CHEMISTRY WORLD CONFERENCE

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CHEMISTRY 2021

BOOK OF ABSTRACTS

CHEMISTRY WORLD CONFERENCE

SEP 06-07, 2021

Theme:

To innovate and integrate advances in Chemistry

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About MAGNUS GROUP

Magnus Group (MG) is initiated to meet a need and to pursue collective goals of the scientific community specifically focusing in the field of Sciences, Engineering and technology to endorse exchanging of the ideas & knowledge which facilitate the collaboration between the scientists, academicians and researchers of same field or interdisciplinary research. Magnus group is proficient in organizing conferences, meetings, seminars and workshops with the ingenious and peerless speakers throughout the world providing you and your organization with broad range of networking opportunities to globalize your research and create your own identity. Our conference and workshops can be well titled as 'ocean of knowledge' where you can sail your boat and pick the pearls, leading the way for innovative research and strategies empowering the strength by overwhelming the complications associated with in the respective fields.

Participation from 90 different countries and 1090 different Universities have contributed to the success of our conferences. Our first International Conference was organized on Oncology and Radiology (ICOR) in Dubai, UAE. Our conferences usually run for 2-3 days completely covering Keynote & Oral sessions along with workshops and poster presentations. Our organization runs promptly with dedicated and proficient employees' managing different conferences throughout the world, without compromising service and quality.

About Chemistry 2021

CHEMISTRY 2021 is one of the most important assemblies for providing a podium within the chemists and chemical professionals. This meeting is assured to exceed your vision about the new approaches and techniques involved in trending discoveries. It also provides you a high quality communication with the global experts representing both academia and industry; and will build collaborations among scientists. The conference scientific program deals with the major areas of specialized topics related to all aspects of chemistry.

KEYNOTE FORUM

DAY 1

CHEMISTRY WORLD CONFERENCE

SEP 06-07, 2021

Alexander Bagaturyants

Federal Research Center Crystallography and Photonics Russian Academy of Science, Russian Federation

Theoretical modelingin organic nanophotonics

Multiscale atomistic simulation methods are applied to studying excited molecules in organic materials and their interaction with neighboring molecules. The formation of exciplexes at the interface between layers of organic molecules in multilayer structures, typical for organic light-emitting diodes and for other devices of organic electronics and photonics, makes an important contribution to their emission spectrum. Adequate models of a complex system containing excited components and suitable methods for the description of charge and/or excitation transfer are considered. These following steps are briefly discussed Multiscale atomistic simulation methods are applied to studying excited molecules in organic materials and their interaction with neighboring molecules. The formation of exciplexes at the interface between layers of organic molecules in multilayer structures, typical for organic light-emitting diodes and for other devices of organic electronics and photonics, makes an important contribution to their emission spectrum. Adequate models of a complex system containing excited components and suitable methods for the description of charge and/or excitation transfer are considered. These following steps are briefly discussed: the construction and use of the library of parameters of the EFP (Effective Fragment Potentials) approximation for the simulation of environment of luminescent dopants and transport molecules in the layers the estimation of the accuracy of the obtained results; the creation of a program complex for the construction of the polarized environment using the library of parameters in the EFP approximation; the investigation of the effect of the polarized environment on the positions of triplet and singlet levels of luminescent dopants; the development and improvement of approaches to the calculation and interpretation of absorption spectra of supramolecular systems using hybrid QM/MM methods; studying the formation of exciplexes forming at the interface between two organic semiconducting layers by molecular dynamics and the calculation of their properties by quantum chemical methods; selection and development of force fields for metal-organic complexes, molecular dynamics simulation of such system using these force fields; the development and improvement of the computational approach based on multiconfigurational quantum-chemical calculations of radiative and intersystem crossing constants; studying spin-mixed states of phosphorescent iridium(III) complexes, the calculation of radiative phosphorescence constants, and analysis of channels of nonradiative phosphore scencequenching.

Audience Take Away:

- The formation of exciplexes at the interface between layers of organic molecules in multilayer structures; the construction and use of Effective Fragment Potentials for the simulation of environment of luminescent dopants and transport molecules in the layers; the effect of the polarized environment on the positions of triplet and singlet levels of luminescent dopants; selection and development of force fields for metal-organic complexes; studying spin-mixed states of phosphorescent iridium(III) complexes, the calculation of radiative phosphorescence constants, and analysis of channels of nonradiative phosphorescence quenching.
- The audience will be able to use this knowledge for the investigation and development of organic multilayer light-emitting and photovoltaic devices.
- This knowledge will help the audience in their work on the development of new promising materials for photonics applications. This knowledge will also be helpful to other faculty for the use of modern methods of multiscale molecular modeling in their research and teaching. This will provide a practical solution to problems that could simplify or make a designer's job more efficient. It will improve the accuracy of a design and provide new information to assist in a design problem.

Biography

Prof. Alexander Bagaturyants was graduated from D.I. Mendeleev Institute of Chemical Technology, Moscow, Russia in 1962, obtained his PhD degree, Dr. Sci. degree, and the academic title of professor in 1968, 1987, and 1992, respectively, in physical chemistry. From 1997 to up to now he is the head of laboratory, chief researcher at the Photochemistry Center RAS, Federal State Institution "Federal research center Crystallography and Photonics Russian Academy of Science" (FRC Crystallography and photonics RAS). His main research interests are in the field of atomistic multiscale simulations of organic functional materials. He is an author of more than 90 research articles and one monograph (MultiscaleModeling in Nanophotonics: Materials and Simulations, Alexander Bagaturyants, Mikhail Vener, Singapore, Pan Stanford Publishing, 2018, 274 Pages, ISBN 9789814774406.)

Fathi Habashi

Laval University, Canada

Metallurgical chemistry

Metallurgical Chemistry gives a brief history of the development of metal extraction technology, then discusses the metal and mineral industries, and physical and physicochemical methods of enriching ores. Various methods of recovering metals from ore: hydrometallurgy, pyrometallurgy, and electrometallurgy are thoroughly detailed. It covers the theory of metallurgical reactions, and reviews pollution problems in the metallurgical industry. It provides an overview of the field that may be useful to persons in a number of disciplines. It will serve as a review for mining, metallurgical, and chemical engineers, as well as geologists and mineralogists. For chemists working in related fields such as refractories, fertilizers, organic solvents, or synthetic resins, and for chemistry students.

Biography

Fathi Habashi is a Professor Emeritus of Extractive Metallurgy, born in Egypt, holds a B.Sc. in Chemical Engineering from Cairo, Dr.techn. from Vienna, and honorary degrees from Oruro in Bolivia, Saint Petersburg Mining Institute in Russia, Technical University of Engineering in Lima, and San Marcos University also in Lima. He held the Canadian Government Scholarship in Ottawa, taught at Montana School of Mines, then worked at the Research Department of Anaconda in Tucson, Arizona before joining Laval in 1970. Habashi desired to develop an integrated understanding of extractive metallurgical processes and to put them into a systematic order within a historical background. He was a Guest Professor in a number of universities and published some textbooks on metallurgy. He edited Handbook of Extractive Metallurgy in 1996 in 4 volumes.

Victor John Law
University College Dublin, Ireland

The application of microwave generated steam ovens for the decontamination of respirators and face masks

During the two influenza pandemic's of this century (caused by H1N1 and SARS-Cov-2), experimental microwave generated steam (MGS), has shown potential, for decontamination of respirators and surgical masks. Recent review articles of the decontamination of single-use face respirators / masks have been primarily performed within the health sector, with particular focus on the disinfection efficiency of the process. However, as with all datasets collected from different research sources, experimental conditions are not reported in a consistent manner. These reports generally provide an overview of MGS microwave conditions, however they did provide sufficient detail in standard microwave engineering terminology from which the thermodynamic of process can be obtained. In particular how the parameters: power density (W L-1) and available energy budget (J s-1 x J = J) is reflected in the processed respirator / mask outcome. The understanding of these parameters and how they influence the decontamination outcome is necessary for further development of the MGS process and enable it to fulfill some of Green chemistry goals (reduce the amount of harmful chemical products in the environment, and limit the number of respirators and masks required to be manufactured. The work reviews the treatment of N95-type respirators, surgical and medical masks, and in this context looks at microwave oven-related injuries and fires. In addition, the thermodynamics of converting liquid-phase water into steam in terms of available microwave power (W) calculated power density (W/ft3, W L-1) and process energy budget verses the decontamination outcome. Using this knowledge, meaningful recommendations can be made on the suitability of individual microwave oven for the treatment, in addition what respirators should be used, or not be used in MGS decontamination process. Finally, if an oven cannot be found, then recommendation for how to go about designing a microwave oven for MGS decontamination is given.

Audience take-away:

- The problems with microwave generated steam (MGS) decontamination of respirators when using a microwave oven, Green chemistry: Using water and a microwave oven enable respirators reuse up 3 times. Thereby not using harmful chemicals and reducing waste.
- Microwave oven-related scald and burns. The thermodynamics of microwave heating and how to keep safe at work and at home.
- A microwave engineering approach to MGS availed power density (W/ ft3, W/L) and energy budget (J s-1 divided by irradiation time = J), or how to choosea suitable microwave oven for MGS.
- What is required to design and build a microwave oven suitable for MGS of respirator decontamination?

Biography

Dr. Victor John Law received his B.Scs. degree from The Open University in 1985 while at the Cavendish Laboratory, Cambridge, U.K. He obtained his Ph.D. degree from the University of Ulster, Belfast, Northern Ireland in 2005. He has been a Senior Research Fellow with University College London, London, U.K and Dublin City University, Dublin Ireland. Since 2012, he has held the post of Senior Research Engineer at University College Dublin, Ireland. Dr. Law has Published over 120 refereed articles (H-index = 19 (mean = 17) for the top 100 publications and holds one patent). His research interests include material processing and microwave and plasma drive circuits.

Osman Adiguzel
Firat University, Turkey

Shape reversibility and the role of thermomechanical treatments in shape memory alloys

Shape memory effect is a peculiar property exhibited by a certain alloy systems in the β-phase fields, and result of thermal and mechanical processes. These alloys have dual characteristics called thermoelasticity and superelasticity, governed by successive thermal and stress induced martensitic transformations, and performed thermally and mechanically, respectively. Thermal induced transformation occurs along with lattice twinning on cooling and ordered parent phase structures turn into twinned martensite structures. Twinned martensite structures turn into detwinnedmartensite structures by means of stress induced transformation by deforming plastically in martensitic condition. Strain energy is stored in the material with deformation and released upon heating, by recovering the original shape in bulk level, and cycles between original and deformed shapes on heating and cooling, respectively. Superelasticity is also a result of stress induced martensitic transformation and performed in only mechanical manner in the parent austenite phase region. The materials are deformed just over Austenite finish temperature, and shape recovery is performed simultaneously upon releasing the applied stress. The ordered parent phase structures turn into the detwinned structures by means of stress induced martensitic transformation, like the deformation step in shape memory. Superelasticity is performed in non-linear way, unlike normal elastic materials, loading and unloading paths in stress-strain diagram are different, and hysteresis loop reveals energy dissipation.Shape memory effect is performed thermally in a temperature interval depending on the forward and reverse transformation, on cooling and heating, respectively, and this behavior is called thermoelasticity. Deformation at different temperatures in intermediate region between Martensite start and Austenite finish temperatures exhibits different behavior beyond shape memory effect and superelasticity, and the materials partially recover original shape. Thermal induced martensitic transformation occurs as martensite variants with the cooperative movement of atoms in <110>-type directions on {110}-type close packed planes of austenite matrix, by means of shear-like mechanism. The {110}- plane family represent 6 planes, and totally 24 martensite variants occur. Copper based alloys exhibit this property in metastable β-phase region, which has bcc-based structures. Lattice invariant shears are not uniform in copper based shape memory alloys, and the ordered parent phase structures martensitically undergo the non-conventional complex layered structures on further cooling.The long-period layered structures can be described by different unit cells as 3R, 9R or 18R depending on the stacking sequences on the close-packed planes of the ordered lattice. The unit cell and periodicity is completed through 18 layers in direction z, in case of 18R martensite, and unit cells are not periodic in short range in direction z. In the present contribution, x-ray diffraction and transmission electron microscopy studies were carried out on two copper based CuZnAl and CuAlMn alloys. X-ray diffraction profiles and electron diffraction patterns exhibit super lattice reflections inherited from parent phase due to the diffusion less character of martensitic transformation. X-ray diffractograms taken in a long time interval show that diffraction angles and intensities of diffraction peaks change with the aging time at room temperature. This result refers to a new transformation in diffusive manner.

Keywords: Shape Memory Effect; Martensitic Transformation; Thermoelasticity; Superelasticity; Lattice Twinning and Detwinning.

Audience take-away:

- Shape memory effect is an interdisciplinary subject and based on microstructure of materials.Crystal structure of copper based shape memory alloys is complicated.
- I will start my presentation with elementary knowledge and continue the importance and application on copper based shape memory alloys. Audience will find the answer of many questions, and my presentation will be beneficial for every delegate and participant.

Biography

Dr Adiguzel graduated from Department of Physics, Ankara University, Turkey in 1974 and received PhD- degree from Dicle University, Diyarbakir-Turkey. He has studied at Surrey University, Guildford, UK, as a post doctoral research scientist in 1986-1987, and studied on shape memory alloys. He worked as research assistant, 1975-80, at Dicle University and shifted to Firat University, Elazig, Turkey in 1980. He became professor in 1996, and he has been retired due to the age limit of 67; following academic life of 45 years. He published over 60 papers in international and national journals; He joined over 100 conferences and symposia in international and national level as participant, keynote speaker with contributions of oral or poster. He served the program chair or conference chair/co-chair in some of these activities. In particular, he joined in last six years (2014 - 2019) over 60 conferences as Keynote Speaker and Conference Co-Chair organized by different companies. He supervised 5 PhD- theses and 3 M.Sc- theses.

SPEAKERS DAY 1

CHEMISTRY WORLD CONFERENCE

SEP 06-07, 2021

CHEMISTRY 2021

Klemen Bohinc
University of Ljubljana, Slovenia

Ions and molecules with internal degrees of freedom

Interactions in electrolyte solutions are of fundamental importance in many chemical and biological systems. These interactions can be altered by the presence of charged molecules/ions, which possess spatially distributed charge. In this presentation, I will consider the influence of charged molecules on the interaction between charged surfaces from theoretical and experimental point of view.

