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Catalysis, Chemical Engineering and Technology Virtual

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CATALYSIS, CHEMICAL ENGINEERING & TECHNOLOGY

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Siew Chun Low[1], Guang Hui Teoh[1], Lei Zhou[1,2]

[1]School of Chemical Engineering, Engineering Campus, Universiti Sains Malaysia, Nibong Tebal, Pulau Pinang, Malaysia.

[2]School of Textile and Garment, Anhui Polytechnic University, Wuhu, China.

The effect of rough interface printing on polymeric membrane via micromolding for membrane distillation applications

Most polymer membranes used for membrane distillation (MD) are low surface energy fluoropolymers. These polymers can form superhydrophobic surfaces through some direct surface roughening techniques. The creation of rough interface through micro-molding is one of the surface roughening techniques reported in this work. The polymer solution is cast on a micro-mold template with a design pattern, thereby preserving the microstructure replicated in the design pattern. In this work, the surface-printed polyvinylidene difluoride (PVDF) membranes mimicked the wavy surface structure of the micro-mold template. After the phase inversion process, the PVDF membrane is spontaneously desquamated from the replica. The prepared membrane exhibits a high static water contact angle (WCA) of over 155° and a low water sliding angle (WSA) of less than 10°, surpassing the superhydrophobic performance standard of a membrane. In direct contact membrane distillation (DCMD), the surface printed PVDF membrane with a hierarchical structure shows a salt rejection rate of more than 99%, and has excellent resistance to complex aquaculture feed solutions containing suspended solids (organic matter), dissolved nutrients (from feed and fish excretion) and microalgae. Based on the findings, the micro-mold templated membrane shows the potential advantage of improving the surface roughness of the membrane, exhibiting excellent WCA and WSA without the need for additional extrinsic additives.

Biography

Dr. Siew Chun Low is an Associate Professor in the School of Chemical Engineering at Universiti Sains Malaysia. She is particularly interested in the use of membranes to control environmental pollution. Thus far, she has published 8 book chapters, more than 110 journal articles with h-index of 23, and received more than 1800 cumulative citations. She also participated in more than 35 conferences, including 1 keynote and 2 invited lectures. Dr. Low is also the subject editor of ASM Science and the guest editor of 2 Special Issues in Journal of Physical Science and Environmental Science and Pollution Research (Springer)

Nataša Novak Tušar [1,2], Andraž Šuligoj[1,3], Urška Lavrenčič Štangar[3]

[1]Department of inorganic chemistry and technology, National Institute of Chemistry, Ljubljana, Slovenia.
E-mail id: natasa.novak.tusar@ki.si, E-mail id: andraz.suligoj@ki.si
[2]Graduate school, University of Nova Gorica, Nova Gorica, Slovenia.
[3]Faculty of chemistry and chemical technology, University of Ljubljana, Ljubljana, Slovenia.
E-mail id: urska.lavrencic.stangar@fkkt.uni-lj.si

Porous materials as supports for photocatalysts in air cleaning applications

The aim of the field of catalyst/photocatalyst design for heterogeneous catalysis is to establish the desired composition and structure of these materials in the form of non-supported or supported systems which form powders, shaped powders (e.g. granules) or coatings. The lecture is based on the case study of porous silica supported titanium dioxide as a coating for photocatalytic removal of organic pollutants from the air. Titanium dioxide (TiO_2) is the most used material for mentioned application due to its interesting characteristics: low cost, high stability, shows high photocatalytic activity, it can promote ambient temperature oxidation of the major class of organic pollutants. However, due to the hindered applications of TiO_2 as non-supported systems for photocatalytic air cleaning, design and development of TiO_2 supported systems are very important. Common support materials are porous materials e.g. SiO_2, Al_2O_3, zeolites (aluminosilicates), carbon etc. These materials exhibit high specific surface areas, high porosities in a variety of pore sizes, and high thermal and mechanical stability, while they are mostly chemically inert. Here, an overview on the design and development of coatings from a) porous SiO_2 supported TiO_2 for removal of volatile organic pollutants from indoor-air under UV light and b) porous SiO_2 supported TiO_2 functionalized with transition metals for removal of volatile organic pollutants from outdoor-air under visible light will be

Biography

Prof. Nataša Novak Tušar has been the head of the Laboratory for catalysts (former Laboratory for environmental sciences and engineering) at the Department of Inorganic Chemistry and Technology at the National Institute of Chemistry in Ljubljana since 2021. Since 2018 she has been a full professor and director of the PhD program "Materials" at University Nova Gorica, Slovenia. She was Individual Marie Curie Fellow at the synchrotron ELETTRA and at the University of Trieste, Italy, from 2003-2004. She is a member of the governing bodies of ENMIX (European Nanoporous Materials Institute of Excellence) and EFCATS (European Federation of Catalysis Societies).

