

JUNE 2022

13-14



*2<sup>nd</sup> Edition of*

**CHEMISTRY  
WORLD  
CONFERENCE**

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**BOOK OF  
ABSTRACTS**

**2<sup>ND</sup> EDITION OF  
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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 2022

With an earnest objective to congregate chemistry professionals, researchers, scientists and pharma industries, Magnus Group proudly enunciates and welcomes you to its 2<sup>nd</sup> Edition of Chemistry World Conference (Chemistry2022), which is going to be held Virtually during June 13-14, 2022.

This year the global summit will move forward with the theme Designing and Bonding the Molecular World of Chemistry with Current Innovations.

Unique and curated agenda for this year is to open doors for many researchers in academia, clinicians and industry representatives to explore disruptive technology and novel platforms, as well as to discuss cost-cutting and productivity-boosting strategies.

The two-day colloquium is designed to foster collaboration and innovation, with Chemistry poster presentations, interactive panel discussions, and visionary keynotes sessions.

We are confident that our conference will provide you with an incredible chance to explore new horizons in your field and we hope to see you at Chemistry 2022.



**KEYNOTE FORUM**

**DAY 01**



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## Karol Hęclic\* and Iwona Zarzyka

Rzeszow University of Technology, Poland

### Molecular modeling of imidazoquinazolinodione derivatives

Imidazoquinazoline derivatives have biological activities in different aspects. Therefore, they are applied as active substances in drug production. Moreover, their physical properties, for example, high decomposition temperature ~400 degree of Celsius make them useful in thermally stable polymers production. Research with molecular modeling methods confirms the structure of imidazoquinazolinodione derivatives and explain the course of the synthesis reaction. Modeling the entire space of solutions, i.e. products of reaction of 1-phenyl-2H,6H-imidazo-[1,5-c]quinazolino-3,5-dione with sequencing moles of ethylene oxide together with appropriate transition states, allowed to clearly define and explain the directions of subsequent reactions. The used methods indicate that molecular modeling, often treated as purely theoretical, finds practical application and can sometimes be the only tool to explain the obtained experimental results.

#### Audience Take-Away:

- How the molecular modeling methods help in prediction and/or confirmation, e.g. imidazoquinazolinodione derivatives structures, and explain the course of the synthesis reaction.
- How the molecular modelling methods, often treated as purely theoretical, have practical application and become the only way to understand some specific reactions.

#### Biography

Karol H. studied at Rzeszow University of Technology, Poland and graduated as M.Sc. of IT systems and Organic synthesis. He received his PhD (Chemical sciences) as a result of research on molecular modeling. Currently, he focuses on the use of molecular modeling to predict the properties of molecules containing imidazoquinoline rings. They can be used in two different ways: as monomers for polymerization and as active substances in drug production.



**Osman Adiguzel**

Firat University, Turkey

## Shape reversibility and thermomechanical reactions in shape memory alloys

Shape memory effect is a peculiar property exhibited by certain alloy systems, called shape memory alloys. These alloys have dual characteristics called thermoelasticity and superelasticity. Shape memory effect is initiated thermomechanical processes in the bulk level, on cooling and deformation and performed on heating and cooling after these processes. Therefore, this behavior is called thermoelasticity or thermal memory. Thermoelasticity is governed by successive thermal and mechanical reactions, in the atomic level, thermal and stress induced martensitic transformations. Thermal induced transformation occurs on cooling with cooperative movement of atoms in  $\langle 110 \rangle$ -type directions on the  $\{110\}$ -type planes of austenite matrix, along with lattice twinning and ordered parent phase structures turn into twinned martensite structures. Twinned structures turn into detwinned martensite structures by means of stress induced transformation by deformation in martensitic condition. This is plastic deformation, 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 performed by mechanically stressing the material at a constant temperature in parent phase region, and can be called mechanical memory, too. The materials are mechanically just over Austenite finish temperature, and shape recovery is performed simultaneously upon releasing the applied stress, by exhibiting the classical elastic material behavior. Superelasticity is also a result of stress induced martensitic transformation, and the ordered parent phase structures turn into the detwinned structures by means of stress induced martensitic transformation. Superelasticity is performed in non-linear way, unlike normal elastic materials; stressing and releasing paths are different in stress-strain diagram, and hysteresis loop refers to energy dissipation. Deformation at different temperatures exhibits different behavior beyond shape memory effect and superelasticity. Copper based alloys exhibit this property in metastable  $\beta$ -phase region, which has bcc-based structures. Lattice twinning is not uniform in these alloys, and the ordered parent phase structures turn into the non-conventional complex layered structures. 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 are 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. 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 new reactions in diffusive manner.