Biography

Klemen Bohinc graduated in the field of Physics at the Faculty of Natural Sciences, University of Ljubljana. In 2001 he received his Ph.D. in Electrical Engineering from the Faculty of Electrical Engineering, University of Ljubljana and in 2012 Ph.D. in Physics from the Faculty of Natural sciences and Mathematics, University of Maribor. Currently he teaches Biomechanics and Biophysics at the Faculty of Health Sciences, University of Ljubljana. His research interests are electrostatics and statistical physics of biological macromolecules/membranes, characterization of nanoparticles as well as microbial adhesion to material surfaces.

Svetlana V. Kochemirovskaia*, VA Kochemirovsky, AG Kuzmin, DA Mokhorov, MN Ryazantsev, AV Isa

Peter the Great St. Petersburg Polytechnic University, Russia

Low-frequency magnetic scanning device for determining the quality of moving metallurgical raw materials

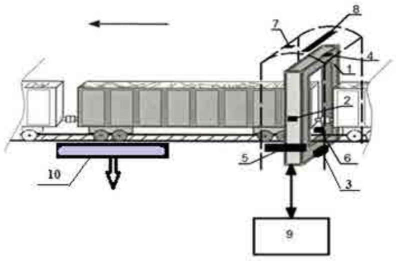
The development of an algorithm for automating the process of measuring the magnetic properties of macroscopic objects in motion is an important problem in various industries, especially in ferrous metallurgy, and in the factories where ferrous scrap is a strategic raw material. The parameter, which basically requires work control, is a hidden mass fraction of a nonmagnetic substance that is present in the ferromagnetic raw material.

Experimental setup and calculation principle is the measuring unit is a solenoid coil located around the railway track. The meter contains two windings: the generating and measuring. The generating winding creates an alternating electromagnetic field with constant parameters of frequency and intensity, in the measuring winding induction current is induced with instantaneous parameters depending on the local properties of the moving core of the solenoid. The object being measured serves as the core. In our case - a moving railway car, the parameters of the measuring device are shown in Table 1.

Figure 1 shows diagram of setup which was used to conduct measurements.Parameters of measuring coil system and electric signals used in measurements are listed in Table 1. Measuring coil system consists of primary and secondary windings.

Table 1: Parameters of the measuring coil system and electric signals used in measureme

Parameter Name	Value	Dimension
Range of alternating current in primary winding	2.00 – 8.00± 0.05	A
Range of alternating magnetic field strength	100 – 1000	A/m
Range of alternating current frequency	20 – 100±1	Hz
Windings real resistance, Ohm - magnetizing winding - measuring winding	1 ± 0.2 12.5 ± 2	Ohm Ohm
Estimated value of the measuring coil cross-section area	43.43 ± 0.01	m2
Reference value of magnetic flux in air	1.9•10-2	Wb
Range of magnetic flux measurement	1.5•10-2–6.0•10-2	Wb
Dimensionsof measuring coil	7190x6040x740	mm



The analytical signal was processed according to the following algorithm:

- calculation of the instantaneous values of the angle of loss as a function of the coordinates along the length of the car,
- calculation of the mass of metal scrap as a function of the integral of the loss angle:

m_src=f(I_φ),

f– is a function describing the dependence of the mass of the core (car with a load) on the integral of the loss angle

- and then the percentage ratio of the mass of the nonmagnetic composition and the ferromagnetic material is calculated:

(M_g-M_m)/M_g *100%=m_n,

Where $\mathbf{M_g}$ is the total weight of the vehicle with a load, measured by means of scales, $\mathbf{M_m}$ is the mass of the ferromagnetic material; **mn** is the percentage of non-magnetic additive.

During the presentation, the error, selectivity and sensitivity of the method will be discussed. Application experience and prospects for improving and reducing the cost of construction. The possibility of using not only for monitoring railway cars, but also freight vehicles and other types of metallurgical raw materials: concentrate, ferroalloys and more.

The proposed method will fully automate the laborious process of quality control of incoming metallurgical raw materials without first unloading the cars. This will allow you to send a complaint to the supplier of low-quality raw materials without overload, evaluation and reclamation. A wagon with low-quality raw materials can be redirected back to the supplier without unloading. This greatly reduces the cost of the process of acceptance, storage and sorting of raw materials at metallurgical enterprises. Information about the system can be laid down in the design at the stage of the logistic study of the roadmap for deliveries and control of finished products. In this case, the process of its installation can be carried out simultaneously with the development of the railway station of a large enterprise. The savings from introducing the system at large metallurgical enterprises can amount to several hundred million dollars a year with a total cost of design and installation costs of 3-4 million dollars.

Biography

Dr. Kochemirovskaia studied Chemistry at the Institute of Chemistry, Saint-Petersburg University 2012. She received her PhD degree in 2017 at the same institution. Since 2020 work in Peter the Great St. Petersburg Polytechnic University as assistant. She has published 13 research articles in SCI(E) journals.

Kseniia O. Ershova*, SV Kochemirovskaia, VA Kochemirovsky, DA Mokhorov, MN Ryazantsev

Nanotechnology Research and Education Centre of the Russian Academy of Sciences, Russia

Influence of atmospheric humidity on the results of determining the age of handwritten inscriptions on questioned documents

Forensic technical examination of documents is in demand to combat the falsification of a document by participants in judicial disputes. Determining the actual date when a certain inscription appeared on a piece of paper is one of the most important and difficult forensic tasks. Written compositions are complex multicomponent mixtures, including dyes, solvents and resins, preservatives, and antioxidants1-4, i.e. complex organic mixtures that undergo changes over time. This is due to numerous technical and legal problems that require description, systematization, and solution.

A typical picture of the evacuation dynamics for volatile components of writing materials is described in most chromatographic studies can be displayed as follows:

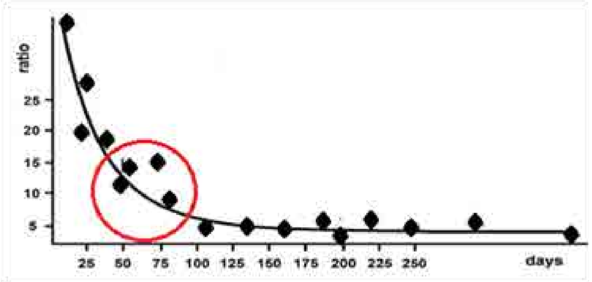


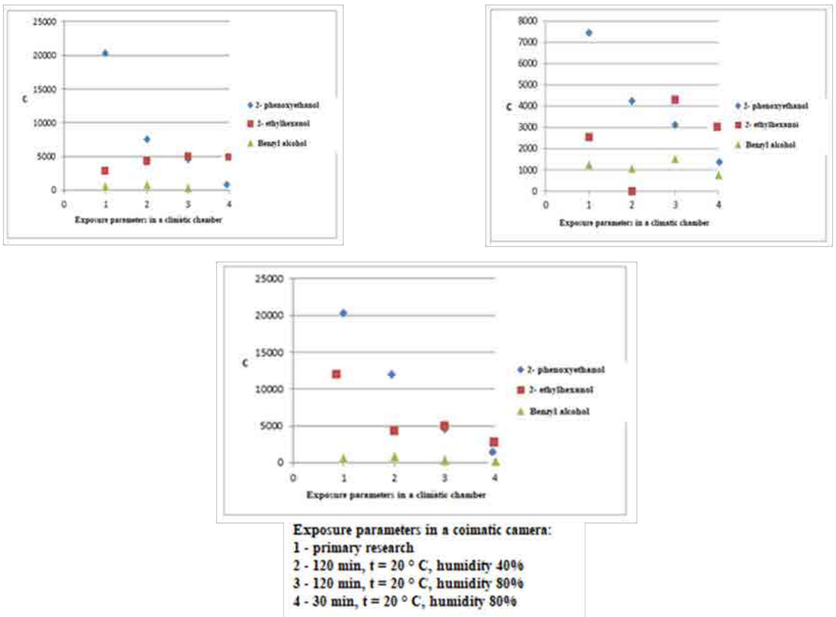
Figure 1: Typical evacuation dynamics for volatile components of writing materials according to chromatographic measurements

Room temperature is believed to be a major factor in aging. However, a much stronger factor of natural influence, in the authors' opinion, should be the atmospheric humidity. In some cases, the amount of 2-phenoxyethanol begins to increase over time according to chromatography-mass spectrometry (red oval in Figure 1).This can be explained by the influence of humidity (Table 1).

Table 1: Some physical and chemical properties of individual ink components*.

	Boiling point (C)	Vapour pressure at 20 C (kPa)	Solubility in water g\l
2-phenoxyethanol	244	0.001	26
glycerol	290	0.0004 (50 C)	unlimited
water	100	0.31	
ethanol	78	5.8	unlimited

As can be seen from Table 1, the two components most frequently analyzed by chromatographic methods: glycerol and 2-phenoxyethanol, are limited or unlimited soluble in water. At the same time, both of them have very high boiling points and low equilibrium vapor pressure (for comparison, the same parameters are given for water and ethanol). This means that in the process of document storage, not pure components, but their diluted aqueous solutions evaporate. In this case, the period of active aging will be determined not by the duration and temperature of storage, but by the number and depth of differences in natural humidity. In particular, this assumption explains the non-monotonic behavior of the time dependence of 2-phenoxyethanol (Figure 1). An experiment was carried out to confirm this assumption. Identical strokes applied at the same time on the same paper were kept in a climatic chamber at the same temperature for different times at different humidity. ChromatekKristall 5000.2 chromatograph was used to study volatile components, and a SenterraBruker Raman spectrometer was used to study dyes. The results of studying the dynamics of volatile components of three arbitrarily selected ballpoint ink are shown in Figure 2 and 3.



Exposure parameters in a coimatic camera:
1 - primary research
2 - 120 min, t = 20 ° C, humidity 40%
3 - 120 min, t = 20 ° C, humidity 80%
4 - 30 min, t = 20 ° C, humidity 80%

Figure 2: Results of chromatographic tests of three ballpoint ink in a climatic chamber

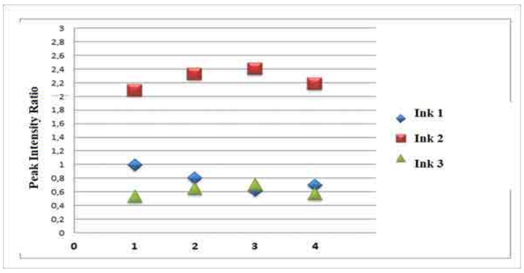


Figure 3: Results of spectroscopic tests of three ballpoint ink in a climatic chamber

The test results show a strong dependence of the content of volatile components on external humidity and an insignificant dependence of the aging parameters of dyes on humidity.

Biography

Dr. Kseniia Ershova (nee Gorshkova) studied Chemistry at the Institute of Chemistry, Saint-Petersburg University 2014. She received her PhD degree in 2018 at the same institution. Since 2020 work in Nanotechnology Research and Education Centre of the Russian Academy of Sciences, Saint Petersburg Academic University. She has published 6 research articles in SCI(E) journals.

Marita Pigłowska*, Beata Kurc
Poznan University of Technology, Poland

Safety issues of lithium-ion cells

Personal electronic devices, electric cars, computers, and emergency power systems all require energy storage. Modern science offers quite a lot of them (electrochemical cells, hydroelectric power stations or thermal stores, flywheels, etc.), but there is still work to improve them.

Lithium-ion cells (LIBs) are one of the most commonly used in smartphones, laptops and electric cars. The advantages of their use are weight, Autonomy, form, can be charge even if not empty, while the biggest disadvantages are their high flammability and relatively high price. Of course, in terms of kinetic and diffusion conditions, it can be postulated that the very diffusion of ions into the porous electrode, as well as their mobility in the electrolytic medium itself, will play a significant role, but as it turns out - only during the so-called conditioning, i.e. the first charge/discharge cycles. In addition, electrostatic interactions do not cause textural and structural changes of the electrode, and thus the cyclical life of (for an example) electrochemical capacitors.

The aspect of safety in electronic devices turns out to be a huge challenge for the world of science. So far, satisfactory power and energy densities, efficiency and cell capacities have been achieved. Unfortunately, the explosiveness, thermal runaway of the cells prevents them from being used in demanding applications such as electric cars at higher temperatures. In LIBs there are different electrolytes used: flammable liquid inorganic electrolytes, and less flammable composite polymer-ceramic electrolytes, ionic liquids (IL), polymeric ionic liquids, polymer electrolytes: solvent-free polymer electrolytes (SPEs), gel polymer electrolytes (GPEs), and composite polymer electrolytes (CPEs). Also, different flame retardants are used to prevent the thermal runaway and combustion of the lithium-ion battery. Due to the low biodegradability of flame retardants, more and more often work is done on ingredients commonly available in nature, such as starch, cellulose or lignin. The main aim of the work is to present the flame retardant properties of starch in a lithium-ion cell and its influence on the electrochemical performance of the graphite anode. In order to show the flame-retardant properties of starch, the Flash point, Self-extinguishing time is determined, and then, in order to check the efficiency of the cell's operation, an electrochemical test is carried out using electrochemical impedance spectroscopy.

Audience take-away:

- It could be interesting topic for the people, who care about our planet and also about the future which is oriented on electric vehicles and the main disadvantage – flammability aspect.
- The audience could use this topic to learn more about inside processes which occur in lithium-ion cells for optimalization of the safe construction of this cell for EVs.
- This topic could be used in automotive industry, as green chemistry aspect, in electrochemical studies, kinetics and catalysis. This provides a practical solution to a problem that could simplify or make a designer’s job more efficient. It gives the improvement of the accuracy of a design of safe LIB and also information to assist in this problem.
- Combining practical knowledge with theory (learning and working in a laboratory has a very big impact on our lives).

Biography

Eng. Marita Pigłowska (graduated in 2021), current master student of Composites and Nanomaterials at Poznan University of Technology. In her scientific carrier she published 9 articles in international reviewed journals. She took part in 2 international conferences (presented topics: flammability of lithium-ion cells (she won the prize for the best student oral presentation) and use fuel cells and batteries in automotive industry). In 2019 she became the winner of the 2nd place in Hydrogen Competition in Poland. In 2021 she won the Veolia contest for the best engineering thesis and took part in Summer School of Veolia.

Ayse Sap*, Mehmet Yaman
Firat University, Turkey

Optimization and validation of HPLC-DAD method for the quantification of curcuminoids in turmeric (Curcuma Longa)

Curcumin and its derivatives named curcuminoids are a naturally occurring polyphenolic compounds extensively marketed as a nutraceutical. The wide therapeutic potential of curcumin is highly explored by the authors. Therefore, many inventions were made by pharma-industries for its clinical use and to bring it to the market as a drug.