Patricia J. Kooyman[1,*], Roald Brosius[2], Jack C.Q. Fletcher[1]

[1]Department of Chemical Engineering, University Of Cape Town, Rondebosch, South Africa, E-mail id: patricia.kooyman@uct.ac.za

[2]Haldor Topsøe A/S, Kgs. Lyngby, Denmark, RBRO@topsoe.com, E-mail id: jack.fletcher@uct.ac.za

Tuning hydrocracking process parameters

Gas- and Coal-to-Liquids processing are attractive routes towards clean liquid transportation fuels (alternative to crude oil refining). The industrial route converts coal or gas to synthesis gas (CO and H_2), followed by Fischer-Tropsch synthesis (FTS) to a wide range of hydrocarbons and subsequent product workup. Hydrocracking of FTS wax (dewaxing) requires a bifunctional catalyst, containing a hydrogenation/dehydrogenation function and an acidic function. We use Pt noble metal (de)hydrogenation / zeolite solid acid.

Two approaches to improve the yield of transportation fuels in the dewaxing process are: synthesis of zeolites with hierarchical pore systems, introducing mesopores, decreasing diffusion limitations and the secondary cracking that results from long residence time in the zeolite pores; and the process parameters a) presence of water in the feed, b) total process pressure.

Water is the main byproduct of FTS, and leaving it in the feed for dewaxing allows the integration of synthesis and hydroprocessing. The presence of water decreases activity and increases selectivity to linear products, both due to competitive adsorption on the acid sites [1].

Surprisingly, when using zeolites, lowering the total process pressure to atmospheric increases the diesel yield dramatically and makes the whole process much more economical [2]. This is in contradiction to previously reported results using amorphous silica-alumina (ASA), where more diesel is formed at higher pressure [3,4].

[1] R. Brosius, P.J, Kooyman, J.C.Q. Fletcher, ACSCatalysis 2016, 6, 7710

[2] R. Brosius, patent WO2020016845A1

[3] D. Leckel, M. Liwanga-Ehumbu, EnergyFuels 2006, 20, 2330

[4] D. Leckel, EnergyFuels 2007, 21, 1425

Biography

Patricia J. Kooyman obtained her MSc from Leiden University, studying the selective reduction of nitrosobenzene over mixed manganese oxides. She obtained her PhD from Delft University of Technology, studying TS-1 zeolite synthesis and catalytic properties. Following a post-doc at Shell research centre (Amsterdam), she learned about TEM from Prof. Zandbergen at the NCHREM (Delft), where she pioneered gas-phase operando TEM. She served as assistant professor in ChemEng at Delft University of Technology before coming to South Africa in 2015 as SARChI Chair Nanomaterials for Catalysis at the University of Cape Town. Her research focusses on heterogeneous catalysis, especially structure-performance relationships.

Grégory Lefèvre[1], Manuel Corral-Valero[2], Teddy Roy[1,2], Thibaut Corre[2], Olivier Delpoux[2], Gerhard Pirngruber[2]

[1]Chimie ParisTech, PSL Research University, CNRS, Institut de Recherche de Chimie Paris (IRCP), F-75005 Paris, France.

[2]IFP Energies nouvelles, Direction Catalyse, Biocatalyse et Séparation, Rond-point de l'échangeur de Solaize, 69360 Solaize, France.

A surface reactivity model of γ-alumina based on DFT-MUSIC hybrid approach and

γ-Al_2O_3 is a transition alumina oxide whose surface chemistry seems to be a key factor in the preparation of heterogeneous catalysts where it is used as a support. The modification and description of its surface are necessary to understand the role of the support on the catalyst preparation by impregnation techniques, and on the obtained catalyst performance. However, the speciation of surface sites of this material confronts several obstacles and implementing them in a surface complexation model is a challenging task. In our approach we combined the MultiSite Complexation Model (MUSIC) with atomistic information from Density Functional Theory and Ab Initio Molecular Dynamics to describe the chemical reactivity of γ-Al_2O_3 surface at the solid liquid interface. This model was first compared to experimental measurements on proton adsorption to evaluate its prediction ability. Then, a multi-technique characterization of phosphate and malonate ions was performed, as these species have been proposed to tune the surface reactivity of this catalyst support during the impregnation step in heterogeneous catalysis preparations. The surface complexation model has been complemented using these experimental results, which allowed to obtain complementary information on the nature and reactivity of the sites involved in the adsorption mechanisms of these species.