**Keywords:** Shape memory effect, martensitic transformation, thermoelasticity, superelasticity, lattice twinning and detwinning.

### Audience Take Away:

- Shape memory effect is a multidisciplinary subject from physics, chemistry to materials sciences and metallurgy.
- Shape memory alloys are functional advanced materials and used shape memory devices in biomedical and other applications. I will introduce the details on thermoelasticity and superelasticity.



## 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 80 papers in international and national journals; He joined over 100 conferences and symposia in international and national level as participant, invited speaker or 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 seven years (2014 - 2020) over 80 conferences as Keynote Speaker and Conference Co-Chair organized by different companies. He supervised 5 PhD- theses and 3 M.Sc.- theses. Dr. Adiguzel served his directorate of Graduate School of Natural and Applied Sciences, Firat University, in 1999-2004. He received a certificate awarded to him and his experimental group in recognition of significant contribution of 2 patterns to the Powder Diffraction File – Release 2000. The ICDD (International Centre for Diffraction Data) also appreciates cooperation of his group and interest in Powder Diffraction File.



## Thomas J. Webster

Interstellar Therapeutics, USA

### Beating COVID with Nano Chemistry

COVID-19 has stopped our normal way of life across all parts of the world. This presentation will cover how nano materials are being used to help prevent, detect, and treat COVID. Specifically, it will cover how self-assembled materials can be formulated to bind to regions of SARS-CoV-2 (the virus that causes COVID) to keep it from attaching to mammalian cells, entering mammalian cells, and replicating. It will emphasize targeting regions of SARS-CoV-2 in therapeutics that have not been mutating, thus, providing a versatile technique to fight COVID. Further, it will demonstrate how such nanomaterials can be used to improve the detection of SARS-CoV-2 as well as prevention. It will include a wide range of research from scientists all over the world, including in vitro and in vivo analysis, and discuss how such nano chemistries can better prepare us for future pandemics.

#### Audience Take Away:

- How nanomaterials are being used to passivate SARS-CoV-2 and treat COVID .
- How nanomaterials are being used to detect SARS-CoV-2 and COVID.
- How nanomaterials may be versatile materials to treat numerous viruses including future SARS-CoV-2 mutations.
- How nano chemistries can be used in diverse fields as tissue engineering to treat viruses.

#### Biography

Thomas J. Webster's (H index: 108; Google Scholar) degrees are in chemical engineering from the University of Pittsburgh (B.S., 1995; USA) and in biomedical engineering from RPI (Ph.D., 2000; USA). He has served as a professor at Purdue (2000-2005), Brown (2005-2012), and Northeastern (2012-2021; serving as Chemical Engineering Department Chair from 2012 - 2019) Universities and has formed over a dozen companies who have numerous FDA approved medical products currently improving human health. Dr. Webster has numerous awards including: 2020, World Top 2% Scientist by Citations (PLOS); 2020, SCOPUS Highly Cited Research (Top 1% Materials Science and Mixed Fields); 2021, Clarivate Top 0.1% Most Influential Researchers (Pharmacology and Toxicology); and is a fellow of over 8 societies.

**POSTERS**  
**DAY 01**



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**Irina Karardjova\*, Valentin Georgiev, Ivanka Dakova**

University of Sofia, Bulgaria

## U determination in wine and honey from bulgaria

Uranium is a toxic metal with low radioactivity which is ubiquitous in the environment. As a result of its natural occurrence, it can be found at different concentrations and in the form of different compounds in rocks, water, soil and air. Additionally, uranium can also enter the environment from anthropogenic sources – for example via the application of phosphate containing fertilizers. Uranium exhibits a chemical toxicity which can, in the case of continuous intake, lead to e.g. nephrotoxicity. Uranium is not readily transferred from soil to crops, and also has a low transfer factor from grass to animals. Nevertheless, as a component of the natural environment, uranium is likely to be present as a trace constituent in all foodstuffs. In the present study U is determined in wine and honey – traditional Bulgarian products. The idea is to find correlation between U content in soil and wine produced from grapes grown and U content in monofloral honey and U content in respective plants from the same region. The regions selected are characterized with relatively high background values for U. Bioavailable content of U in soil was determined using two extractants – 0.04 M acetic acid and 0.05 M EDTA (ammonium salt) widely accepted as suitable for assessment of mobile U, which might be accumulated by plants. In order to fulfil these tasks analytical procedures have to be developed for U determination by sensitive instrumental methods ICP-OES, ICP-MS.