In this study, a simple, rapid and sensitive High-Performance Liquid chromatographic (HPLC) method for simultaneous determinations of curcumin (C), desmethoxycurcumin (DMC) and bis-desmetoxycurcumin (BDMC) was optimized and validated.

Separation of curcumin, DMC and BDMC was performed using C18 column. Six factors including the solvent type, ratio of mobile phase, flow rate of mobile phase, column temperature, enjection volüme, and wavelength were investigated. Taking into consider retention time, peak area, resolution and tailing factor, the optimum conditions were preferred: methanol as solvent, THF/Citric A (40/60) as mobile phase, rate of mobile phase = 0,5 mL/min, temperature of column = 300C, injection volume= 20 microliteri and wavelength = 425 nm.

Audience take-away:

- This research can help listeners about method validation and optimization in HPLC analysis.
- The method is further used to determine ppm levels of curcumin derivatives and recovery was found to be 90%.
- The proposed analytical method can be used for the quantification of curcumin in medicinal plants.

Biography

Ayşe is a PhD student at the Firat University, Turkey and graduated as MS in 2013 at the same institution.

Seongwoo Woo
Addis Ababa Science & Technology University, Ethiopia

Improving the fatigue of newly designed mechanical system subjected to repeated impact loading

To Improving the fatigue of newly designed mechanical system subjected to repeated loading, this paper develops parametric accelerated life testing (ALT) as a systematic reliability method to produce the reliability quantitative (RQ) specifications—mission cycle—for recognizing missing design defects in mechanical products as applying the accelerated load. Parametric ALT is a way to enhance the prediction of fatigue failure for mechanical systems subjected to repeated impact loading. It incorporates: A parametric ALT plan formed on the system BX lifetime, a fatigue failure and design, customized ALTs with design alternatives, and an assessment of whether the last design(s) of the system fulfils the objective BX lifetime. A BX life concept with a generalized life-stress model and a sample size equation are suggested. A domestic refrigerator hinge kit system (HKS), which was a newly designed mechanical product, was used to illustrate the methodology. The HKS was subjected to repeated impact loading resulting in failure of the HKS in the field. To conduct ALTs, a force and momentum balance was utilized on the HKS. A straightforward impact loading of the HKS in closing the refrigerator door was examined. At the first ALT, the housing of the HKS failed. As an action plan, the hinge kit housing was modified by attaching inside supporting ribs to the HKS to provide sufficient mechanical strength against its loading. At the second ALT, the torsional shaft in the HKS made with austenitic ductile iron (18 wt% Ni) failed. The cracked torsional shaft for the 2nd ALTs came from its insufficient rounding, which failed due to repeated stress. As an action plan, to have sufficient material strength for the repetitive impact loads, the torsional shaft was reshaped to give it more rounding from R0.5 mm to R2.0 mm. After these modifications, there were no problems at the third ALT. The lifetime of the HKS in the domestic refrigerator was assured to be B1 life 10 years.

Audience take-away:

- New design methodology for mechanical systems.
- Directly applicable in field to improve the fatigue of product.
- Parametric accelerated life testing (ALT) as a systematic reliability method to produce the reliability quantitative (RQ) specifications.

Biography

Dr. Woo has a BS and MS in Mechanical Engineering, and he has obtained PhD in Mechanical Engineering from Texas A&M. His major research is in energy system such as HVAC and its heat transfer, optimal design and control of refrigerator, reliability design of mechanical components, and failure Analysis of thermal components in marketplace using the Non-destructive such as SEM & XRAY. Especially, he developed parametric accelerated life testing (ALT) as new reliability methodology. If there is design fault in the mechanical system that is subjected to repetitive stress, it will fail in its lifetime. Engineer should find the design faults by parametric ALT before product launches. In 1992–1997 he worked in Agency for Defense Development, Chinhae, South Korea, where he has researcher in charge of Development of Naval weapon System. In 2000-2010 he had been working as a Senior Reliability Engineer in Side-by-Side Refrigerator Division, Digital Appliance, SAMSUNG Electronics, where he focused on enhancing the life of refrigerator as using parametric the accelerating life testing. Now he is working as associate professor in mechanical department, Addis Ababa Science & Technology University.

Mohd Sajid Ali*, Hamad A Al-Lohedan
King Saud University, Saudi Arabia

Interaction of anticancer drug gemcitabine with human plasma protein: Experimental and computational analysis

The interaction of common anticancer drug gemcitabine with human serum albumin (HSA), an important plasma protein, has been studied in details. A slight hyperchromic shift in the difference UV absorption spectra of HSA on the addition of gemcitabine gave a primary idea of the possible complex formation between them. Inner filter effect played an important role in the observed fluorescence quenching of HSA by gemcitabine that can be understood by comparing the observed and corrected fluorescence intensities obtained at $\lambda ex = 280$ nm and 295 nm. There was a large difference between the observed quenching at these two excitation wavelengths that becomes negligible after the correction of inner filter effect (IFE). Quenching of intrinsic fluorescence of HSA by gemcitabine increases with increase in temperature which suggested the existence of dynamic type of quenching. Overall, gemcitabine shows weak to fair interaction with HSA with binding ratio of around 1. Secondary structural analysis showed that low concentrations of gemcitabine didn't affect the native structure of protein, however, higher concentrations affects it slightly with partial unfolding. Molecular docking simulation was also performed to understand the mode of binding as well as the most preferred binding site of gemcitabine into HSA.

Audience take-away:

- From this research, the effect of IFE, a known phenomenon in the fluorescence spectroscopy and causes the fluorescence decrement of the fluorophore by absorbing some of the radiations falls on the sample, on the fluorescence quenching of a protein by a ligand could be understood if one is considering the different excitation wavelengths for the study.
- The observed quenching will be dependent on the extent of the absorption of the light at a particular wavelength. Thus, if the study would be carried out at two excitation wavelengths which have different absorbances, the quenching will be different in each case; however, correction of the IFE could give the clear picture.
- The binding extent of a pharmacological active compound with plasma proteins like serum albumin is an important factor in understanding its therapeutic action.
- The substances which bind strongly take more time to release from the binding proteins while very weak or no binding may cause the drug not to reach at its site of action. From this study it can be seen that serum albumin are good carrier for the gemcitabine.
- This research is helpful in teaching as well as in research. In the teaching the inner filter effect could be demonstrated to the students and how it affects the actual data at various wavelengths could also be taught. In fluorescence spectroscopy related research, the understanding of the IFE and its correction are necessary.

Biography

Dr. Ali Studied M.Sc. Chemistry from the Aligarh Muslim University, Aligarh, India in 2002. He then joined the research group of Prof. Kabir-ud-Din at the same institute and received his Ph. D. degree in 2006. During briefly teaching in an engineering college, he got an independent postdoctoral research project named "Young Scientist Fellowship" award in 2008 and remained to stay in the same research group to accomplish the goals of the project. In 2010 he joined the Department of Chemistry, College of Science, King Saud University as an Assistant Professor. He is now working as an Associate professor in the same institute. He has published more than 70 research articles in SCI(E) journals.

Yasemin Yildiz
Sakarya University, Turkey

Is it possible to remove SARS-CoV-2 with membranes in water and wastewater?

Several agents around the world have caused the pandemic. Looking at the last 17 years, it is seen that there have been three major outbreaks caused by the coronavirus. The World Health Organization (WHO) announced on March 11, 2020, that the most recent epidemic, SARS-CoV 2, had turned from an epidemic into a global pandemic. The main transmission route of the virus aerosol/droplet inhalation and person-to-person contact, even so, there is evidence to suggest the presence of viral RNA in wastewater. This evidence raises the need for a better understanding of wastewater, among other risk factors for human health.

A potentially deadly virus for SARS-CoV-2 and some precautions should be taken to conduct scientific tests. For this reason, some studies use murine hepatitis virus (MHV) instead of SARS-CoV-2 to test against the dangers specified in the Biosafety and COVID-19 (SARS-CoV-2) guidelines. It is known that the membranes used for virus separation are mostly microfiltration and ultrafiltration. Pore size and virus size compatibility are important for good separation in these membranes. The penetration of small virus particles into the pores of the membrane shortens the life of the membrane.Some studies overcome this difficulty with coating.

This study focuses on the current knowledge about SARS-CoV-2 and its presence in wastewater/water, the use of membrane technologies to remove SARS-CoV-2 in wastewater/water, and the impact of SARS-CoV-2 on public health. Although available data for eradicating SARS-CoV-2 by purification techniques are limited, the membrane could be a promising technique to mitigate the impact of the ongoing COVID-19 outbreak.

Audience take-away:

- Information will be gained on the relationship of waste with covid and its impact on public health.
- The focus will be on the possibility of covid contamination of wastewater and its removal by membranes.
- By integrating this method into cities' wastewater management, the spread of the virus can be significantly reduced.

Biography

Dr. Yasemin studied Chemistry at Sakarya University, Turkey, and graduated as MS in 2008. She then joined the research group of Neutec. Ltd. She has been working as a lecturer at Sakarya University since 2010. She received her Ph.D. degree in 2014 at the same institution. As a lecturer, Dr. Yasemin Yıldız received an invitation from the University of Pristina to study at the Chemistry Department, Faculty of Education at Prizren University, in 2014. Her research was related to membrane preparation, extraction and metals separation, membrane stability, and lifetime during her visit.

magnus
Group

POSTERS DAY 1

CHEMISTRY WORLD CONFERENCE

SEP 06-07, 2021

Maria Guć*, Grzegorz Schroeder
Adam Mickiewicz University in Poznan, Poland

Use of molecularly imprinted polymers (MIPs) and magnetic molecularly imprinted polymers (magMIPs) in flowing atmospheric-pressure afterglow mass spectrometry (FAPA-MS)

Polymers with a molecular imprint, selective for the following compounds were obtained: flavonoids – quercetin; female sex hormones – estrone and β-estradiol; non-steroidal inflammatory drugs – naproxen, diclofenac, and ibuprofen; herbicides – 2, 4-dichlorophenoxyacetic acid (2, 4-D) and 4-chloro-2-methylphenoxyacetic acid (MCPA), flavonoid glycosides – rutin and cyanogenic glycoside – amygdalin. For selected MIPs, magnetic analogs were synthesized by the core-shell method. The magnetic core consisted of $Fe3O4$ nanoparticles, coated with a polymer obtained by the same synthesis as MIPs. The use of a magnetic core allowed for the fast and efficient magnetic separation process of mag-MIPs from solutions with neodymium magnet (few seconds). In addition, the use of spherical $Fe3O4$ nanoparticles as a magnetic core surrounded by a polymer coating of mag-MIPs resulted in the location of specific recognition sites in the outer layer of the material, rendering them more accessible during the analyte binding, thus increasing the efficiency of mag-MIPs in comparison to MIPs. MIPs and mag-MIPs were used for the analysis of chemical compounds by the two techniques ESI-MS and FAPA-MS. In the FAPA-MS method, MIPs/mag-MIPs are introduced into the sample, where the analyte is bound in the polymer structure. The MIPs/mag-MIPs along with the bound analyte are then isolated from the solution and analyzed directly from the polymer structure. The thermally released analyte is ionized with low-temperature plasma under atmospheric pressure and, together with the carrier gas, transported to the mass spectrometer, where the ions are analyzed. This approach not only shortens the time and simplifies the analysis protocol, but in many cases significantly lowers the limit of detection of low-molecular-weight organic compounds, solves the problem of fragmentation, dimers formation, sodium ions adducts, complex formation, and solvent interactions. Different types of plasma torches were tested (V-FAPA, L-FAPA). Moreover, the lower consumption of solvents makes the proposed method environmentally friendly and compliant with the principles of Green Chemistry. A protocol combining the use of MIPs/mag-MIPs with FAPA-MS analysis was successfully applied to the analysis of real samples.

In the last stage of the research, it was shown that the polymer structure itself does not adversely affect living organisms, therefore MIPs/mag-MIPs can be used in environmental samples. Toxicity tests were carried out on two types of organisms: Daphnia magna Straus and Tetradesmus obliquus (Turpin) M.J. Wynne. It was proved that the initial assumptions were correct and the combination of the technology of producing polymers with a molecular imprint with the method of direct FAPA-MS analysis with plasma ionization solves many complex analytical problems.

The proposed methods can be successfully used in the pharmaceutical industry for the determination of active substances in drugs or their residues, e.g. in sewage, in the medical industry, for example, for the determination of substances in the blood, in sport for the determination of prohibited substances from urine or blood, in the cosmetics industry for analysis substrates, products, or wastewater, and the protection of the environment.

Audience take-away:

- Methods of obtaining selective Molecularly Imprinted Polymers (MIPs) and their magnetic analogs (mag-MIPs) for the isolation and pre-concentration of analytes will be presented.
- The direct Flowing Atmospheric-Pressure Afterglow Mass Spectrometry (FAPA-MS) analysis of bound small organic compounds from MIPs/mag-MIPs structures will be presented. It is a new analytical technique using low-temperature plasma ionization that allows qualitative and quantitative analysis of a compound from a solid phase.
- Various types: V-shaped and L-shaped plasma torches will be presented.
- Analytical parameters for the technique combining the use of MIPs/mag-MIPs and the ESI-MS and the new technique using MIPs/mag-MIPs in FAPA-MS analysis will be compared. The results obtained for the analysis of environmental samples will be presented.
- Discussion of the toxicity of the obtained polymeric materials on organisms, while using them for the analysis of environmental samples, e.g. water from rivers, lakes.

Biography

M.Eng. Maria Guć studied Chemistry at the Adam Mickiewicz University in Poznań, Poland, and graduated MS in 2016. During her master's degree, she started her studies, at the Faculty of Chemical Technology at the Poznań University of Technology and graduated Bachelor of Engineering in 2019. Immediately after graduation fellowship supervised by Prof. Grzegorz Schroeder at the Department of Supramolecular Chemistry, Faculty of Chemistry, Adam Mickiewicz University in Poznan. She is a Ph.D. student at the same university. She publishes articles in the field of analytical, bioanalytical, and supramolecular chemistry.