Biography

Grégory Lefèvre has completed his PhD from University of Nancy, France. He is a senior researcher in French National Center for Scientific Research and Associated Professor at Paris Sciences et Lettres University. He has worked in the solid-solution interface field for more than twenty years and has published 91 papers in reputed journals and hold 2 patents.

José C. Conesa

Institute of Catalysis and Petroleum Chemistry, CSIC, Spain. E-mail id: jcconesa@icp.csic.es

Computing with hybrid DFT methods interfaces between semiconductors

Band offsets between semiconductors determine the direction of electron transfer at their interfaces. Two methods are used to compute such offsets from first principles: alternating slabs put in contact, without empty spaces between them, and separate calculations of each material surface confronted with empty vacuum space. The first method has the risk of introducing distortions due to insufficient epitaxial match, leading to bandgap changes; the second neglects electron transfer at the interface, implying also a spill of electronic density into the vacuum space which is not present in the real interfaces. Here results will be compared using both approaches for different interfaces: anatase TiO_2/ZnO (relevant for photocatalysis), and a comparison of interfaces between $CuGaS_2$ and either ZnS or CdS, relevant for photovoltaic materials, will show the effects of significant epitaxial mismatch. The same comparison will also be made in the PbTe|TiO_2 (rutile) and diamond|α-tin; the system $BiVO_4$/NiOOH (relevant for photoelectrochemistry) will be also studied. The method will be based on using for the bulk phases hybrid DFT methods providing bandgap values coincident with the experimental ones, transferring subsequently to the interfaces the distances between the band positions and the profile of the electrostatic potential as previously suggested (C.G. Van de Walle & R.M. Martin, PRB 1987, 35, 8154). In all cases it will be ensured that all interfaces are nonpolar according to Tasker's criterium. A critical analysis of any relevant differences found will be presented.

Biography

J.C. Conesa entered the ICP staff in 1979; he was ICP Director, being now ICP Ad Honorem Professor. He was first in Spain using SR techniques to study heterogeneous catalysis, and first in CSIC to use quantum calculations to understand them. Expert in XPS and FTIR (including *operando*), EPR, UV-Vis-NIR. He analyzed CeO_2-supported oxides, recently for H_2 production. He keeps interest in photocatalysis and photoactive solids. He belongs to the Steering Committee of AMPEA, a JP of the European EERA devoted to sustainable energy. His over 200 articles and book chapters received > 9900 citations; his Hirsch index is h=57.

Giuseppina Iervolino

[1]Department of Industrial Engineering, University of Salerno, Italy, E-mail id: giiervolino@unisa.it

Advacend oxidation process for environmental purpose: the application of heterogeneous catalyst

In recent years, research towards innovative and effective technologies and processes for water treatment and energy recovers has become increasingly popular. In particular, as regard the water contamination much attention has been paid to specific contaminants such as azo dyes or heavy metals such as arsenic which can be found in water due to natural action. For this kind of pollutant it is necessary the application of strongly effective processes able to completely remove this pollutants from water. The advanced oxidation processes represent a very interesting alternative to the conventional processes for water treatment. In particular, in recent years, interesting innovations have been proposed for photocatalytic processes or for processes based on non-thermal plasma where heterogeneous catalysts are used. The efficiency of innovative photocatalyst and of very strong oxidizing species obtained with non-thermal plasma, was demonstrate for the degradation of azo dye, herbicides and metals. At the same time the heterogeneous photocatalysis process has been studied and its aspects have been investigated for the valorisation of the organic substances present in the waste water in order to produce hydrogen. For this purpose, various catalytic formulations have been studied, also immobilized on easily recoverable supports in order to make the catalyst recyclable. This presentation will illustrate some interesting applications of heterogeneous photocatalysis and non-thermal plasma both for the abatement of contaminants in the liquid phase and for the production of hydrogen from waste substances present in wastewater.