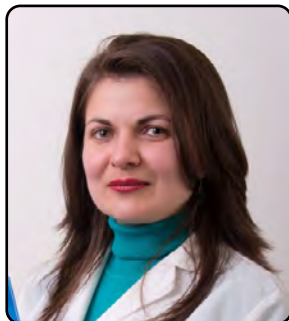
Systematic interference studies were performed for the influence of major components of wine and honey on the accuracy of U determination. Suitable element was proposed for internal standard calibration. In addition, for very low concentrations, solid phase extraction was applied using ion imprinted polymer as a sorbent. Results obtained showed relatively low correlation coefficients between U content in soil (for both extracts) and U content in wine. Most probably plant physiology prevents biouptake of U from soil. Almost the same is valid for honey. Very low correlation coefficients were defined between monofloral honey and U content in plants. From such point of view honey could not be accepted as suitable bioindicator for environmental pollution.

### Audience Take Away:

- The study refers to systematic investigations on U determination in wine and honey – development of analytical procedure. Assessment of correlation coefficients between U content in grapes and wine produced and plants and monofloral honey collected from the same region with typically high background values for U.
- The study will help wine and honey producers to improve technology for wine and honey production. In addition, the study is important for consumer for assessment of safety of widely consumed products – wine and honey.

### 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.

**Tanya Yordanova\*, Ivanka Dakova, Irina Karadjova**

University of Sofia St. Kliment Ohridski, Bulgaria

**Determination of  $Sb^{III}$  and  $Sb^V$  in water samples based on highly selective solid-phase extraction with polyvinyl imidazole**

Antimony is a chemical element that occurs in the environment as a result of natural and anthropogenic processes and its biogeochemical cycle is nowadays sufficiently characterized. Toxicological profiles and bioaccumulative properties of particular Sb species are well known – the inorganic chemical forms are much more harmful than organic species, especially the lower oxidation state  $Sb^{III}$ . In this sense, reliable knowledge about Sb speciation is essential taking into account significant differences between toxicity and bioavailability of trivalent and pentavalent forms. This work is focused on the preparation of vinylimidazole-based polymeric material and its further application as a sorbent for non-chromatographic speciation analysis of inorganic antimony in water samples. The polymer was synthesized by radical polymerization of vinylimidazole as a functional monomer, acetonitrile as a solvent, trimethylolpropane trimethacrylate as a cross-linking agent and 2,2'-azo-bis-isobutyronitrile as an initiator. Extraction efficiency and selectivity of the prepared material toward inorganic chemical species of antimony ( $Sb^{III}$  and  $Sb^V$ ) were studied by batch method.

Several parameters such as pH of the aqueous media, amount of the polymeric sorbent, time of sorption, type and concentration of the eluent solution were investigated in order to define the optimal chemical conditions for selective separation and enrichment of both  $Sb^{III}$  and  $Sb^V$ . Inorganic Sb species at trace levels were separated by quantitative retention of  $Sb^V$  at pH 5-6 for 25 minutes followed by elution with 0.1 M citric acid and ICP-MS measurement. The supernatant solution, containing  $Sb^{III}$ , was removed and treated with conc. HCl in order to convert  $Sb^{III}$  in negatively charged chloride complex and then 100 mg of sorbent material were added. Quantitative sorption was achieved for 15 min and after that, elution of  $Sb^{III}$  was carried out with 0.1 M tartaric acid for 20 min followed by measurement with ICP-MS. Additionally, total concentration of antimony can be determined in a parallel sample after preliminary conversion of  $Sb^{III}$  to  $Sb^V$  by oxidation with  $H_2O_2$  and subsequent extraction according to the procedure described for the retention of  $Sb^V$ . Thus a simple analytical scheme for speciation and determination of inorganic Sb in natural and bottled waters based on two sequential extraction steps was developed.

**Audience Take Away:**

- Synthesis and application of vinylimidazole-based polymeric sorbent.
- Non-chromatographic approach for speciation analysis of antimony.
- Fast and reliable analytical procedure for determination of  $Sb^{III}$  and  $Sb^V$  in water samples.