Tanya Yordanova*, Ivanka Dakova, Irina Karadjova
University of Sofia “St. Kliment Ohridski”, Bulgaria

Determination of labile copper species in water samples based on solid-phase extraction with ion-imprinted polymer

The toxicity, bioavailability and mobility of copper in aquatic environment strongly depend on its speciation rather than on total Cu concentration. Various approaches have been developed for quantitation of mobile and bioavailable metal fractions e.g. methods based on voltammetric measurements, DGT and PLM techniques as well as speciation codes like Visual MINTEQ, WHAM etc. Ion-imprinted polymers(IIPs) are synthetic smart materials with artificially generated recognition sites able to specifically rebind a target chemical species, i.e. the imprinted ion. Taking into account their high selectivity toward free metal ions, solid phase extraction (SPE) by IIP could be a good approach for fast and reliable quantitation of free copper in natural waters as well as its labile chemical species. For this purpose, Cu(II)-IIP has been prepared by copolymerization of methacrylic acid as a monomer, trimethylolpropanetrimethacrylate as a crosslinking agent and 2,2'-azo-bis-isobutyronitrile as an initiator, in the presence of 4-(2-pyridylazo)resorcinol as a chelating ligand and Cu2+ as a template ion. The chemical structure and morphology of the Cu(II)-IIP have been characterized using elemental analysis, FTIR and SEM. Selectivity of the synthesized IIPtoward labile Cu(II) species was evaluated in a batch system. The optimal pH values for the quantitative sorptionof Cu(II) was 7-8, and complete desorption was achieved by elution with 1 M HNO3. Cu(II)-IIP has been successfully appliedfor separation of labile copper species in model solutions containing chelating agents as EDTA, glycine, citric, tartaric and humic acid and in real samples (surface waters) followed by instrumental measurement using ETAAS or ion-selective electrode. The concentrations of labile copper species determined by the proposed SPE procedure were in a good agreement with the values calculated by Visual Minteq.

Acknowledgement: The authors gratefully acknowledge the financial support provided by the Bulgarian National Scientific Foundation (Grant DN 19/10 SmartSpeciation).

Audience take-away:

- The main principles of ion-imprinting technique in a polymer matrix.
- A simple and reliable procedure for fast solid-phase extraction of labile Cu species in natural water samples.
- The great potential of ion-imprinted polymers in speciation analysis of trace copper in aquatic systems.

Biography

Dr. Yordanova studied Chemistry at the Sofia University, Bulgaria and graduated as MS in 2010. She then joined the research group of Prof. Karadjova at the Department of Analytical Chemistry, Faculty of Chemistry and Pharmacy, Sofia University St. Kliment Ohridski. She received her PhD degree in 2014 at the same institution. After defense of her PhD thesis, she obtained the position of Chief Assistant Professor at the same department. She has published 12 research articles and 1 book chapter.

Ivanka Dakova*, Irina Karadjova
Sofia University “St. Kliment Ohridski”, Bulgaria

New polymeric ionic liquid as a smart material for As(V)/As(III) speciation analysis

During the last years, the introduction of the functional groups such as ionic liquids into polymers is giving rise to a new class of smart materials called polymeric ionic liquids (PILs). Due to their specific properties emanating from the ionic liquid units and their intrinsic polymeric nature, PILs find applications in various areas, such as analytical chemistry, biotechnology, gas separation, catalysis, etc. In this study we report the synthesis and characterization of new polymeric ionic liquid and its application for arsenic determination and speciation in surface waters. PIL was synthesized via chemical modification of polymeric precursor. In the first step, poly(glycidyl methacrylate-co-trimethylolpropanetrimethacrylate) particles were prepared by precipitation copolymerization in porogen solvent. These polymer particles were further modified by chemical binding with 1-methylimidazole (MIA) to obtain PIL material ‑ poly(MIA). The new synthesized poly(MIA) was characterized using elemental analysis, Fourier transform infrared spectroscopy, scanning electron microscopy, and nitrogen adsorption–desorption measurements. The effect of the porogen solvents acetonitrile, toluene and methanol on particle size and morphology was established. The adsorption properties of poly(MIA) toward As(III) and As(V) were studied by batch procedure. An excellent separation of As(V), selectively adsorbed on the poly(MIA), from As(III) was achieved at pH 7–9 for 20 minutes. A nitric acid was found to be the most efficient eluent for quantitative desorption of the retained As(V). The maximum adsorption capacity of poly(MIA) toward As(V) was 14.3 μmol/g polymer. The kinetic data were well described by pseudo-second-order equation while Langmuir model is best fitted to isotherm data. Experiments performed for selective determination of As(VI) in surface waters showed that the interfering matrix does not influence the extraction efficiency of poly(MIA). The analytical procedure for As(V) determination in surface waters was developed and validated through analysis of certified reference materials.

Acknowledgements: We acknowledge the financial support from the Bulgarian National Scientific Foundation (Grant DN 19/10 Smart Speciation).

Audience take-away:

- The audience will learn about the synthesis and characterization of a new polymeric ionic liquid and its application for As(III)/As(V) speciation analysis.
- The audience will get an understanding on the parameters that need to be controlled to ensure quantitative sorption / desorption of the studied arsenic species.
- The audience will learn about the analytical characteristics (LOD, LOQ, RSD) of the proposed analytical procedure for As (III) / As (V) speciation analysis.
- The research shows a new type of polymer materials that could be of interest to researchers working in polymer and analytical sciences.

Biography

Dr. Ivanka Dakova studied Chemistry at the Sofia University, Bulgaria and graduated as MS in 1984. She received her PhD degree in polymer science from the Sofia University, in 1994. In 1999, she joined the Laboratory of Analytical Atomic Spectroscopy in Faculty of Chemistry and Pharmacy, Sofia University. In 2012, she obtained the position of an Associate Professor. Her major research interests are focused on the preparation and application of ion imprinted polymers and organic-inorganic hybrid materials for separation and preconcentration of trace elements and speciation analysis.

Penka Vasileva*, L Djerahov, I Karadjova
University of Sofia "St. KlimentOhridski", Bulgaria

Adsorption of chromium(III) and manganese(II) on PVA-PEO-TEOS membranes doped with gold nanoparticles: Equilibrium and kinetic study, analytical application for simultaneous speciation of chromium and manganese

Trivalent chromium and divalent manganese adsorption was studied in a batch mode with PVA-PEO-TEOS membranes doped with starch-coated gold nanoparticles (Au-Starch NPs) at 298.15 K. Equilibrium and kinetic behaviours, as well as analytical application of the hybrid nanocomposite membranes as a sorbent for simultaneous chromium and manganese speciation were the focus of this work. The employed organic polymers poly(vinyl alcohol) (PVA) and poly(ethylene oxide) 400 (PEO) are not toxic and biocompatible in nature; tetraethoxysilane (TEOS) was used as a precursor for the inorganic polymer silica in the hybrid polymer matrix. Solutions of PVA, PEO and pre-hydrolysed TEOS were mixed with Au-Starch NPs dispersions and cast hybrid nanocomposite membranes were obtained under drying at 50 °C. The physico-chemical characteristics of gold nanoparticles and hybrid membranes were studied by XRD, TEM, SEM and AFM observations, FTIR and UV-vis spectroscopy, DSC analysis. Gold nanoparticles were uniformly distributed in the PVA-PEO-TEOS membranes without any aggregation. Even more the presence of Au-Starch NPs in the hybrid membranes remarkably increased their mechanical stability, the most probably because of their crosslinking role. The extraction efficiency of PVA-PEO-TEOS/Au-Starch NPs membranes toward environmentally relevant Cr and Mn species was studied at various pH values. Results obtained indicate that adsorption process attained equilibrium in 12 hours at optimal pH 9. Cr(III) and Mn(II) selectively sorbed on the membrane surface, while Cr(VI) and Mn(VII) remained in the solution. The adsorption behaviour of Cr(III) and Mn(II) was studied by isotherm (Langmuir, Freundlich, Temkin, and Dubinin–Radushkevich (DRK)) and kinetics (pseudo-first order, pseudo-second order, sigmoidal) models. The adsorption data were best fitted by Langmuir model, following sigmoidal kinetic model including three stages: inducement, precipitation and equilibrium periods. A simple and sensitive analytical procedure was developed for separation and speciation of Cr and Mn species in aquatic environment using dispersive solid phase extraction of Cr(III) and Mn(II) by PVA-PEO-TEOS/Au-Starch NPs membranes prior to Cr(VI) and Mn(VII) determination in the supernatants. After sorption at optimal conditions, the effluate solution was easily decanted and Cr(VI), as well as Mn(VII), was measured using ETAAS; the membrane was washed twice with doubly distilled water, dissolved in aqua regia, diluted to desired volume and Cr(III) and Mn(II) measured again by ETAAS. The determination limits achieved for toxic species Cr(VI) and Mn(VII) is 0.05 µg/L, which fulfils the requirements for their monitoring in surface water bodies under the demand of Water Frame Directive. In addition, if necessary Cr(III) and Mn(II) might be determined in the same sample with even lower determination limit of 0.005 µg/L. Relative standard deviation for all determinations varied between 6 to 11% for Cr and Mn concentrations in the range 0.05-50 µg/L. The analytical method developed was validated for Cr(VI) by parallel analysis using standard method based on diphenylcarbazide. The accuracy of Mn(VII) quantification was confirmed by added found method. The developed analytical method was applied to the simultaneous speciation of chromium and manganese in river water samples from national monitoring points.

Acknowledgements: We acknowledge the Bulgarian Scientific Fund, Project, DN19/10, “Smart speciation”.

Audience take-away:

- Ecofriendly method for synthesis of gold nanoparticles and their incorporation in hybrid organic-inorganic polymer matrix.
- Selective sorption of Cr(III) and Mn(II) onto self-standing PVA-PEO-TEOS/Au-Starch NPs membranes with promising results regarding simultaneous speciation analysis of chromium and manganese.
- Simple analytical procedure for selective determination of Cr(III)/Cr(VI) and Mn(II)/Mn(VII) in surface waters usable in routine analytical practice.

Biography

PenkaVasileva received M.S. in Chemistry and Ph.D. in Chemistry from Sofia University “St. Kliment Ohridski”, Bulgaria in 1981 and 2003, respectively. She currently serves as an Associate Professor at the Department of Inorganic Chemistry, Faculty of Chemistry and Pharmacy, Sofia University “St. Kliment Ohridski”, Bulgaria. She has long-term interests in synthesis and characterization of noble metal nanoparticles, oxide nanostructures, new composite and hybrid nanomaterials. Her research is focused on design and application of nanomaterials as optical sensors, antibacterial agents, (photo)catalysts and sorbents for solid-phase extraction in analytical chemistry. She has published more than 65 research articles in SCI(E) journals.

Irina Karadjova*, V Georgiev, I Dakova
University of Sofia "St. Kliment Ohridski", Bulgaria

Ion imprinted polymers for uranium determination by ICP-MS

Recently, there has been an increased demand for developing methods that are suitable for separation and trace level determination of uranium from various types of samples including surface waters, food, biological samples and industrial effluents. This demand is two-fold, firstly, because of the large requirement for uranium in the atomic energy programme and secondly due to the very high toxicity of uranium. Serious problem is pollution of Both groundwater and surface water by uranium, which gets seeped from the mining and milling leachates as well as from the normal run-off associated with mining sites. Chemical immobilization, trapping and surface imprinting as enrichment procedure in combination with sensitive instrumental method for quantification are the most used approach uranium determination in various matrices. IIPs are generally prepared from a reaction mixture composed of a functional monomer, a crosslinker, an initiator and a template . IIPs are developed in a similar way to imitate key and lock mechanisms for recognition and removal of the targeted ions. Thus, IIPs offer excellent selectivity and specific affinity for a given ion. The aim of the present study is synthesis and characterization of ion-imprinted polymer sorbents and their application for U determination. Experimental design includes synthesis of polymer matrix using vinyl monomers e.g., methacrylic acid, acrylamide, styrene, 4-vinylpyridine crosslinked by ethylene glycol dimethacrylate or divinylbenzene in the presence of template such as: uranyl ion, 1-(prop-2-en1-yl)-4-(pyridin-2-ylmethyl) piperazine, salicylaldehyde cross linked in the presence of uranyl template, chitosan. The composition, structure and morphology of the polymer particles obtained are characterized using elemental analysis, FTIR, SEM and BET analyses. The optimal parameters for the quantitative sorption of uranyl ions are defined and the extraction efficiency of synthesized polymers is compared and discussed. The desorption behavior of retained uranyl in the presence of different elution agents: 3M HCl. 2M HNO3, 0.05M EDTA was also studied. Analytical procedure for the determination of kinetically labile uranyl species was developed and characterized (LOQ, RSD, repeatability, selectivity).

Acknowledgements: We acknowledge the Bulgarian Scientific Fund, Project, DN19/10, "Smart speciation".

Audience take-away:

- Synthesis of various ion imprinted polymers for uranyl ions.
- Selective sorption of uranyl ions. Determination of kinetically labile uranyl species.
- Simple analytical procedure for selective determination of uranyl in various samples.

Biography

Prof. Dr. Irina Karadjova studied Chemistry at the Faculty of chemistry and pharmacy, University of Sofia "St. Kliment Ohridski", Sofia, Bulgaria and graduated as MS in 1981. She then joined the research group of Prof. D. Tsalev at Department of Analytical chemistry of same faculty. She received her PhD degree in 1992 at the same institution. From 1992 to 2019 she obtained the position of an Associate Professor and then full Professor at the Faculty of chemistry and pharmacy. She is a Head of Laboratory for Analytical Atomic Spectrometry. She has published more than 70 research articles in SCI(E) journals with more than 1500 citations.

Maja Molnar*, MelitaLončarić, VesnaRastija, ValentinaPavić
Faculty of Food Technology Osijek, Croatia

Optimization of rhodanine derivatives synthesis in deep eutectic solvents using different green techniques

Increasing need in drug consumption during last few decades, lead to the development of the pharmaceutical industry, thus increasing the synthesis of compounds with positive effects on human health. Mass production leads to the increased waste production and environmental pollution. Therefore, emphasis is placed on the green production methods and technologies. In organic synthesis, pollutants can be various solvents as well as catalysts. It is also important to reduce the energy consumption that can be achieved by using ultrasound and microwave irradiation. One of the green approaches in the synthesis is utilization of deep eutectic solvents (DESs), which can be used both as solvents and catalysts. DESs are composed of biodegradable and environmentally benign components. The advantages of the deep eutectic solvents are low toxicity, low inflammability, high availability, high recyclability, low volatility and low price. Among the many desired compounds that are synthesized today, rhodanine derivatives are compounds that have been increasingly synthesized due their significant biological activities such as antibacterial, antimalarial, herbicidal, antifungal, antitumor, insecticidal, antiviral, anti-inflammatory and cardiotonic activities. It has been reported that rhodanine derivatives can potentially be used in the treatment of obesity, cystic fibrosis, diabetes, Alzheimer's disease, thrombocytopenia, cancer, sleep, mood and central nervous system disorders as well as chronic inflammation.