Biography

Giuseppina Iervolino was graduates at “University of Salerno” with honors in Environmental Engineering in 2013, with the thesis entitled "*Removal of arsenic from drinking water by a photocatalytic oxidation and adsorption process*". In 2017, at University of Salerno, she obtained the PhD title in “Industrial Engineering” (Chemical Engineering curriculum) with the thesis entitled "*Advanced Oxidation Processes for Food Industry Wastewater Valorization and Treatment* ". Actually she is “Assistant Professor” at the Department of Industrial Engineering of the University of Salerno. Her research activity is focused on environmental issues concerning the water treatments (both wastewater, both for drinking purposes) and the valorization, with H2 production, of organic substances present in the industrial wastewater, with particular reference to the application of advanced oxidation processes, studying innovative catalysts and photocatalysts, the reactor configurations and light source. In addition, she is working on two innovative research line: the application of "Non Thermal Plasma" technology for the removal of not easily biodegradable contaminants from wastewater, and the electrification of industrial processes for hydrogen production.. Giuseppina Iervolino is the author, at the month of February2022, of 45 publications with indexing SciVerse Scopus®, with ISBN / ISSN and DOI number with 1040 citations and h-index of 18**)**

Raffaella Mancuso

Laboratory of Industrial and Synthetic Organic Chemistry (LISOC)-Department of Chemistry and Chemical Technologies, University of Calabria, Arcavacata di Rende (CS), Italy.

Pd-Catalyzed Carbonylation of Sulfurated Substrates Under Aerobic Conditions

The PdI_2/KI-catalyzed oxidative carbonylation of alkyne derivatives suitably substituted with a nucleophilic group -YH (Y = O,NR) has proved to be a powerful methodology for the construction of functionalized heterocycles in a multicomponent fashion starting from simple building blocks. Oxidative carbonylations are carried out in the presence of an external oxidant, necessary to reoxidize the Pd(0) formed in the course of carbonylation to catalytically active Pd (II). This kind of reactivity, unfortunately, cannot be applied to substrates bearing a thiol nucleophilic group (Y = S), owing to the wellknown instability of the -SH group to oxidizing agents, including oxygen. This problem has so far hindered the development of PdI_2/KI-catalyzed oxidative carbonylation processes for the synthesis of sulfurated heterocycles.

In this Keynote it will be shown the synthesis of different types of molecules, containing sulfur, by Pd-catalyzed oxidative carbonylative S-cyclization process, starting from suitable acetylenic substrates bearing a masked thiol function, still nucleophilic enough to promote a carbonylative S-cyclization process, but sufficiently stable under the oxidative conditions.

Biography

Prof. Mancuso received the PhD in “Methodologies for the Development of Molecules of Pharmacological Interest” at the University of Calabria (2006). She won a “Young investigator research project” on 2007. After a post-doc stage at Iowa State University (USA) (2008) she came back to University of Calabria. She joined the University of Barcelona (Spain) in 2012. In 2018 she received her second PhD degree in “Environmental, Construction and Energy Sciences and Engineering”. She is currently Associate Professor at the University of Calabria (Italy). Prof. Mancuso received a “Research Award” in September 2017 in the field "Innovation in Organic Synthesis". Current scientific production include 122 papers in international peer-reviewed journals, 8 patents and more than 170 communications in national or international conferences. She is an international referee in the field of Multidisciplinary and Organic Chemistry, and editorial board member of international journals.

Kristijan Lorber[1,2] and Petar Djinović[1,2]

[1]Department of Inorganic Chemistry and Technology, National Institute of Chemistry, Ljubljana, Slovenia.
[2]University of Nova Gorica, Nova Gorica, Slovenia.

Photothermal methane and CO_2 conversion to syngas under mild conditions over metal@semiconductor catalyst

Photo-thermal reduction of atmospheric carbon dioxide into methane, methanol and carbon monoxide under mild conditions over suitable (photo)catalysts is a feasible pathway for production of fuels and platform chemicals with minimal involvement of fossil fuels.
The methane dry reforming reaction (DRM) converts methane and CO_2 into syngas, a mixture of H_2 and CO. When illuminated by white light, the $2Ni/CeO_{2-x}$ catalyst enables conversions of both CH_4 and CO_2 beyond thermodynamic equilibrium, while the energy efficiency reaches 33 %. The DRM reaction is sustained in a purely photocatalytic mode without external heating when illuminated by 790 mW cm^{-2} of white light with CH_4 and CO_2 rates equaling 0.21 and 0.75 mmol $(g_{cat}*min)^{-1}$, respectively. At a constant catalyst temperature of 400 °C, the reaction selectivity expressed as H_2/CO ratio increases from 0.23 to 0.59 in light-assisted mode compared to the experiment in the dark. The theoretical analysis of Ni/CeO_{2-x} optical properties agree with *in-situ* UV-Vis DRS results and show that the presence of partly reduced Ce^{3+} sites is crucial for extending the optical absorption of Ni/CeO_{2-x} into the visible light range. The strong electromagnetic near field enhancement was identified as the dominant source of visible-light-induced rate acceleration and occurs mainly over nickel nanoparticles which are the active sites for methane activation. This work identifies sub-stoichiometric Ni/CeO_{2-x} photocatalyst as highly efficient for boosting methane activation by visible light illumination under mild conditions.