**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\*, Mariya Mitreva and Irina Karadjova**

Sofia University, Bulgaria

**Studies on the effect of functional monomers and chelating ligands on the properties of Fe(II) ion-imprinted polymers designed for iron speciation**

Iron is one of the most essential, chemical elements in an aquatic environment due to its role of catalyzer in phytoplankton photosynthesis and its involvement in metabolic processes – nitrate reduction, nitrogen fixation and respiration. Total dissolved Fe concentrations in an aquatic environment include kinetically labile complexes of Fe(II) and Fe(III), organically bound Fe and colloidal Fe species. The selective determination of dissolved species of both Fe(II) and Fe(III) at environmentally relevant very low concentrations is an actual task in environmental analytical chemistry. In this work, we report a study on the effect of template species – Fe(II) complexes with 4-(2-pyridylazo)resorcinol or 2,2'-bipyridine as well as the functional monomers: acidic (methacrylic acid) and neutral (hydroxyethyl methacrylate) on the extraction efficiency and applicability of Fe(II) ion-imprinted polymers (Fe(II)-IIPs) for iron speciation in surface waters. The polymers were synthesized by precipitation copolymerization of functional monomer, trimethylolpropane trimethacrylate (crosslinking agent) and 2,2'-azo-bis-isobutyronitrile (initiator) in the presence of template and characterized by elemental microanalysis, scanning electron microscopy and Brunauer–Emmett–Teller analyses. Extraction efficiency was examined by batch solid-phase extraction. The optimization experiments showed quantitative sorption of both Fe(II) and Fe(III) ions on the surface of Fe(II)-IIPs at pH 7, however selective sorption of only Fe(II) could be achieved in the presence of fluoride ions as a masking agent for Fe(III).

The desorption behaviour of both Fe(II) and Fe(III) was also identical and loaded Fe species were eluted quantitatively with 4 M HNO<sub>3</sub>. The kinetic studies indicated that the adsorption of Fe(II) ions best fitted with the pseudo-second-order kinetic model. The equilibrium experimental data of adsorption processes with different synthesized sorbents were well fitted by Langmuir isotherms models. Under the optimum conditions pH 7 and equilibrium time of 30 min the highest extraction efficiency and selectivity toward Fe(II) was achieved for Fe(II)-IIP containing methacrylic acid and Fe(II)-4-(2-pyridylazo)resorcinol complex as a template. The analytical procedure for Fe speciation was developed and validated with this sorbent.

**Audience Take Away:**

- Synthesis and characterization of new Fe(II) ion-imprinted polymers and their application for Fe(II)/Fe(III) speciation analysis.
- Evaluation of the influence of a functional monomer and type of chelating agent on the extraction efficiency and applicability of Fe(II) ion-imprinted polymers.
- Simple analytical procedure for the determination of Fe(II) and Fe(III) in surface waters was developed and characterized.

**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. She has published 50 research articles in SCI(E) journals.





**P. Vasileva\*, L. Djerahov, I. Karadjova**

University of Sofia, Bulgaria

## Direct and selective quantification of Cr(VI) in waste waters with raffinose capped silver nanoparticles as sensitive optical sensor

In the present study, a new method for direct and selective determination of Cr(VI) in the presence of Cr(III) in water samples is presented using raffinose capped silver nanoparticles (Ag/Raff NPs). The nanoparticles used were obtained by one-step, one-phase “green” synthesis based on chemical reduction of Ag<sup>+</sup> using D-(+) raffinose as both reducing and capping agent, and sodium hydroxide as a reaction catalyst. Careful kinetic studies and optimization of the response time of the optical sensor ensured selective, accurate and reliable determination of Cr(VI) in waters in only 5 min. The method is based on the variation of LSPR absorption band intensity as a result of electrostatic interaction between the negatively charged Ag/Raff NPs and positive Cr(III) ions, *in-situ* produced by chemical reduction of Cr(VI) with ascorbic acid at pH 4, combined with the fast kinetics of Cr(III) coordination to the –OH groups of capping agent on the nanoparticle surface, causing further the nanoparticle aggregation. A standard addition calibration method for Cr(VI) quantification in real water samples, based on systematic study of matrix interferences, is proposed.