In this work Knoevenagel condensation of salicylaldehydes and rhodanine was conducted under different conditions. Initially, reaction was performed in 20 different DESs at 80 °C in order to find the suitable reaction media. Choline chloride based DESs are synthesized from choline chloride as a hydrogen bond acceptor and 20 different hydrogen bond donors (carboxylic acids, sugars, ureas or amides). The best reaction media was proven to be ChCl:acetamide DES, with the highest product yield of96.3 %, followed by ChCl:malonic acid, ChCl:levulinic acidand 1,3-dimethylurea with the yields of 91.1 %, 85.8 % and 80.1 %, respectively. Reaction of rhodanine and salicylaldehyde was performed in four mentioned DESs under microwave and ultrasound irradiation, and with DES as a catalyst in order to find the best reaction conditions.

Audience take-away:

- In this presentation, positive aspects of rhodanine derivatives will be presented and their biological activities will be explained.
- Audience will learn about deep eutectic solvents properties and their proper use in the synthesis of organic compounds.
- The use of green synthesis techniques, as well as their advantages and disadvantages will be explained.

Biography

Dr. Maja Molnar studied at the Faculty of food Technology Osijek, getting her PhD diploma in 2011. She has been working at the Faculty of food Technology since 2007, teaching General and Analytical Chemistry. Her research work accompanies an application of green chemistry methods in the synthesis of heterocyclic compounds. She is mainly focused on the synthesis of biologically active compounds, such as coumarin, quinazolinones, rhodanines, pyridine derivatives.

Michał Rombel*, Andrzej L Dawidowicz
Maria Curie-Sklodowska University, Poland

The influence of protein precipitation methods on uncontrolled conversion of cannabidiol to 9-tetrahydrocannabinol during analysis of plasma samples

The growing popularity of supplements containing cannabidiol (CBD), mainly CBD oils, in self-medication of humans and the increased interest in this compound in different preclinical and clinical trials stimulates the development of procedures of CBD analysis in plasma for the study of CBD pharmacology in people and animals or in establishing dose–therapeutic effect relationships of this compound. Preliminary removal of protein by its precipitation from plasma is still one of the willingly applied plasma sample preparation methods in many analytical procedures estimating plasma drug concentration, including CBD. The present paper shows that a significant amount of CBD transforms to 9- tetrahydrocannabinol (9-THC) in a hot GC injection system when acidic precipitation agents, such as TFA, TCA, $HClO_4$, $H2SO_4$, $ZnSO_4$ or $CHCl_3$, are used for plasma protein precipitation. The transformation degree depends on the temperature of the GC injector, the concentration of the precipitation agent and the incubation time of plasma with the precipitating agent. At the CBD plasma concentration equal to 50 ng/ml, which is approximately a mean level for patients treated for epileptic syndromes, the CBD transformation degree can exceed 20%. The presented results are important not only for analysts cooperating with pharmacologists and for medicine doctors examining the activity of CBD-containing drugs in the therapeutic process, but also for forensic scientists who may erroneously find innocent people guilty of using marijuana or its preparations.

Audience take-away:

- Plasma protein precipitation is willingly applied in procedures of CBD analysis.
- CBD transforms to 9-THC in GC injector when acidic precipitation agents are used.
- The transformation degree of CBD to 9-THC in GC injector can exceed even 20%.
- The presented results are important both for clinical and forensic investigators (80).

Biography

Michał Rombel studied Chemistry at the Maria Curie-Sklodowska University in Lublin, Poland and graduated as MS in 2019. Then he began studying at the Doctoral School of Quantitative and Natural Sciences and joined the research group of Prof. A. L. Dawidowicz at the Institute of Chemical Sciences - Chromatography Department at the University mentioned above.

KEYNOTE FORUM

DAY 2

CHEMISTRY WORLD CONFERENCE

SEP 06-07, 2021

Puru Jena

Virginia Commonwealth University, USA

Chemistry beyond conventional wisdom

The chemistry of elements in the periodic table, created by Mendeleev in 1869 before the discovery of the electron and the knowledge of quantum mechanics, can be explained in terms of their valence electrons and the orbitals they occupy. For example, noble gas atoms, with filled outer electron orbitals (ns^2np^6) are chemically inert. Similarly, zinc, with an outer electron configuration of filled s shell ($4s^2$) is divalent and interacts weakly another Zn atom. But bulk Zn is not chemically inert; it is metallic. Zinc assuming an oxidation state of +III and noble gas atoms forming chemical bonds at room temperature are against conventional wisdom. In this talk I will discuss ways in which zinc can be in a +III oxidation state and noble gas atoms, including argon, can form a covalent bond at room temperature. These unexpected features are made possible by the use of highly stable super-electrophilic clusters. In particular, $BeB^{11}(CN)^{12}$ and $BeB^{23}(CN)^{22}$ clusters, which are, respectively, stable as tri-anion and tetra-anion in the gas phase, can make Zn to assume +III oxidation state. On the other hand, $B^{12}(CN)^{11}$- cluster can bind argon with a binding energy of 0.6 eV. These results, based on density functional theory with dispersion correction, have predictive capability and provide a path to manipulate text book chemistry. The rational design of clusters with electron affinities far exceeding those of halogen atoms and their ability to promote chemical reactions once thought impossible can usher a new era in chemistry.

Audience take-away:

- How chemistry of elements can be fundamentally changed?
- How such knowledge can be used to promotereactions, once thought impossible?
- How this knowledge can create new materials with tailored functionalities?

Biography

Dr. Jena's honors include: Presidential Medallion from Virginia Commonwealth University (2011); Jefferson Science Fellow at the US Department of State (2007); David Hare Professorship lecture at the Indian Association for Cultivation of Science, Kolkata, India (2005); Fellow of the American Physical Society (2000); Outstanding Faculty Award from the State Council of Higher Education of Virginia (2001); University Award of Excellence (1993) and Outstanding Scholar Award (1987) from Virginia Commonwealth University; and Chair of the Gordon Conference on Metal-Hydrogen Interactions (1993). He has served as a member of numerous scientific panels at the National Science Foundation, Department of Energy, and Army Research Office. He was a member of the Executive Committee in 2003 that drafted the report on the "Basic Research Needs for the Hydrogen Economy" for the Department of Energy. He has also served on the Virginia Governor's task force on green energy technologies and on the Presidential Commission on bilateral scientific collaboration between USA and Russia (2011).

Francesco Parrino
University of Trento, Trento, Italy

Mechanistic insights on heterogeneous photocatalysis for the synthesis of high-value added compounds

Heterogeneous photocatalysis is an advanced oxidation process which exploits the property of irradiated semiconductors to generate electrons and holes which in turn initiate useful redox reactions. The classical field of application of photocatalysis has been the environmental remediation, due to the ability of radical oxygen species thereby generated to oxidize almost every organic and inorganic pollutant. However, the technical and economic hurdles encountered when trying to scale up photocatalytic water treatments, along with the concomitant discovery of very selective photocatalytic processes caused recently a dramatic change of scenario. In fact, the mild operative conditions, the possibility of exploiting solar light irradiation, and of using water as the solvent make photocatalysis a promising alternative to traditional organic syntheses, in compliance with the principles of “green” Chemistry. In this way it is possible to perform a great variety of organic and inorganic reactions such as partial oxidations, reductions, coupling reactions, and polymerizations.

The present paper presents some photocatalytic syntheses such as partial oxidation of alcohols to aldehydes, the vanillin production, the synthesis of elemental bromine, and the limonene epoxidation. These reactions will be used as paradigmatic examples to highlight the basic mechanisms of photocatalysis. The remarkable results in terms of yield of reaction and the appealing reaction conditions make industrial implementation of these reaction a step closer to industrial implementation. Therefore, some engineering issues such as optimization, intensification, and reactor design will be also presented.

Audience take-away:

- The audience will learn the basic mechanisms of photocatalysis and some of the most industrially promising applications.
- Photocatalysis is an intrinsically interdisciplinary field of research which can be approached starting from different perspectives and competences.
- Photocatalysis can be successfully integrated with other processes synergistically providing process intensification.

Biography

Dr. Francesco Parrino graduated in Palermo in 2005 in Chemical Engineering cum laude and got a PhD in Inorganic Chemistry in 2009 at the Friedrich-Alexander University of Erlangen-Nürnberg (Germany). His research activity deals with the preparation and characterization of photocatalysts for degradation of pollutants and for green synthesis of organic molecules. He is the Member of the "Italian Chemical Society" Trentino AA-ST Section, Division: Chemistry for Technologies, Member of the "Italian Chemical Association for Engineering" and review editor of the Journal "Frontiers in Environmental Chemistry". He is coauthor of several papers and communications in international conferences on these topics. Citations 986, h index 19 (Scopus).

Maxim Mironov

SPC Biomicrogel Company Ltd, Russia

Bio-based membranes for separation of water/oil mixtures

The pollution of water sources with petroleum products is one of the most important and actual ecological problem. Every year, oil spills create a serious damage to the ecosystem, which leads to the death of plants, algae, birds and fish. At the same time, wastewater from steel and metallurgical plants, domestic wastewater and storm water cause significant environmental damage.

There are various technologies for water treatment from petroleum products available. Special place among them is occupied by membrane because they have many advantages such as high technological efficiency, multiple use capability and environmental friendliness. Besides, membranes can use for oil spill response, filtration of waste water, separation of technical water and other application. Development of bio-based membranes for separation of water/oil mixture is one of the perspective ways for protective of environmental from pollutions. In this work the review about bio-based membranes made from natural materials is presented. Methods of preparation, microstructure and properties of textile and aerogel membranes are discussed. It is shown that textile membranes have a number of advantages over aerogel membranes, such as low cost and simple production technology. Cotton textiles modified by biopolymers occupy a special place among perspective eco-friendly products for separation of oil/water mixtures and mixtures of organic solvents, fats, vegetable oil with water.

Microgels are polymer colloid particles with diameter less than 1 micron that can swell in water. Our research program is focused on the modification of biopolymers in aqueous suspensions and production of commercially available microgels for the modification of cotton textile under trademark Spilltex®.These biopolymers are obtained from natural raw materials, for example food industry waste, such as beet pulp. They are non-toxic and do not contain substances that can contaminate environment. demonstrates super hydrophilic properties. Flow of purified water through the membrane is more than 30 times higher than for similar membranes. These type membranes can be used in petroleum, chemical and even in food industries, because they are made from biodegradable materials. Membranes are easy regenerated by washing in water, which allows it to be used repeatedly. Various industrial applications of membranes Spilltex® will be demonstrated including gravitation separation of wastewater and full-scale water treatment from petroleum products.

Audience take-away:

- Actual data about bio-based membrane from different research group.
- Preparation methods, microstructure and properties of aerogel and textile membrane.
- Technical information about cotton textile membrane modified by polysaccharide microgels (Biomicrogels®).
- The presented results can be used in the development of filter systems for the separation of water / oil mixtures.

Biography

Since 2006 Maxim Mironov has been the research group leader and assistant professor at Ural Federal University. Since 2009, he became the Chairman of MCR 2009 in Yekaterinburg, Russia. Since 2012, he has been the R&D director at «SPC BIOMICROGEL» COMPANY LTD.At the 2013 he graduated as a PhD degree at the Ural Federal University. He has published more than 120 research articles in SCI(E) journals and he is the author of 24 patents.

SPEAKERS DAY 2

CHEMISTRY WORLD CONFERENCE

SEP 06-07, 2021

Nunzio Cardullo*, Vera Muccilli, Corrado Tringali
University of Catania, Italy

Natural and synthetic polyphenols as carbohydrates hydrolyzing enzymes inhibitors

Carbohydrates are among the main nutritious components of human diet. Normally, the blood sugar level after meal highly responses to the digestion of carbohydrates, mainly starch. They are initially hydrolysed by salivary and pancreatic α-amylase to reducing into oligosaccharides. Then, the reducing sugars are digested by pancreatic α-glucosidase to glucose that enters blood circulation. Therefore, retarding the starch digestion by inhibiting the activity of essential hydrolysing enzymes, namely α-amylase and α-glucosidase, is beneficial to health as it alleviates the stimulation to pancreatic islet B cells. Furthermore, controlling postprandial blood sugar level is useful in regulating some glycometabolism-related diseases, for example type 2 diabetes. Type 2 diabetes develops in adulthood and is mainly related to incorrect lifestyles (sedentary life), industrially sourced food and some chronic degenerative diseases. Furthermore, in chronic conditions, hyperglycaemia causes the onset of other diseases (retinopathy, nephropathy, heart attacks, etc.) and an increase in the production of reactive radical species, with consequent oxidative damage to the involved tissues.

In 2019, diabetes has been included in the top 10 global causes of death, thus, there is an urgent need in the search of new and effective antidiabetic drugs, besides considering certain side effects showed by commercial antidiabetic drugs. The inhibition of the activity of α-amylase and α-glucosidase is an established protocol in the search for potential antidiabetic agents with hypoglycaemic activity.Given the slight or absent side effects on naturally occurring compounds, the search is pointed to the discovering of new hypoglycaemic agents from natural sources. In the last decade, an increasing number of papers has been dedicated to the hypoglycemic effect of natural extracts and their main constituents. Among natural products, some polyphenols occurring in edible plants showed promising α-glucosidase and/or α-amylase inhibitory activity. Moreover, the well-known antioxidant properties of polyphenols represent a further advantage in the search for potential dual-action antidiabetic agents, with both hypoglycemic and antioxidant activity.

Tannins, flavonoids and phenolic acids are natural products belonging all to the polyphenol family and are considered promising lead compounds in the search for new anti-diabetic drugs. Some authors have discussed their structure-activity relationship, however the exact inhibition mechanisms of α-glucosidase α-amylase by polyphenols are still unclear. In this scenario, we have focused our research activity on the study of hydrolysable tannins, such as C-glucosidicellagitannins and galloylated glucoses; phenolic acids, such as rosmarinic and chlorogenic acids; and bisphenolneolignans, such as magnolol, as α-glucosidase and α-amylase inhibitors. Consequently, several analogues and derivatives of the above-cited natural polyphenols have been synthesized and evaluated as hypoglycemic agents. UV and fluorescence spectroscopy have been employed to deeply analyze the inhibition mechanism of the most promising hypoglycemic agents as well as binding mode analyses of these compounds using molecular docking simulations have been performed.