Biography

Petar Djinović has completed his PhD from Faculty of Chemistry and Chemical Technology in Ljubljana, Slovenia, and postdoctoral studies at Max Planck institute for Kohlenforschung, Germany. He is the senior research associate at the National Institute of Chemistry, and assistant professor at the University of Nova Gorica. His research interests are mechanistic analyses of catalytic and photocatalytic CO_2 conversion reactions. He has published more than 70 papers in reputed journals.

Anita Šalić

University of Zagreb, Faculty of Chemical Engineering and Technology, Marulićev trg 19, HR-10000 Zagreb, Croatia, E-mail id: asalic@fkit.hr

Intensification of sustainable biodiesel production: *The power of microscale*

The global energy market has evolved dynamically in recent decades with continuous efforts to advance technologies for production of sustainable and environmentally friendly energy sources. One of the examples of such advanced technologies is the enzyme catalysed production of biodiesel performed in microreactors. Biodiesel production on a large, batch scale, is mainly performed as transesterification catalysed by alkaline catalysts. Therefore, an alternative approach which combines sustainable and environmentally friendly catalyst like enzyme lipase and continuous transesterification on microscale should lead to process intensification. All the known benefits of microreactor technology such as the large surface area to volume ratio and the intensification of mass and energy transfer combined with a short residence time result in higher conversions and productivities of those achieved in meso and macro-reactors. Another advantage of microtechnology is the possibility to combine several process steps on the one unit. On that way microreactor for biodiesel production and microseparator for purification of produced biodiesel can be connected in series, leading to the development of an integrated system on a single microunit.

Different approaches, such as transesterification catalysed with free and immobilized enzyme for biodiesel production on a microscale, application of deep eutectic solvents as extraction and stabilization media, microextraction and cross-flow filtration for biodiesel purification, used during development of a fully integrated system for biodiesel production will be presented.

Biography

Anita Šalić, obtained her PhD in 2015 from University of Zagreb by working on implementation of microreactor technology in to chemical and biochemical reactions. During her research work she has co-authored 32 original scientific papers published in Web of Science journals, 10 scientific and professional papers in other journals and proceedings, and 4 book chapters. She has actively participated in several national and international scientific conferences where she has delivered more than 50 presentations. She received the Croatian Annual Award for Science for young scientist in the field of technical sciences.

Lindomar Alberto Lerin[1], Valentina Venturi[2], Simona Aprile[1] and Pier Paolo Giovannini[1]

[1]Department of Chemical, Pharmaceutical and Agricultural Sciences, University of Ferrara, Ferrara, Italy.
E-mail ids: lrnldm@unife.it, prlsmn@unife.it, gvnppl@unife.it.

[2]Department of Environmental and Prevention Sciences, University of Ferrara, Ferrara, Italy,
E-mail id: vntvnt@unife.it

Lipases-catalyzed esters synthesis with pharmacological activities

Currently, products labeled as natural have been an important attribute when choosing a product. Products obtained by biotechnological processes, including those obtained by enzymatic biocatalysis, are labeled as natural, thus satisfying this trend. Biotechnological processes have several environmental advantages compared to traditional acidic or basic catalysts generally used in chemical synthesis. In this way, the use of enzymes, such as lipases, in biotechnological processes reduces the production of waste, accelerates the rate of reactions under mild conditions of temperature and pressure, facilitates the recyclability of catalysts and reagents and the processing of the products, and can be applied to many organic transformations. These characteristics integrate several principles of green chemistry. The enzymatic synthesis of esters of aromas, fragrances, or compounds with pharmacological activities, such as antioxidant, antimicrobial, anti-inflammatory, neuroprotective, among others, has become a subject of scientific and industrial interest. Thus, lipase-catalyzed reactions for the synthesis of esters of secondary plant metabolites, such as geraniol and eugenol, have gained highlights because they are major constituents of several essential oils and are commercially available in large quantities. Thus, the optimization of process conditions for the synthesis of esters in solvent-free systems either under batch or continuous-flow mode, using methodologies that minimize the number of tests and maximize the observation of the effects of independent variables, such as substrates

