect” and <RE-O₄8f> bond may have a significant effect on the bulk modulus. The bimodal effect means certain properties of lanthanide elements and compounds will not change linearly with the increase of atomic number of lanthanides but present two peaks or two valleys in Eu and Yb positions.

liyuhong@lzu.edu.cn
Structural, dielectric and impedance study of a new lead free ferroelectric (Ba, M) (Ti, M') O3, M=Ca; Sr and M' = Sn; Zr ceramics

HOUDA MSOUNI1,2, A Tachafine1, D Fasquelle1, M El Aatmani1, J-C Carru2, M El Hammou1 and A Zegzouti1
1Cadi Ayyad University, Morocco
2University of the Littoral Opal Coast, France

The dielectric properties and microstructure of co-doped B-site and A-site BaTiO3 solid solution of the type (Ba, M) (Ti, M') O3 were investigated. The influence of extremely small amount of Sr, Sn, Zr and Ca dopants on the microstructure and the dielectric characteristics of BaTiO3 were studied systematically. These compositions were designed using the conventional mixed oxide technique and the XRD analysis results indicated that no secondary phase was formed. The microstructure of sintered pellets was studied by SEM at room temperature. The dielectric measurements showed that the BSTZ ceramic present the highest permittivity at 25°C and 100kHz with the value of 2600, whereas the crystallite size was found to approach 32.3 nm. The BaTiO3 ceramic with Sr at A-site has no phase transition above room temperature, while ceramics with Sn at B-site present ferroelectric – para-electric transition with sharp transition. Finally, the ceramic with Zr at B-site exhibit normal ferroelectric-para-electric transition with Tc=97°C. The effect of doping was been studied and analyzed using the AC complex impedance spectroscopy technique to obtain the electrical parameters of polycrystalline samples in a wide frequency range at different temperatures. The piezoelectric properties were also studied.

houda.msouni@gmail.com

Structural evolution of pearlite in steels with different carbon content under drastic deformation during cold drawing

E Brandaleze and M Romanyuk
Universidad Tecnológica Nacional, Argentina

Steel wires, under severe cold drawing deformation, develop high strength. High carbon steel (C>0.80%) has a great demand in the steel market because of the extremely high strength (5-6 GPa). For this reason, it is relevant to increase the knowledge on the structural evolution and deformation mechanisms involved during wiredrawing process due to their critical applications, among which we can mention wires for: Bridges, cranes and tire cord. The mechanical behaviour aptitude is determined by torsion test. When the fracture surface is flat, the wire is apt. On the opposite, an irregular fracture surface (delamination) means poor mechanical properties. This paper presents a comparative study on steel wires (0.80% C) that presented normal behaviour and delamination problem during torsion test, in order to compare the structural evolution at high deformation. The deformation mechanisms and cementite stability was analyzed. The microstructural study was carried out applying light and Scanning Electron Microscopy (SEM). Finally, the structural information was correlated with results of Differential Scanning Calorimetry (DSC) and thermodynamic properties obtained by Fact Sage simulation. The structural study verified the presence of curling phenomenon in both steels products. It was possible to verify differences (~26%) in the interlaminar spacing (λ) of the pearlite between wires that present normal and delaminated behaviour under torsion test. The ductility loss (in the delaminated wire) is promoted by multiple causes: Higher interlaminar spacing, high nitrogen content in the product and the presence of dynamic strain aging, which is promoted by cementite destabilization and the formation of ε carbide.

ebrandaleze@frsn.utn.edu.ar
Study of the structural and morphology features of Bi2O3 nanoparticles

Mohammad Sideeq Rather
National Institute of Technology-Srinagar, India

An improved way and surfactant free approach has been employed for the synthesis of Bismuth oxide (Bi2O3) nanoparticles at very low temperature of 110°C. This new approach is based on a reaction of bismuth powder and de-ionized (DI) water without the use of any additives or surfactants. XRD and SEM have been employed to characterize the Bi2O3 nanoparticles. By the morphological investigations using SEM, it was observed that the grown Bi2O3 products are having dimensions in the range of 3 nm to 25 nm. The reported method besides being organics free is economical, fast and free of pollution, which will make it suitable for large scale production.

sideeq.rather@gmail.com

Protein antifouling properties of a chemical vapor deposited alkyl-functional carboxysilane coating characterized using quartz crystal microbalance

Shyam V Vaidya¹, Alfredo R Narváez¹, Min Yuan¹, David Daghfal¹, James Mattzela² and David Smith²
¹Abbott Laboratories, USA
²SilicoTek® Corporation, USA

The protein resistant properties of a chemical vapor deposited alkyl-functional carboxysilane coating (Dursan®) were compared to that of an amorphous fluoropolymer (AF1600) coating and stainless steel by studying non-specific adsorption of various proteins onto the coating surfaces using quartz crystal microbalance with dissipation monitoring (QCM-D). A wash solution with non-ionic surfactant, polyoxyethylene glycol dodecyl ether (or Brij 35), facilitated 100% removal of residual bovine serum albumin (BSA), mouse immunoglobulin G (IgG), and normal human plasma proteins from the Dursan surface, whereas these proteins remained adsorbed on the bare stainless steel surface. Mechanical stress in the form of sonication demonstrated robustness of the Dursan coating to mechanical wear and showed no impact on the coating’s ability to prevent adsorption of plasma proteins. Surface delamination was observed in case of the sonicated AF1600 coatings and it led to adsorption of plasma proteins. The combination of the robust alkyl-functional carboxysilane coating (Dursan) and non-ionic surfactant in the wash buffer that we have reported here is certainly a step forward toward mitigation of surface biofouling in biotechnological applications, specifically in case of automated immunoassay analyzers, reagent manufacturing, and filling setups.

shyam.vaidya@abbott.com