Audience take-away:

- Nature provides a huge library of compounds with known and yet undiscovered biological properties.
- Most of the natural compounds we usually take with diet carry out beneficial health effects (nutraceuticals) and preventive action towards several diseases every day.

- Medicinal chemistry and organic chemistry are useful tools to study and understand the mechanisms of action of natural compounds as well as to obtain new molecules with enhanced biological activity.
- Simple and generally available spectroscopic techniques (UV, fluorescence, NMR) allows the study of the mechanisms of inhibition and or interaction of small molecules with biological targets.

Biography

Dr. Nunzio Cardullo studied Chemistry at the Catania University (Italy) and graduated as MS in 2012. He attended the International PhD in Chemical Sciences at the University of Catania and received the PhD degree in 2016defending his work on the "Synthesis of natural-derived polyphenols as potential anticancer agents". During his PhD he spent three months at the University of Helsinki where he developed part of his research. Since 2017 He has held a postdoc position at the Department of Chemical Sciences (University of Catania) and here he took two teaching positions in Organic Chemistry. He has published 24 research articles in SCI(E) journals.

Diana-Ioana Buliga*, Aurelian Cristian Boscornea, Ioan Calinescu, Aurel Diacon, Ioana Popa

University Politehnica of Bucharest, Romania

Optimization of ultrasound-assisted extraction of chlorophylls from spinach by- products using response surface methodology and stabilization of the extracted pigments by encapsulation

Chlorophylls are tetrapyrrole derivatives with coplanar system of conjugated double bonds which form an aromatic structure with delocalized electron density at the orbitals level. Typically found in higher plants are chlorophyll-a and chlorophyll-b, in various proportions depending on the maturity and species of the vegetal material and also on the light exposure, stress etc. Being widely available in nature, the natural pigment can represent a solution of environmentally friendly textile dyeing option. However, its easily degradable nature stands in the way of utilizing chlorophyll at its maximum potential. The aim of this study was to develop a mathematical model for the optimization of chlorophyll extraction from fresh spinach leaves using ultrasound-assisted extraction (UAE) and ethanol 96% as extractive solvent. The UAE equipment comprises in a Hielscher UP200H Ultrasonic Processor, a jacketed reactor, heating plate equipped with a temperature control and magnetic stirring units. In order to decrease the number of experiments and, consequently, the volume of used solvent, the developed method was optimized with the use of Design of Experiments approach. The optimization of the extraction method was carried out by employing the Box-Behnken response surface methodology (RSM) and its application with selected input variables such as solid/solvent ratio, ultrasound (US) power and stirring rate to the determination of the optimal conditions to maximize the concentration of chlorophyll extraction. The JMP software (Cary, N.C., USA) was used to design the experiment. The extracts were spectrophotometrically analysed in triplicate and the concentrations of chlorophyll-a and chlorophyll- b were calculated using molar extinction coefficients.

The answers evaluated in this experimental set were the concentrations of chlorophyll-a and chlorophyll-b. The levels of the evaluated factors were determined. Optimization results showed good agreement between predicted and experimental values of chlorophyll-a and chlorophyll-b yields with a high coefficient of determination (R2 = 0.93 and R2 = 0.93, respectively). The optimum solvent/solid ratio, US power and stirring rate, which lead to achieving maximum concentrations of chlorophyll-a and chlorophyll-b (148.8 mg/L and 67.7 mg/L, respectively) were 4.3:1, 120 W, and 1000 rot/min, respectively. Due to the light and heat sensitive nature of the extract, it was further stabilized. The encapsulation strategy involved the silanization of the chlorophyll extract by reaction with 3- aminopropyltriethoxysilane (APTES), followed by a hydrolysis step in the presence of tetraethyl orthosilicate (TEOS) and cetyltrimethylammonium bromide (CTAB) (as stabilizing agent) for the generation of silica. The degradation studies showed an improved stability to storage conditions of the encapsulated chlorophyll compared with the pure compound.

Acknowledgement: This paper was supported by a University Politehnica of Bucharest grant “Inginer in Europa” in online system registered at ME under no. 140/GP/19.04.2021, by using the special situation financing fund which cannot be integrated in the form of financing for higher state education institutions.

This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI– UEFISCDI, project number PN-III-P1-1.1-TE-2019-1387 (contract number TE141/2020), within PNCDI III.

Audience take-away:

- Advantages of the Design of Experiments studies which imply fewer experimental runs, a better process understanding in a shorter time period and overall, lessened research and development cycles.
- A method of chlorophyll stabilization through encapsulation, which enhances the possible uses of this natural pigment.
- To reconsider the utilization of some natural products in various domains of interest.

Biography

Eng. Diana-Ioana Buliga studied Chemical Engineering at the Politehnica University of Bucharest (UPB) and graduated as engineer in 2018. She then joined the research group of associate professor Dr. Eng. Aurelian Cristian Boscornea from the Dyes and Pigments group from the same institution. She obtained her master's degree in 2020 after finishing the Biofuels, Biorefineries and Conex Technologies master program at UPB. She is currently developing her PhD thesis under the coordination of Prof. Dr. Eng. Ioan Calinescu. She has published two research articles and participated at eight national and international conferences.

Domenico Cautela
Stazione Sperimentale Per Le Industrie Delle Essenze E Dei Derivati Dagli Agrumi, Italy

Occurrence and analysis of betainized compounds in fruits

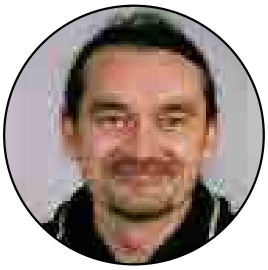
Betainized Compounds are a group of low molecular weight compounds, highly soluble in water, derived from amino acids in which the nitrogen atom is fully methylated.These substances are ubiquitous in the vegetal world and tend to accumulate, through specific biosynthetic pathways, in the cytoplasm and intercellular fluids, where they exert protective functions for proteins, nucleic acids, and cell membranes in response to abiotic stresses.Recently, a group of betainized compounds have been suggested to play a role in health effects in relation to a vegetable and fruit consumption or Mediterranean diet. The content of betainized compounds appears to be species specific and can help to characterize vegetable sources and their derivatives, such as fruit juice.This presentation focuses on the occurrence and distribution of Betainized Compounds in fruits and on the analytical techniques for their analysis.

Audience take-away:

- Application of analytical methods for the determination of betainized compounds in vegetables and fruits.
- Development analytical tool for food authenticity.
- Associations of betainized compounds with dietary and metabolic biomarkers.

Biography

Dr. Cautela studied Food Science and Technology at the "Università degli Studi di Milano"and graduated as MS degree "cum laude", in 2000. He received a PhD degree in 2011 at the "Seconda Universita degli Studi di Napoli". Since 2004 he is a researcher at the SSEA "Experimental Station for the Industry of the Essential oils and Citrus products. Since 2018, he is also Fixed-term professors of Food Chemistry (9 credits, 72 hours) at Università Telematica "E-CAMPUS", Novedrate (Italy). He has published more than 37 research articles index in Scopus.



Tomasz Panczyk*, Pawel Wolski, Patrycja Wojton
Polish Academy of Sciences, Poland

Interaction of human Telomeric i-motif DNA with Single walled carbon nanotubes : Insights from molecular dynamics simulations

Telomeres are terminal fragments of chromosome composed of highly repetitive sequences of nucleic bases (TTAGGG):(CCCTAA). We can distinguish guanine rich (G-rich) and cytosine-rich (C-rich) strands within the double stranded telomeric DNA. The biological role of telomere is protection of chromosome and regulation of cellular aging. Telomeres play also important role in the development of cancer. An interesting feature of telomeric part of the DNA is that they can form non canonical spatial structures. So, the G-rich strand can form G-quadruplexes (Gq) and the C-rich strand can form intercalated, quadruple helical structure called i-motif (iM). G-quadruplexes can form at neutral pH but they need monovalent ions (Na^+,K^+) to be stabilized. I-motif has been described in literature as a structure which can exist only at a reduced pH when one of cytosines become protonated.

The biological function of Gq as telomerase inhibitor is well-known and it is considered as important target in anicancer drugs development. Biological function of iM is less recognized though it was found that carboxylated single wall (but not multi-wall) carbon nanotubes are one of few factors which can stabilize i-motif selectively. Moreover, it was also shown that carboxylated carbon nanotubes are able to inhibit telomerase activity though the mechanism of that process is still unknown.

Selective induction and stabilization of telomeric iM by carboxylated single walled carbon nanotubes is a very interesting phenomen. Therefore, this work is devoted to the analysis of the interaction of carbon nanotubes with iM at the atomic level using molecular dynamics simulations. We study two kinds of i-motifs differing by the protonation state of cytosines, i.e. unprotonated ones representative to neutral pH and with half of the cytosines protonated and representative to acidic conditions. These i-motifs interact with two kinds of carbon nanotubes differing mainly in chirality and on-tip functionalization by amino groups or by guanine containing residues. We found that protonated i-motif adsorbs strongly, though not specifically, on the nanotubes surfaces with its 3' and 5' ends directed towards the surface and that adsorption does not affect the i-motif shape and hydrogen bonds existing between C:C+ pairs. The functional groups on the nanotube tips have minimal effect either on position of i-motif or on its binding strength. Unprotonated i-motif, in turn, deteriorates significantly during interaction with the nanotubes and its binding strength is rather high as well. We found that (10,0) nanotubes destroy the i-motif shape faster than (20,0). Moreover the i-motif either tries to wrap the nanotube or migrates to its tip and become immobilized due to interaction with guanine residue localized on the nanotube tip and attempts to incorporate its 3' end into the nanotube interior. We can thus conclude that single walled CNT cannot directly stabilize the structure of unprotonated i-motif due to simple physical interactions being a result of the specific shape of CNTs. We observed rather reverse effect – narrow CNT turned out to be more effective in deteriorating the iM structure.

Acknowledgment: This work was supported by Polish National Science Centre grant 2017/27/B/ST4/00108.

Audience take-away:

- The audience can learn about the importance of noncanonical DNA structures in suppression of telomerase activity, i.e. the enzyme which is responsible for the infinite proliferative capacity of cancer cells.
- The audience can learn about the role of carbon nanotubes as specific factor affecting the stability of the noncanonical i-motif structure.
- The knowledge about mechanisms of the above mentioned processes, coming from molecular dynamics simulations, can help in designing of novel anti-cancer drugs or selective drug delivery systems.

Biography

Prof. Tomasz Panczyk studied Chemistry at the Department of Chemistry, Maria Curie-Sklodowska University in Lublin, Poland and graduated in 1997. He then joined the research group of Prof.Wladyslaw Rudzinski at the same Department and started his PhD. He received his PhD degree in 2001 at the same institution. Since 2001 he has been employed in Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences in Krakow. Since 2009 he is a Life Member of Clare Hall college in Cambridge, UK. He has published more than 80 research articles in SCI(E) journals.

Fatih Piskin*, Taner Ozdal
Mugla Sitki Kocman University, Turkey

Combinatorial development of proton conducting oxides for hydrogen separation membranes

Separation membranes allow purification of hydrogen from gas mixtures produced by various methods, such as the reformation of natural gas, coal gasification, or the gasification of municipal waste. Hydrogen separated in this way may be used in fuel cells to generate electricity or may be fed directly to the natural gas grid to temporarily storage. It is likely that the current network of natural gas will soon be transformed into a "gas" grid where hydrogen would be an essential ingredient. All these require the use of efficient separation membranes, which would make the easy availability of hydrogen possible as is currently the case for natural gas. Thus, the separation membranes would have a much wider scope than normally anticipated and therefore there would be a need for separation membranes that are more efficient and in particular of low cost.

The current study concentrates on proton conducting oxides that can operate at temperatures higher than 450 °C and applicable to the steam reformation of natural gas including the water-gas shift reactions. Proton conducting oxides used for this purpose are quite attractive due to their high hydrogen selectivity and superior tolerance to possible toxic gases (e.g. CO, H2S, etc.) that may be present in the gas mixtures.

The current study adopts a membrane design methodology based on combinatorial material science. This approach makes use of a magnetron sputtering system whereby a material library of thin-film membranes is produced in a single experiment. The library is then screened by four-probe resistivity and electrochemical impedance measurements so as to identify the compositions that are highly reactive with hydrogen. A map of reactive index prepared in this way is used to determine candidates for hydrogen separation. The membranes are then fabricated in the form of discs and tested for hydrogen permeability. In the current study, BaZr0.80Y0.20O3-SrCe0.95Yb0.05O3 heterostructures are investigated using the above methodology.

Acknowledgement: This work was supported by TUBITAK (The Scientific and Technological Research Council of Turkey) with project Number 119M065, which the authors gratefully acknowledge.

Audience take-away:

- Material development has traditionally followed a Darwinian scheme which involved limited variation at given time and a selection resulting in slow evolution. In the context of material development, this approach requires a careful pre-consideration in altering the material composition and detailed characterization with regard to both the resulting structure and the properties.
- Combinatorial approach is an alternative method whereby a large number of samples each with a different composition are produced in a single experiment yielding the so-called material library. These are then screened in a fast manner using a suitable method identifying the compositional field with the required properties. If necessary, the process may be repeated for the second time by re-examining the selected field to pinpoint the exact composition(s).

Biography

Dr. Piskin studied Materials Science and Engineering at the Anadolu University, Turkey. He then joined the Energy Storage Materials Laboratory in Middle East Technical University. He received his MS and PhD degree in 2013 and 2018, respectively in the same university. After one year visiting researcher fellowship supervised by Prof. Bilge Yildiz at Massachusetts Institute of Technology, USA, he obtained the position of an Assistant Professor at Mugla Sitki Kocman University, Turkey.

Yahia F. Makableh*, Rama Al-Abed
Jordan University of Science and Technology, Jordan

Improved perovskite life time by using nano-polymer matrix sandwich structure

The stability of Perovskite materials life time by using Nano-polymer sandwich structure is investigated. A Perovskite composite is used consisting of the structure FAxMA1-xPbI3. The x ratios varied as 0.8,0.5 and 0.2. Two different polymers are used namely PMMA and Polyaniline. The polymers thicknesses were varied by using a spin coating method before and after the deposition of the Perovskite structure. X-ray diffraction and Uv-Vis-Nir spectroscopy are used for the analysis of the life time. Thus far over 75 days material life time is observed without any noticeable decomposition of the Perovskite layer, when compared to a reference sample. The study is performed at room temperature and open atmosphere without any special equipment to preserve the Perovskite from degradation.