Biography

Lindomar Alberto Lerin received his D.Sc in Biochemistry from the Federal University of Rio de Janeiro shortly after graduating in Biological Sciences. Currently working as a research fellow in the Department of Chemical and Pharmaceutical Sciences at the University of Ferrara. His works deal with the bio-based circular economy using Green Technologies as Biotechnological Processes, mainly in the enzymatic processes optimization, with the development of enzymatic biocatalysis for the bioproducts synthesis, in particular lipases esterification in batch, fed-batch, continuous flow, and bubble column reactor, as well with the use of experimental design methodology (DOE) to maximize the biocompounds production.

Blaž Likozar,[1,2,3] Miha Grilc,[1] Matej Huš[1]

[1]Department of Catalysis and Chemical Reaction Engineering, Kemijski inštitut, Ljubljana, Slovenia,
E-mail id: blaz.likozar@ki.si

[2]Pulp and Paper Institute, Ljubljana, Slovenia.
[3]Faculty of Polymer Technology, Slovenj Gradec, Slovenia.

Engineering Multi-scalar Process Digital Twinning: From Atoms to Plants

The future presents us with many difficult challenges, which are related to the increase of the world's population, the elevation of the quality of life, but still the limited natural resources of the Earth. Chemical process engineering experienced a rise with the boom in oil refining in early twentieth-century US. Today, engineering faces challenges related to the harvesting, conversion and storage of renewable energy, the capture, storage and use of carbon dioxide, and other sustainable sources such as biomass. However, due to critical raw material sources (*eg* H_2 production), limitations in terms of thermodynamics (*eg* CO_2) and volatile changing composition (*eg* biomass), the challenges are not easily solved, so they often need a fully integrated treatment, from the atomic structure of catalysts. This spans to factories, measuring several kilometers. On the other hand, the rise of computing power, digitalization and the deployment of digital twins allows us to solve, predict, and improve complex chemical transformations, from electrons to (bio) refineries, which is still in its infancy. Examples of how models describe conversions will be presented.

Biography

Blaž Likozar, the head of the Department of Catalysis and Chemical Reaction Engineering. Prof. Blaž Likozar (M) (40 years). Department head, programme head, project head, *etc*. Background: PhD in chemical engineering (2008); post-doc in Austria and USA. The participation in EU/projects: the PI in 15 H2020, 2 ERA-NET, & 5 ERDF projects, etc. Other useful information: 239 peer-reviewed research documents, > 4000 citations, and the *h*-index of 30; SusChem, EERA Bioenergy, EFCE Chemical Reaction Engineering Working Party, EFCE Energy Section & NATO ET/SET member; SRIP CE vice-chair; an editor, reviewer and author.

A Krishna sailaja

Department of pharmaceutics, RBVRR Women's college of pharmacy,
Affiliated to Osmania University, Hyderabad, India.

Formulation Of Mefenamic Acid Loaded Polymeric Nanoparticles By Ionotropic Gelation Technique

Mefenamic acid is used for the treatment for rheumatoid arthritis, post operative pain and dysmenno-reha.It is chemically [2-[(2, 3-dimethylphenyl) amino] benzoic acid], an anthranilic acid derivative, whichh is a prostaglandin inhibitor. It is water insoluble, bitter drug with good oral bioavailability (but poor physico chemical parameters, aqueous solubility) are responsible for its decreased biological activity. It is available as tablets, capsules and suspensions. Nanoparticles have shown significant advancements in delivery of drugs and biomolecules. The primary objective of this investigation was to develop and characterize polymeric nanoparticles of Mefenamic acid. Mefenamic acid nanoparticles were prepared by ionic gelation technique by changing the polymers and stabilizers.

For ionic gelation technique, Chitosan was used as polymer and Sodium tripolyphosphate as cross linking agent. Five formulations were prepared by varying the concentrations of polymer and drug. The mean particle diameter and zeta potential value of the best formulation (F2) was found to be 194.6nm and -35.3 mV respectively. FTIR studies showed the absence of chemical interaction between Mefenamic acid and polymer and the encapsulation of drug into the nanoparticles. The SEM results indicated that Mefenamic acid nanoparticles were found to be spherical in shape. The Invitro drug release studies showed that the drug release followed Higuchi pattern with fickian diffusion. The drug release was sustained till 11hrs following first order rate constant for the best formulation.