Analytical figures of merit, the validation method and application to real samples are presented. The calibration curve for Cr(VI) is linear in the range 2.5 - 7.5  $\mu\text{mol L}^{-1}$ , limit of quantification achieved is 1.9  $\mu\text{mol L}^{-1}$ , and values of relative standard deviation vary from 3 to 5 % for concentration level 1.9 - 7.5  $\mu\text{mol L}^{-1}$ . The interference studies performed in the presence of various metal ions show very good selectivity of Ag/Raff NPs toward Cr(VI) species. The observed selectivity of the optical response of raffinose capped silver nanoparticles towards Cr(VI) is achieved because of optimally selected combination of two key parameters in the procedure: *in situ* reduction of Cr(VI) with ascorbic acid in the presence of raffinose capped silver nanoparticles and optimal contact time of 5 min between the analyte and the optical probe. The added-found method is used to confirm accuracy and precision of developed analytical approach. The analytical procedure was validated by comparative analysis of underground waters, polluted with Cr(VI) from chromium plating factory, with the standard method based on spectrophotometry using diphenylcarbazide (ISO 11083: Water Quality —Determination of Chromium(VI)—Spectrometric Method Using 1,5-Diphenyl- carbazide). Very good agreement between the results obtained undoubtedly validates the analytical probe developed (raffinose capped silver nanoparticles) for selective quantification of Cr(VI) and confirms the applicability of the developed analytical procedure for routine application in the laboratory practice. The analytical approach developed might be used also as a fast screening method on site.

### Audience Take Away:

- Ecofriendly new method for synthesis of raffinose capped silver nanoparticles under ultrasonic irradiation and their application as sensitive LSPR-based optical sensor for direct quantification of Cr(VI) in waste waters.
- Careful optimization of sensor response time for reliable and selective determination of chromium(VI) without the separation of chromium(III) in water.
- Simple analytical procedure for selective quantification of Cr(VI) in waste waters characterized by a short reaction time, stable optical signals, simplicity, high selectivity and relevancy in routine analytical practice.

### Biography

Penka Vasileva 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.



**Heba S. A. Elzahabi\***

Al Azhar University, Egypt

## Quinoxaline antiviral motif between history and future: Urgent need for new antiviral

Struggling for the development of antiviral drug is a pivotal issue because of many reasons, e.g., existence of the chronic viral infections, e.g., hepatitis C virus (HCV), the emergence of new viral infections, e.g., corona virus and the development of resistance to currently used antiviral drugs. The progress of the antiviral research provided different antiviral agents. For example, European patent application by Donald Delong encouraged co-administration of ethyl-quinoxaline carboxylate and adamantanes in fighting influenza virus. In Swedish study, indoloquinoxaline (B220) attracted the attention as efficient antiherpes agent (Fig. 1). Hydroxy analog (9-OH-B220) was also reported as efficient antiviral agent that formed thermal stable complex with DNA. Later on, compound B220 was explored for inhibitory activity against HSV-1, cytomegalovirus and varicellae zoster virus. In 2007 quinoxaline carboxylic ester, opavirline was subjected to the investigation for the treatment of HIV infection (Fig. 1). Considering opavirline as a non-nucleoside reverse transcriptase inhibitor (NNRTI) paved the way to apply it in a study that explored the mutations of drug resistance. Consequently, it explored adaptation to a mutated NNRTI binding site with small reductions in binding affinity. Further, indoloquinoxaline was considered as potential semisynthetic antiviral scaffold that was designed via modification of indoloquinoline alkaloid, e.g., ellipticine. This alkaloid was proved to be natural anticancer agent with low safety margin. So, innovative researches modified it to antiviral indoloquinoxalines. Also, the category of NNRTI included quinoxaline scaffold (S-2720) that exhibited potent inhibition activity against HIV-1 RT and HIV-1. The library of quinoxaline derivatives included some difuryl quinoxaline compounds with promising antiviral activity. In 2012, some thioamide triazoloquinoxalines displayed promising antiviral activity against herpes simplex. Recently the light was focused on simple dihydroxyquinoxaline scaffold that promoted ATPase catalytic activity of herpes simplex. On continuation of our previous work to develop new antiviral agent and with the guidance of the previously mentioned data, it was the idea to develop new quinoxaline derivatives to investigate their antiviral activity. Ethyl (6,7-dimethyl-2-oxo-3,4-dihydroquinoxalin-3-yl)acetate and ethyl (6-methyl-2-oxo-3,4-dihydroquinoxalin-3-yl) acetate (1a,b), 3-methylquinoxalin-2(1H)-one (4) and 1,4-dihydroquinoxaline-2,3-dione were the starting precursors for nine novel quinoxaline compounds, 3a, 6, 10, 13, 15, 16, 17, 18, and 20, via adopting different nucleophilic reactions. The synthesized compounds were tested for their antiviral activity against HCV, HBV, HSV-1, and HCMV. Concomitantly, their safety profile was investigated as well as their selectivity against the viral strains. The Virology Unit at the University of Alabama recorded that, two compounds, 1a and 20, exhibited highly potent activity against HCMV with lower IC<sub>50</sub> values (> 0.05 μM) compared to ganciclovir (IC<sub>50</sub>, 0.59mM). Compounds 1a and 20 also exhibited low cytotoxicity together with a high selectivity index.