Audience take-away:

- This study shows new methods of preserving the lifetime of Perovskite structures without decomposition.
- Perovskite structures are widely investigated due to their importance in the photovoltaic applications.
- Yet most Perovskite structures faces decomposition after few hours or few days. Hence this research is showing long life time without any Perovskite decomposition due to the suggested structure.
- This research is part of team work consists of several previous and new masters students working on the Perovskite structure design and investigation to greatly enhance the life time of this material.

Biography

Dr. Yahia Makableh has earned his earned his PhD degree from the University of Arkansas. His research was focused on investigating InAs quantum dots solar cells and device fabrication and characterization. Additionally, he is working on plasmonic effect, surface modification using anti reflection coating and hydrophobicity. He has published several papers in technical journals such as APL, SOLMAT and others. Currently he is an assistant professor at the Nanotechnology Institute at Jordan University of Science and Technology working on novel materials and structures for high performance solar cells and photo detectors, Optical Nanomaterials especially Perovskite materials.

Lorena Memushaj*, Jona Keri
Aldent University, Albania

Symptoms, causes and treatment of people with food allergies in tirana, albania

A food allergy occurs when the body’s immune system sees a certain food as harmful and reacts by triggering an allergic reaction.There are two categories of food allergy. Immunoglobulin E (IgE) mediated is where symptoms result from the body’s immune system making antibodies called IgE. This type of food allergy can trigger anaphylaxis, life-threatening allergic reactions. Non-IgE mediated is where other parts of the body’s immune system react, causing symptoms, but does not involve the IgE antibody. Many non-IgE reactions are believed to be T-cell mediated. Symptoms include tingling in the mouth, itchy skin rash, swelling of the face or throat, shortness of breath, nausea, abdominal pain and diarrhea. A study was conducted through a prepared questionnaire that would test 250 people suffering from food allergies. The aim of this study is to monitor symptoms, causes and treatment of people with food allergies in Tirana, Albania.

During the statistical processing of the data collected, it is observed that most common symptoms in people suffering from various food allergies were urticaria (40.91%), skin rash (40.91%), difficulty breathing (31.82%), swelling of the face (31.82%) and the others exhibited various symptoms such as abdominal pain, diarrhea, nausea or vomiting, dizziness to fainting. The persons who had shown a mild degree of allergy were (26.09%), persons who had shown a moderate degree of allergy (26.09%) accompanied by medication recommended by the doctor. In the same percentage were persons who had an immediate reaction associated with hospitalization and anaphylactic shock (47.83%).Referring to the medications used in cases of mild food allergy, patients stated that 13.64% of them did not find it necessary to use any medication and the symptoms were gone within 24 hours. 9.09% of them had used Epinephrine in cases of anaphylactic shock. 50% of patients always carried an antihistamine drug with them and 27.27% consistently used alternative medication.

The sample is not comprehensive and the results can not be generalized because the sample was taken from the city of Tirana. The recommendation of food allergy is to avoid exposure to the food until your doctor's appointment. Information and care should be added to kindergartens, schools and media on the identification, treatment and management of people with food allergies.

Keywords: Food allergy, symptoms, Epinephrine, antihistamine, alternative medication.

Audience take-away:

- The importance of food allergies, what and how they cause them.
- Methods of identifying diagnoses.
- Methods of prevention and treatment.
- Underlining the drugs used (pay attention to reactions with other drugs that the patient administers).
- Alternative medicine as a treatment option.

Biography

Dr. Lorena Memushaj studied Food Chemistry at Faculty of Natural Sciences; Tirana University and graduated MS in 2010. She received her PhD degree in 2016 at the same institution. Experienced university lecturer in Food and : Analytical Chemistry at the Department of Pharmacy; Faculty of Medical Sciences; Aldent University, Tiranë, Albania. Skilled in food technology, food microbiology and also quality and safety of food products.

Dr.N.Gokarneshan*, B.Padma, R.Haripriya and A.J.Abisha Raju
Dr. SNS Rajalakshmi College of Arts and Science, India

Lotus fibre : The new generation natural fibre

Sustainability issues in Textiles have paved way for exploration of many new fibers from renewable sources. Many researches are done to refine the extraction process, test and identify the hidden properties and to characterize the fiber for its unique property. By default, all the natural fibers are sustainable in every dimension of analysis. Each country has their traditional textiles made from ecofriendly materials. Lotus fabric of Cambodia has the same significance but is less popular compared to other natural fibers. It is the eco-friendliest fabric in the world and commonly referred as sacred fabric, which was once used only by the monks. This article explains the history of lotus fiber, separation of fiber, spinning, weaving, properties, popular brands, end uses and market share of lotus fabric which can be an eye-opener of how sustainability is meticulously planned which is the reason for good quality fabrics at slightly higher pricing. Awareness gained on lotus can be applied in exploration of few other natural resources and organic wastes for textiles.

Audience take-away:

- Audience will be able to get useful insights on the topic and get ideas to extend research in the area.
- Little research has been done in the area and therefore the presentation would help the audience to exploit the properties of the fibre and explore in different areas of applications. With regard to design, development of new products are possible.

Biography

Dr.N. Gokarneshan got his PhD in 2008. He has academic experience spanning over 25 years and industrial experience of about 10 years, He has authored 15 books, published over 200 papers in various leading journals, contributed many book chapters for edited books, presented papers in conferences. He is editorial board member in journals and also serving as reviewer. His areas of interest include Textile science, Textile chemical processing, Technical textiles and Fabric formation. He is a recipient of many awards and recognitions. He is presently working as Dean at the department of costume design and fashion at Dr.SNS Rajalakshmi College of Arts and science, Coimbatore, India.

POSTERS DAY 2

CHEMISTRY WORLD CONFERENCE

SEP 06-07, 2021

Julia Godlewska*, Bartosz Cieśla, Piotr Bruździak
Gdańsk University of Technology, Poland

K-peptide and osmolytes in solution – spectroscopic and theoretical studies

K-peptide (GILQINSRW) – a short 9 amino acid fragment of the hen egg white lysozyme has the ability to form amyloid structures, thus it can serve as a model for studies of interactions between pathological amyloid structures and various compounds generally known as osmolytes. Two of them – trimethyl-N-oxide (TMAO) and dimethylsulfoxide (DMSO) has been selected on the basis of their structural simplicity and known influence on proteins. TMAO is a strong to moderate stabilizer which promotes aggregation, DMSO is a popular anti-freeze agent. Our goal was to get an overview of possible interactions in aqueous solution of both K-peptide and on of osmolytes. ATR-FTIR spectroscopy (Thermo Nicolet 8700 equipped with single reflection diamond cell GoldenGate ATR accessory) was used to analyse weak interactions in solutions. Due to relatively low concentration of the K-peptide it was not possible to study directly its vibrational structure, instead we had to focus on the shape and shifts of vibration bands of TMAO or DMSO in solutions. The concentration of osmolytes was kept constant to diminish the influence of their dissolution (it could potentially change interaction between the same solute molecules in a solution and affect the shape of FTIR spectra) while concentrations of the K-peptide varied. A variant of the derivative spectra method was used to isolate and boost spectroscopic signals indicating interactions. Some of the changes visible in spectra were similar to those caused by hydration/dehydration of osmolytes, indicating an important role of the solvent in interactions. Moreover, we used DFT calculations to assign and confirm the peak shifts. For a practical reason, N-acetyl-glycine-methylamide (NAGMA) was used as a model of the full K-peptide. All calculations were performed with the GAUSSIAN 09 v.D1 software using a well-established set of DFT method and basis set – B3LYP/6-311++G(d,p), including the GD3-BJ dispersion correction.

Acknowledgement: This work was funded by the National Science Centre, Poland (grant 2017/26/D/NZ1/00497). Calculations were carried out at the Academic Computer Centre in Gdańsk.

Audience take-away:

- Weak interactions between various solutes can have an immense influence on properties of peptides and proteins in solutions.
- Direct interactions are generally unfavorable in such solutions.
- Water plays an important role as an intermediary between solutes.

Biography

Julia Godlewska is second year Chemistry student at the Gdańsk University of Technology, Poland. In February 2021, she joined Prof. Bruździak's research group at the Department of Physical Chemistry at Gdańsk University of Technology. Moreover, she is a Vice-president of the Science Circle "SimLE", which deals with the development of technologies for the space industry. Their rocket took part in a competition - Spaceport America Cup in June 2021 and will take part in European Rocketry Challenge in October 2021.

Elidia Maria Guerra*, M. O. Diniz, D. T. Cestarolli, R. F. Bianchi
DQBIO/CAP/UFSJ, Brazil

Electrical characterization of V_2O_5/POMA deposited by casting technique

Conductive polymers derivates, such as poly-o-methoxyaniline (POMA), have been broadly using in different applications due to their similar characteristic of polyaniline. POMA can intercalate intoV_2O_5 matrix to improve their structural and electrical properties, and thin films of V_2O_5/POMA can be deposited by different techniques to extender their technological applications after intercalation reactions. V_2O_5 was prepared by sol-gel route. POMA was polymerized from its monomer, o-methoxyaniline, by intercalation reaction into the V_2O_5 matrix. After intercalation reaction, it was possible to note that the structure of the inorganic and organic materials was preserved from the results of DRX, FTIR and SEM. The use of deposition technique by casting for application as component in ammonia sensor,indicated that the parameter as resistance, interface effects and conductivity slightly change with the deposition technique compared with layer by layer deposition.A goodtheoretical–experimental fitting was observed between the Z' curves and between the Z" curves, accordingto the theoretical model proposed. In both components, the numerator is much higher than the denominator, so we can infer that the real component (Z') is approximately proportional to the bulk resistor (R) and that the imaginary component of complex impedance (Z'´) is approximately proportional to the bulk resistor squared (R2). Finally, these results indicated that the R is mostly responsible for the ammonia gassensitivity obtained by the Z' measurements and indicate also that R2 isassociated with the ammonia gas sensitivity obtained from the Z'´measurements. Therefore, in the presence of ammonia gas, the film presented a sensitivity in both real andimaginary components of CI with a good reliability confirmed by the theoretical Cole–Cole model.

Audience take-away:

- In generally, the sensor can be used form ammonia gas detection.
- Sensitivity component can be used possibilitya low-cost device.
- The device can be easy to handle.

Biography

Dr. Elidia Maria Guerra studied Chemistry at the Sao Paulo University, Ribeirao Preto, Brazil,graduated in 2002 and post-graduated as Ph.D in 2007.Follow this, during her two Postdoctoral she was supervised by Prof. Dr. Marcelo Mulato(University of São Paulo) in 2007-2009 and by Prof. Dr. Rodrigo F. Bianchi (Federal University of OuroPreto) in 2009. She obtained the position of an Associate Professor II at the UFSJ.

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Universidad Autónoma de Chile, Chile

Trichloroisocyanuric acid mediated oxidative rearrangement of tetrahydro-b-carbolines

Spirooxindoles are exceptional and versatile scaffolds, and thus have been extensively studied in the fields of synthetic and pharmaceutical chemistry. The unique three-dimensional spiro system may be the main cause for the bioactivities of spirooxindoles. Especially, spirooxindoles have been considered to exhibit antitumor, antimicrobial, antioxidant, anti-inflammatory, antiviral and other bioactivities. Due to all these pharmaceutical potencies of spirooxindole derivatives, chemists have been inspired to establish various synthetic routes for this class of compounds. One of them is a multi-reactive centered reagent, which is beneficial in chemical synthesis due to their advantage of minimal material utilization and formation of less by-products.

In this work we employed the safer multi-reactive centered reagent (MRCR) trichloroisocyanuric acid (TCCA). TCCA is a reagent with three reactive centers, and was employed here in the synthesis of spirooxindolesfrom various N-protected tetrahydro-b-carbolines. Particularly, TCCA is inexpensive and produces essentially the nontoxic cyanuric acid as a by-product, which can be easily separated from the reaction mixture.The reaction proceeded via oxidative rearrangement and produced spirooxindoles in good to excellent yields (up to 99%). The optimized protocol consisted in 0.35 equivalents of TCCA and THF/water (1:1) as the solvent at room temperature for 30 minutes. Diversely substituted spirooxindoles and naturally occurring (±)-coerulescine and (±)-horsfiline were furnished in excellent yields using the optimized reaction conditions. To demonstrate the commercial importance of this protocol, gram-scale reactions to produce (±)-coerulescine and (±)-horsfiline with yields of 93% and 90%, respectively, were carried out. In addition, this synthetic strategy is amenable for the generation of a library spiro-compounds and their derivatives, which can be further utilized in the drug discovery process.

Audience take-away:

- Multi-reactive centered reagents are beneficial in chemical synthesis due to their advantage of minimal material utilization and formation of less by-products. Trichloroisocyanuric acid (TCCA), a reagent with three reactive centers, was employed in the synthesis of spirooxindoles.Low equivalents of TCCA were required to give spirooxindoles up to 99% yield.
- This protocol was proven for the gram-scale total synthesis of natural alkaloids such as coerulescine andhorsfiline in excellent yields.
- An operationally simple and high yield protocol for the synthesis of spirooxindoles from the corresponding tetrahydro-b-carbolines (THBCs) using the inexpensive TCCA.
- To demonstrate the commercial importance of this protocol, it also carried out gram-scale reactions to produce bioactive compounds yields above 90%.
- This synthetic strategy is a menable for the generation of a library spiro-compounds and their derivatives, which can be further utilized in the drug discovery process.

Biography

Dr. Nachtigall studied chemistry in Brazil, in a sandwich doctorate program between the University of Campinas (Brazil) and Indiana University (USA) in the group of Prof. Dr. David Clemmer and obtained a Postdoctoral degree in Max-Planck-Institut für Kohlenforschung. Specialist in the study by mass spectrometry, Dr. Nachtigall works as a professor at the Autonomous University of Chile, has more than 40 publications in ISI journals, 3 USPTO patents, and her main line of research is based on the development of new, more effective catalysts and the study of organic reaction mechanism using MALDI-MS and ESI-MS techniques.