Key words:- Entrapment efficiency, Loading capacity, Particle size, zeta potential

Biography

Dr. A.Krishna sailaja pblished more than 140 research papers in national and International journals of high repute. She delivered more than 30 lectures in national and International conferences and webinars. Filed 4 patents in novel drug delivery system. Published 5 books. Received best scientist award and best faculty award for her Professional contribution. Currently working as Associate Professor and Head, Department of Pharmaceutics, RBVRR Women's college of pharmacy, Affiliated to Osmania university, Hyderabad, India.

Rosa Alicia Saucedo-Acuña[1]*, Karen Zulema Meza-Valle[2], Judith Virginia Ríos-Arana[3], Guillermina Martínez-Moreno[4], and Juan Carlos Cuevas-González[5]

[1]Institute of Biomedical Sciences, Universidad Autónoma de Ciudad Juárez, Juárez, Chihuahua, México, E-mail id: rosauced@uacj.mx

[2]Institute of Biomedical Sciences, Universidad Autónoma de Ciudad Juárez, Juárez, Chihuahua, México, E-mail id: mvz.karenmeza@gmail.com

[3]Institute of Biomedical Sciences, Universidad Autónoma de Ciudad Juárez, Juárez, Chihuahua, México, E-mail id: jrios@uacj.mx

[4]Institute of Engineering and Technology, Universidad Autónoma de Ciudad Juárez, Juárez, Chihuahua, México, E-mail id: gemartin@uacj.mx

[5]Institute of Biomedical Sciences,Universidad Autónoma de Ciudad Juárez, Juárez, Chihuahua, México, E-mail id: juan.cuevas@uacj.mx

Development of an artificial scap based on pectin-allantoin hydrogel for the treatment of skin wounds

The last two years several approaches reported the use of natural compounds for medical applications. Particularly fresh hydrogels on base of Aloe vera reported an excellent influence on wound contraction. However, the use of fresh hydrogels implies the reduction of mobility and the special care of an open wound during the health process. The development of a film of pectin enriched with allantoin could remedy this inconvenience. To obtain the film, Pectin was enriched with Allantoin in 1:1 relation, and the mixture was plasticized with glycerol. The characterization and a comparative topical study between Aloe Vera hydrogel and a film of Pectin-Allantoin on the skin wound healing process was investigated in female Wistar rats. Pectin-Allantoin film exhibited very similar wound contraction as Aloe vera fresh hydrogel, reducing 25% the total healing time. A magnificent result because the Pectin-Allantoin film covered the wound as an artificial scap on the skin only the early seven days until the body begins to build its natural scab. These results show that with this proposal is possible reached a remarkable healing process using a flexible film of Pectin-Allantoin as an artificial scap making easier the wound care.

Biography

I am doctor in Materials Sciences, I work at Universidad Autónoma de Ciudad Juárez, I founded the Applied Chemistry Group in this university. My research is focused on chemical applications to Environmental and Biomedical Sciences. I was CO president of 2020 National Congress of SMEQ, editor of the abstract book, guess editor of ECS Transactions, I have responsible of 13 research projects, wrote a book, 19 papers, 3 book chapters, 64 meetings publications, a laboratory practices manual, reviewed a book by McGrawHill. And in 2021, I received the recognition as outstanding woman in Sciences by Chihuahua State Government.

Angelo Lucia

[1]Department of Chemical Engineering, University of Rhode Island, Kingston, RI, USA, E-mail id: alucia@uri.edu

Enzyme Catalysis in Metabolic Networks

Enzymes are highly regulated biological catalysts that have turnover numbers that can vary from 10^{6} to 10^{-1} s^{-1}. Recently, Lucia and coworkers have developed and studied a Nash equilibrium approach to metabolic network modeling where enzymes are treated as players in a multi-player game. In this work, explicit inclusion of enzyme-substrate reactions at the cellular length scale and protein docking information at the molecular length scale are described. This multiscale information allows the direct (1) computation of cellular enzyme concentrations, (2) incorporation of genetic modification of enzymes, and (3) encoding age-related changes in enzymatic behavior (e.g., protein misfolding) within any pathway. Molecular length scale binding histograms are computed using protein-ligand docking and directly up-scaled to the cellular level. Numerical examples are presented to illustrate key ideas. Numerical results show that the proposed approach provides a wealth of quantitative enzyme information.