### Audience Take-Away:

- Audience will discover and detect concise profile of different quinoxaline compounds that are rationalized to be testified against different viral infections, two derivatives could be lead compounds for further investigation as they explored potent activity than standard antiviral with high safety margin.
- Definitely, this research will promote and expand the work on different quinoxalines and their isosteres to get simpler and more potent new antiviral agent via lead optimization approach.
- To get more improvement, further bioavailability studies will be done with in-vivo studies to complete the profile of the research.



## Biography

Heba Elzahabi is a professor in pharmaceutical medicinal chemistry. She received her B. Sc. in 1993 from Cairo University, college of pharmacy, M. Sc. Degree on studying the anticonvulsant activity of some novel diphenic acid derivatives in 1998 from Al-Azhar University, college of pharmacy. She achieved her PhD study (2003) on investigating the anti-inflammatory, analgesic activity of novel quinoxalines. She achieved researches on new anticancer agents e.g. in-vitro study against enzymes involved in cancer, researches in organometallic chemistry to testifying the effect of metal chelation on the therapeutic action, with handling a full thermal analysis of organometallic compounds.

**SPEAKERS**

**DAY 01**



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**Hui Sun**

Ningxia University, China

## Controlled fabrication and morphological transformation of polymeric bowl-shaped nanoparticles

**B**owl-shaped nanoparticles are asymmetric hollow structures with a single large opening on the surface. As a classical kind of asymmetric nanoparticle, bowl-shaped nanoparticles have shown advantages in loading and delivery of large sized cargoes, catalysis and energy storage. However, also due to the asymmetric structure, the controlled fabrication of bowl-shaped nanoparticles is still challenging. The self-assembly of amphiphilic polymers is powerful tool to prepare functional soft nanomaterials. Herein, we demonstrate a versatile strategy for preparing nanobowls with precisely controlled openings and interior holes based on the synergy of hydrogen bonding and  $\pi$ - $\pi$  interaction of amphiphilic homopolymers. A series of azobenzene pendants containing amphiphilic homopolymers were synthesized via RAFT polymerization. Upon adding water to the solution of the homopolymers, the high local viscosity of the preformed large compound spheres provided by non-covalent interactions hinders the homogeneous shrinkage of the spheres, leading to the formation of bowl-shaped nanoparticles. The intermediates of bowl-shaped nanoparticles were tracked by investigation into the kinetic process of assembly, and we also proposed a formation mechanism of the bowl-shaped nanoparticles.

In addition, the sizes of the openings and interior holes can be well controlled by molecular weight, initial concentration and concentration of ions. Based on the aforementioned design principle of amphiphilic polymers to prepare bowl-shaped nanoparticles, we also induced amphiphilic homopolymers that only form nanospheres by adding  $\pi$ - $\pi$  interaction donors. Taking advantage of the UV-induced isomerization of azobenzene group, we also investigated the controlled transformation of amorphous bowl-shaped nanoparticles to crystalline ellipsoids, which opens new avenue for the transformation of amorphous nanomaterials to crystalline ones. Overall, we proposed the strategy to prepare bowl-shaped nanoparticles via the self-assembly of amphiphilic homopolymers via the introduction of non-covalent interactions and realized the controlled shape transformation of bowl-shaped nanoparticles.

### Audience Take Away:

- The structure and functions of bowl-shaped nanoparticles.
- The design principle of amphiphilic polymers to prepare bowl-shaped nanoparticles and the formation mechanism.
- How to control the sizes of openings and interior holes of bowl-shaped nanoparticles?
- The controlled dis-assembly and re-assembly of bowl-shaped nanoparticles induced by UV light.

### Biography

Dr. Sun obtained his BS, MS and PhD degrees from Tongji University during 2013 to 2019 under the supervision of Prof. Jianzhong Du. Then he joined School of Chemistry and Chemical Engineering of Ningxia University. Dr. Sun focus on the development of new building blocks, self-assembly methods and functionalities of amphiphilic macromolecules. He has published more than 20 research papers including Nat. Commun., JACS, Chem. Sci. and so forth.