Tatjana Gazivoda Kraljevic*, Ivana Sokol, Andrijana Meščić Macan, Domagoj Drenjančević, Sandra Liekens, SilvanaRaić-Malić

University of Zagreb, Croatia

Synthesis of novel 3-substituted coumarin derivatives by transition metal-catalyzed reactions and their antimicrobial and antitumoral evaluations

Coumarin has an important place in medicinal chemistry, as molecules incorporating the coumarin scaffold show a broad spectrum of pharmacological activities, including anticancer, antimicrobial, antiviral, antioxidant, anticoagulant, anti-inflammatory, and anti-enzymatic. The aim of our study was to synthesise new coumarin-based compounds by using transition metal-catalysed reactions and evaluate their antibacterial and antitumor potential. A series of 7-hydroxycoumarin derivatives with aliphatic and aryl moiety attached directly at C-3 of coumarin ring and through the ethynyl or 1,2,3-triazole linker were prepared by Pd-catalysed or click reaction. The 3-substituted coumarin derivative bearing bistrifluoromethylphenyl at the C-4 position of 1,2,3-triazole showed strong and selective antiproliferative activity against cervix adenocarcinoma (HeLa) cells. The 7-hydroxy-4-methylcoumarin with a phenyl ring directly attached to coumarin at C-3 showed good potency against MRSA and VRE strains. The promising antiproliferative activity of coumarin derivative bearing 3,5-ditrifluoromethylphenyl substituent and antibacterial activity of coumarin derivative with aromatic moiety suggest that further enhancements could be obtained by structural optimisation of the coumarin core.

Audience take-away:

- Synthesis of 3-substituted coumarin derivatives by Pd-catalysed reactionwill be presented.
- Synthesis by Cu(I) catalysed click reactions of coumarin derivatives substituted with 1,2,3-triazole ring will be presented.
- Results of antiproliferative and antimicrobial evaluations of novel coumarin derivatives will be presented and the influence of substituents on biological activity will be explained.

Biography

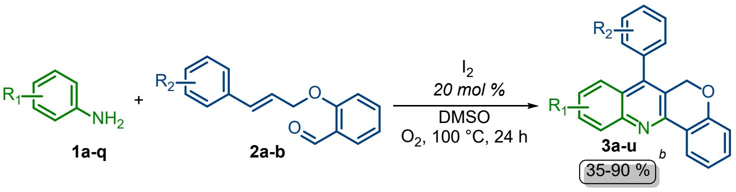
Dr. Tatjana Gazivoda Kraljević graduated in 2000 at the University of Zagreb, Croatia Faculty of Chemical Engineering and Technology and obtained her PhD in 2007 at the Faculty of Science. She has been working at the Faculty of Chemical Engineering and Technology since 2000, currently as vice-dean of education, teaching Organic Chemistry, Heterocyclic Chemistry, Modern Methods of Organic Synthesis, Organic Chemistry in Drug Development and Structure determination of Organic Compounds. Her research interest is focused on the development and synthesis of novel biologically active heterocyclc compounds such as purine isosters, pirimidine and coumarin derivatives by using transition metal catalysed reactions and the green synthetic approach.

Angélica Peñaranda Gómez*,Yaneth M. Brand, Liliana Betancurt Galvis,Carlos E. Puerto Galvis, Vladimir V. Kouznetsov
Universidad Industrial de Santander, Colombia

Synthesis of chromeno[4,3-*b*]quinolines through an imine formation/aza-Diels-Alder/aromatization tandem reaction under metal-catalyst and photosensitizer-free conditions and their in vitro antiviral activity

Chromeno [4,3-*b*]quinolines have emerged as an important class of tetracyclic O- and N-heterocyclic compounds because of their broad biological activities. Particularly, the chromenoquinoline skeleton is found in a variety of potential bioactive entities, such as β-selective estrogen ligands (ERβ), antitumor agents and anti-inflammatory derivatives. Furthermore, due to their fluorescent properties, some chromeno[4,3-*b*]quinoline analogues have been used in fluorescent probes to study cell permeability and live cell imaging of thiols and amino acids. Owing to their biological and fluorescent properties, synthetic and medicinal chemists are focusing their efforts in developing easy-to-handle and practical protocols for the synthesis of substituted chromeno[4,3-*b*]quinolines. Approaches such as the aza-Diels-Alder/aromatization, the tandem aza-Diels-Alder/halogenation and the oxidative arylation/cyclization tandem reactions catalysed by copper catalysts have been reported for the construction of chromenoquinoline derivatives.

Tandem reactions, a well-defined sequential process in which multiple chemical steps occurs one after another, without the need for external intervention for the formation of multiple bonds in a single operation, have become a useful and important strategy to construct complex organic molecules of great interest to scientists in both academia and industry. Besides the undeniable benefits of these protocols: time, effort and cost savings, these processes are often associated with the use of transition metal catalysts, toxic reagents and harsh conditions. Thus, in continuation of our studies on the imine Diels-Alder and the Povarov reactions, we report an improved, non-toxic, transition metal free, I_2/DMSO-catalysed tandem reaction between arylamines 1a-q and O-cinnamyloxy salicylaldehydes 2a-*b* to synthesize 7-aryl-6H-chromeno[4,3-*b*]quinolines 3a-u (Scheme 1).



Scheme 1. Synthesis of 7-aryl-6*H*-chromeno[4,3-*b*]quinolines 3a-u catalysed by the I_2/DMSO system.

All products 8a-u were obtained as stable solids and were fully characterized by IR, mass spectrometry and NMR (^{1}H, ^{13}C) Techniques. Finally, the antiviral profile of the synthetized compounds 3a-u were studied against infected Vero CCL-81 cells with the Zika virus. Compounds were identified as the most promising agents by exhibiting an inhibitory concentration of 77 and 57 PFU/mL, respectively, and with an antiviral activity of 25 μg/mL for both agents, which were substituted with electro-withdrawing groups on the quinoline moiety.

Acknowledgments: We thank the Colombian Institute for Science and Research (COLCIENCIAS) under the project No. 111574455595 contract 648-2017 for the financial support. A.P.G. thanks the fellowship given by Universidad de Antioquia under the contract 20730003-028-2018 and the project 648-2017.

Audience take-away:

- Organic and green chemistry, catalysis, tandem reactions, first steps in drug discovery (Synthesis and preliminary biological evaluation), reaction mechanism.
- This work will be of interest to the organic chemistry industry since a series of small molecules with a complex structure were easily prepared through a green, cheap and efficient methodology.
- The major advantage in comparison with the previous works is avoiding the use of metal and expensive catalysts that would be a big problem in scaling these protocols at industrial scale.
- Moreover, the synthetized compounds can be used for material science applications, medicinal or biological studies. Finally, the described tandem process involves a series of important chemical transformation in organic chemistry that can be used as an example for middle and advanced chemistry courses.

Biography

Angelica Peñaranda obtained in 2014 her Bachelor Degree in Environmental Chemistry at Universidad Santo Tomas (Colombia). In 2015, she joined to the Laboratorio de Química Orgánica y Biomolecular-LQOBio under the supervision of Prof. Dr. Vladimir Kouznetsov, PhD, DScand in 2020 she received her Master Degree in Chemistry from the Universidad Industrial de Santander (Colombia). Her main interests are related with the synthesis of small and complex molecules under green approaches for materials and pharmaceutical purposes, exploring the photo- and physicochemical properties of these derivatives and their biological properties as well. Currently, she is working at CENS group epm analyzing and studying polychlorinated biphenyls in liquids by Gas Chromatography techniques.

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Edible food packaging formulations based on renewable resources

In a context of increasing the world's population and resources consumption one of the greatest challenges of our society is to produce innovative materials by valorization of the renewable resources with the attempt to diminish the dependency of European companies on petroleum-based plastics. The aim of the paper is to develop bioformulations based on the revalorization of casein as a source of protein material. Boric acid was used to produce cross-linked casein, gelatin and casein–gelatin blend (with the contents of casein in the range of 0 to 30 wt% with respect to gelatin) edible films with adequate properties to ensure the safety and preservation of food by inhibiting pathogenic microorganisms and generating zero waste after consumption.The aqueous solutions of gelatin and casein were prepared by dissolving in distilled water, in concentrations of 10% and 7.5%, respectively (weight percent). The gelatin was hydrated with distilled water at room temperature and then dissolved in a water bath at 55 °C for 30 min. The casein was dispersed in distilled water at room temperature, after which sodium hydroxide (NaOH) were added under constant magnetic stirring until pH 7.0 was reached. Zetasizer was used to analyse the particle dimension of casein. Morphology by scanning electron microscopy (SEM), Fourier transform infrared spectroscopy, water absorption and rheology were used to explain the interaction between gelatin and casein.Water absorption is dependent on the composition of the samples and the immersion time. The introdution of casein into edible food formulations does not lead to a decrease in the transmittance. Smooth structured films were obtained due to casein, which is a poorly organized protein. Rheological properties of casein-gelatin wetted filmsshowed that the addition of casein significantly enhanced them. Further study needs to be done to elucidate the mechanism of increase in rate of storage modulus during the annealing stage.

Acknowledgement: This work was supported by a grant of the Romanian Ministry of Education and Research, CCCDI - UEFISCDI, project number PN-III-P2-2.1-PED-2019-2878, within PNCDI III" (BioMatFood), under the Contract No 379PED/2020.

Audience take-away:

- It is possible to open up new markets and increase demand for sustainable bio-waste products.
- Packaging of edible foods will improve consumer satisfaction.
- Environmental sustainability will be improved through a circular approach, water consumption and CO2 emissions in manufacturing processes will be reduced.

Biography

Dr. M. Rapa studied chemical engineering at University Politehnica of Bucharest and graduated as MS in 2002. She received her PhD degree in 2011 at the same institution. She is expert in polymer science, processing of biodegradable polymers designed to various areas at laboratory and pilot scales; testing of physical, mechanical and thermal properties of polymeric compounds, electrospinning. Dr. M. Râpă was first author on 25 ISI articles, co-author on over 60 ISI articles, 340 citations, 11 h-index, and has participated in over 30 research projects.

Patrycja Mała*, Henryk Koroniak, Christian Marcus Pedersen
Adam Mickiewicz University, Poland

Self-promoted glycosylation for the synthesis of N-glycosylsulfonyl amides

N-linked glycopeptides are naturally occurring glycosyl amides involved in various biological events e.g., processes on the cell surface. Synthesis of N-linked glycopeptides is intrinsically challenging since it requires control of stereoselectivity. Typically, in such glycoconjugates asparagine residue is attached to the suitable carbohydrate structure through the β-glycosidic linkage [1]. Apart from glycosyl amides, glycosylsulfonamides have emerged as another noteworthy class of glycosides due to their antitumor activity and inhibition potency toward carbonic anhydrase.

Here we demonstrate a direct, self-promoted glycosylation method for the formation of N-glycosides bearing both, the amide and the sulfonamide functions. The developed N-glycosylation is a two-component reaction, analogous to the previously reported method employing glycosyltrichloroacetimidate (TCA) donors and N-sulfonylcarbamate acceptors. In this work, N-sulfonyl amides have been investigated as another example of electron-poor acceptors. Due to the electron-withdrawing character of the sulfonyl moiety, the acceptors can activate the acid-labile TCA donors leading to glycosidic bond formation. Hence no additional catalysts, promoters, or additives have to be added.

The scope of various TCA donors and sulfonamide acceptors equipped with different protective groups have been studied in a series of glycosylations. Certain trends in terms of reactivity were observed based on the obtained results. The anomeric configuration of the donor has been found to influence the stereoselective outcome. Glycosylations using α-configured TCA donors resulted in high β-selectivity. The reaction takes place in several commonly used organic solvents. Interestingly, the glycosylations carried out at benign temperatures afforded the O-glycosides predominantly. However, these derivatives easily rearranged at elevated temperatures giving the corresponding β-N-glycosides.

Audience take-away:

- The audience will learn about the novel N-glycosylation method requiring no catalysts, promoters, or scavengers.The developed glycosylation is an example of the additive-free reaction and therefore it complies with current trends in organic synthesis.
- The reaction deals with one of the major importance in the preparation of glycosides which is the control of stereoselectivity.
- The presented studies regard the synthesis of biologically relevant compounds.

Biography

Patrycja Mala studied Biological Chemistry at the Adam Mickiewicz University, Poland, and graduated as MSc in 2017. She then undertook PhD studies in the research group of Prof. Henryk Koroniak at the aforementioned university. During her scientific career, she pursued internships in the research group of Assoc. Prof. Christian Marcus Pedersen at the University of Copenhagen. In 2019, she was awarded the DAAD One-Year Research Grant for Doctoral Candidates and worked under the supervision of Prof. Alexander Titz at the Helmholtz Institute for Pharmaceutical Research Saarland. Patrycja Mała is a co-author of the two scientific articles.

Ioana Stanciu
University of Bucharest, Romania

Rheological behavior of olive oil used as biodegradable lubricant

The main objective of a lubricant is to reduce frectionan wear. But also, it is responsible for heat evacuation. Taking into account their nature, there are mineral, synthetical, vegetal or animal lubricants. Untill the XIX-thcentury, the manufacturing process of lubricants has been based on vegetal and animal recources. In southern country, the olive and corn poppyoils were used meanwhile in northern country the rapeseed oil was used. These oils have a high degree of biodegradability even today. But when the mankind has discovered that oil could be processed for having lubricants and fuels at acceptable costs, the importance of vegetal resources had been reduced, but these petroleum-based lubricants has a strogly negative impact on the environment.

This proposes three relationships of dynamic viscosity temperature dependence for olive oil. The purpose of this study was to find a polynomial or exponential dependence between temperature and dynamic viscosity of olive oil, using the Andrade equation changes. Equation constants A, B, C and D were determined by fitting polynomial or exponential. Thousands of years, this oil was used for cooking, cosmetics and soap, but also as fuel for lamps. This proposes the relationship to describe the dependence of the dynamic viscosity of a olive oil, on the temperature. Experimental data for one type of olive oil were used to calculate the accuracy the proposed models. Equation constants were determined by exponential or polynomial beast curves obtained at different shear rates using the program Origin 6.0. The correlation coefficients thus obtained varied between 0.8754 and 0.9999.

Biography

She is a teacher of chemistry and physics in middle school. She graduated from the Faculty of Chemistry of the University of Bucharest in 1998. Studies Master she made in the same college and she has completed in 2001. She obtained a Ph.D. in chemistry in 2008 after 6 years of research stage, in which she obtained multi-grade oils based on synthetic polymers. Since 2005 she has participated in numerous national and international conferences, she has been publishing papers in journals national and international for study multi-grade oils, canola oils and sunflower oil. She continued the research by studying oils and get new rheological models describing their behaviour.

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