Biography

Professor Angelo Lucia has completed his PhD from the University of Connecticut, USA and. He is the Chester H. Kirk Chair of Chemical Engineering at the University of Rhode Island. He has published more than 100 papers in reputed journals and has been serving as an editorial board member for the Journal of Global Optimization and Spring Nature Operations Research Forum.

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Shima Masoumi and Ajay K. Dalai

[1]CREST Bioenergy Center, North Carolina A&T state university, North Carolina, USA,
E-mail id: smasoumi@ncat.edu
[2]Department of Chemical and Biological Engineering, University of Saskatchewan, Saskatchewan, Canada,
E-mail id: ajay.dalai@usask.ca

NiMo carbide supported on chemically prepared activated carbon from algal derived hydrochar for hydrodeoxygenation of algal biocrude oil

Hydrothermal liquefaction of microalgae as a third generation of biofuel feedstock under milder reaction conditions was studied for the production and characterization of biocrude oil and hydrochar. The optimum yield of biocrude oil (57.8 wt.%) and highest energy recovery (85.3 %) was obtained with 75 wt.% of methanol in water at 272°C, 11.5 MPa, and reaction time of 35 min. This study also focused on the utilization of hydrochar-based catalysts as a renewable carbonaceous material to improve the overall economy. The chemically prepared activated carbon with specific surface area of 631 m^2/g was obtained, which also revealed total pore volume and average pore size of 0.36 cm^3/g and 8.2 nm, respectively. The use of novel NiMo carbide catalysts supported activated carbon obtained from chemical activation of algal hydrochar for the catalytic hydrodeoxygenation of algal biocrude oil was investigated. The synthesized catalysts were screened through hydrodeoxygenation (HDO) reactions of HTL algal biocrude oil to produce liquid hydrocarbon fuels. The NiMo carbide synthesized through co-impregnation and carbothermal reduction showed high activity for oxygen removal due to its high acidity and higher active phase exposure to active hydrogen. The upgraded biocrude oil at reaction condition of T=400 ºC, t=2.7 h and 10 wt.% of catalyst loading revealed an oxygen reduction percentage of 94% with HHV of 43.9 MJ/kg.

Biography

Shima Masoumi has completed her Ph.D. from University of Saskatchewan, Canada. I am currently a postdoc at North Carolina A&T state university, CREST bioenergy center. Her research interests focus on production of renewable energies. She has published high quality papers in reputed journals and has been serving as a speaker to Catalysis, Chemical Engineering and TechnologVirtual-2022.

Daouia Medine, Kheir Eddine KHODJA, Feth Allah Allal, Amira Bouanani and Zohra Bengharez

Laboratory of Advanced Materials and Physicochemistry for Environment and Health, Djillali Liabes University of Sidi Bel Abbes, Sidi Bel Abbes, Algeria. E-mail id: dmedine@yahoo.fr

Green and effective adsorbent based on alginate and local arabic gum for cationic dye removal. Kinetic study and optimization using a full factorial experimental design

The discharge of dye effluents into aquatic environments without proper disposal poses veritable threats to the quality of water as well as to the public health. Thus, the treatment of these effluents constitutes a real challenge to be taken up. For this,extensive works have been carried out on the development of sustainable and green effective adsorbent materials. Recently, polysaccharides such as sodium alginate, chitosan and gum, have seen intense research activity because they are biodegradable, efficient, inexpensive and eco-friendly materials and that could be low-cost-alternative adsorbents for wastewater treatment. The present study is focused on Methylene Blue (MB) removal from aqueous solution using alginate/ local Arabic gum composite. Design of experiments based on a full factorial at two levels was applied to investigate the effect of parameters namely pH, contact time, initial MB concentration and adsorbent mass. The analysis of variance (ANOVA) results indicated that pH, initial MB concentration, contact time, biocomposite mass and the interaction term (initial concentration MB–contact time) have a significant influence on MB removal yield with Pvalue <0.05. Among the studied variables, contact time was found to be the most consequential factor for MB removal with Pvalue <0.0001. The prescribed first-order regression model fitted well to the experimental data with a high coefficient of determination (R^2=0.970). The optimal values of pH, adsorbent mass, initial MB concentration and contact time were 10.8g, 50 mg/L and 100 min respectively. Under these optimum conditions, the MB removal was about 84,25% which was very close to the predicted value by the statistical design (80.44%).

Biography

I am Medine Daouia, professor-researcher at Sidi Bel Abbés University. I have completed my PhD from INRS (Énergie Matériaux Telecommunications Research Center), University of Québec, Canada. Currently, my field research is advanced materials for environment and health