**Roksana Trznadel\*, Piotr Ruskowski, Lech Celewicz**

Adam Mickiewicz University, Poland

## Synthesis of gemcitabine phosphotriester hybrids and their initial in vitro evaluation

A number of important biological properties is assigned to the analogs of nitrogen bases, pyrimidine and purine nucleosides, and nucleotides. These are mainly antitumor and antiviral activities, but also antibacterial, antiparasitic, antifungal, and antimalarial. Currently, there are over forty effective analogues which have been approved by the US Food and Drug Administration (FDA). Gemcitabine (2',2'-difluoro-2'-deoxycytidine (dFdC)) is one of interesting examples of this group of cytostatic agents. dFdC is the only cytidine analogue approved by the FDA which effectively affects solid tumors. Among others, it is used to treat metastatic pancreatic, ovarian or non-small cell lung cancer. We present here a general synthesis' method of gemcitabine phosphotriester hybrids with other nucleoside analogues and non-nucleoside compounds of both natural and synthetic origin. To the bioconjugation there were used among others 3'-azido-3'-deoxythymidine (AZT), metronidazole (1-[2-hydroxyethyl]-2-methyl-5-nitroimidazole, MTZ) or metformin.

The first approach was based on the triester method with 1-(mesitylene-2-sulfonyl)-3-nitro-1H-1,2,4-triazole (MNST) via coupling reagent. In comparison, in the second approach there was used only 4-chlorophenyl phosphoroditriazolidate as a phosphorylating agent prepared by reaction of 4-chlorophenyl phosphorodichloridate with 1,2,4-triazole in the presence of triethylamine in acetonitrile without MNST. We also present the initial cytotoxic activity of the target 5'-phosphoramidates derivatives. This parameter was determined as a result of the sulforhodamine B test (SRB). The compounds were tested against five human cancer cell lines: cervical (HeLa), nasopharyngeal (KB), liver (HepG2), lungs (A-549), glioblastoma (U87), and also normal human dermal fibroblast cell line (HDF).

The work was supported by grant no. POWR.03.02.00-00-I023/17 co-financed by the European Union through the European Social Fund under the Operational Program Knowledge Education Development.

### Audience Take Away:

- Drawing attention to the benefits of bioconjugation commonly used in the field of medical chemistry.
- Gaining knowledge of phosphorus chemistry in medical chemistry.
- Approximation of the me-too drug methodology.

### Biography

In 2016 Roksana completed her MSc of Chemistry specialised in biological chemistry, currently PhD student at Department of Medicinal Chemistry of Adam Mickiewicz University in Poznań. So far she has been a co-author of two papers in reputed journals. Her scientific interests are widely speaking organic synthesis in field of drug design, referring mostly to synthesis of derivatives of pyrimidine nucleoside analogues.



**Iwona Budziak-Wieczorek\*, Marta Arczewska, Daniel M. Kamiński**

University of LifeScience in Lublin, Poland

## **Cocrystal formation of natural flavonoids: synthesis, physico-chemical assessment, antioxidant and spectroscopic studies**

In recent years, special interest in the prevention and treatment of many civilization diseases is caused by polyphenol compounds that are widespread in the plant world. Dietary flavonoids exert various biological activities like cardioprotective, chemopreventive, and neuroprotective effects which are attributed to their antioxidant, anti-inflammatory, and signaling properties. However, their poor solubility in aqueous solutions and the associated limited bioavailability exclude the development of effective and stable pharmaceutical formulations or dietary supplements. A number of methods are known to improve the pharmacokinetic profile of bioactive compounds, for example, using salts, amorphous dispersions in a polymer matrix, an inorganic matrix as a carrier, nanoparticles, and cocrystals. Especially, crystal engineering and cocrystallization techniques appear as a promising way to modify the bioavailability (e.g., solubility, permeability, and stability) and other physicochemical properties for a wide range of bioactive compounds. Cocrystals are single phase materials composed of two or more different molecular and/or ionic compounds generally in a stoichiometric ratio, bound by noncovalent interactions, predominantly hydrogen bonds, which are neither solvates nor simple salts.

The aim of the presentation is to show the results including the development of the synthesis of new crystalline forms of (-)-epicatechin, (+)-catechin and cardamonin with commonly used cofomers which are included in the list of compounds authorized for the safe use as additives to food products, pharmaceutical preparations, and dietary supplements. The chemical characteristics of the obtained cocrystals were confirmed by single crystal X-ray diffraction, FTIR, and Raman techniques. Structural studies were based mainly on the analysis of interactions occurring in the molecular structure, e.g. hydrogen bonds,  $\pi\cdots\pi$  interactions and supramolecular synthons.

### **Audience Take Away:**

- Bioavailability of natural flavonoids and effective methods used for improving their solubility or permeability of drug or active pharmaceutical ingredient (API).
- Cocrystallization method of active pharmaceutical ingredient with appropriate cofomers as a promising approach for enhancing oral bioavailability.
- Structural characterization of cocrystals by X-ray diffraction, FTIR and Raman spectroscopy.

### **Biography**

Iwona Budziak-Wieczorek graduated from the Faculty of Chemistry of the Jagiellonian University in Krakow in 2016. She works as a research assistant at the University of Life Sciences in the Department of Chemistry in Lublin (Poland). She wrote a doctoral thesis titled *Bioavailability of natural bioactive compounds – physicochemical and model studies* which is to be defended in 2022. She is interested in cocrystallization methods of natural flavonoids as well as solubility and permeability study. The purpose of her research is to synthesise new cocrystals of poorly water-soluble natural bioactive flavonoids. She has published 11 research articles in SCI(E) journals.

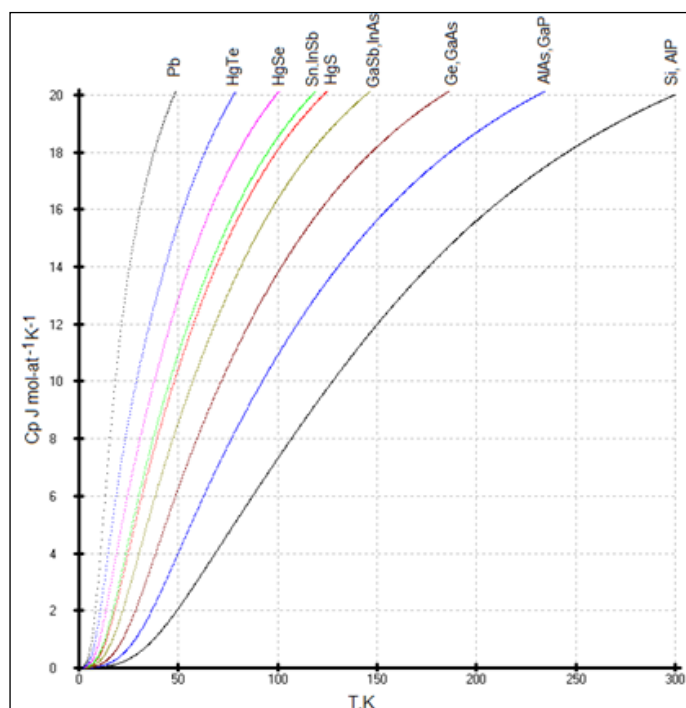
Valery vassiliev

Moscow State University, Russia

## Heat capacities $c_p(t)$ of the isostructural sphalerite phases as a single system in solid state

This work proposes a new vision on the description of heat capacities of diamond-like compounds with sphalerite structure. The 4th group of diamond-like elements consists of, in addition to diamond, silicon, germanium, alpha tin, and diamond-like lead. Flerovium ( $^{114}\text{Fl}$ ) closes this group. There should be no other elements in this group according to the fine structure constant or the Sommerfeld constant  $\alpha$ . In this case, the sphalerite structure has the ultimate value of the heat capacity  $C_p = 30.5 \text{ J mol}^{-1} \text{ K}^{-1}$  or  $3.67 R$ , and it falls on 114th element ( $^{114}\text{Fl}$ ). This quantity arises when plotting the isotherms  $\text{Ln}(C_p/R)$  vs  $\text{Ln}(N)$ . The heat capacities of sphalerite phases were considered as a single system.

**Keywords:** Fine structure constant;  $A^{\text{III}}B^{\text{V}}$ ,  $A^{\text{II}}B^{\text{VI}}$  Phases; Pure Elements IV Group; Ultimate value  $C_p$ ; Entropy; Similarity Method; Objective Function.



Heat capacities of sphalerite phases at the region of temperature 0-300K





**Dr. N. Goakrneshan\*, PG Anandhakrishnan, Dr. NeetiKishore, and Obulam Vidya Sagar**

Hindustan Institute of Technology and Science, India

## Technical aspects of areca fibres

Betel nut is one of the important fruits cultivated in tropical parts of the world. It generates a huge quantity of husk, which is a source of areca fiber. Both fine and coarse fibers are available in the husk. Different properties of fine areca fiber have been analyzed for qualifying its ability to convert into spun yarn. Fine areca fiber has good physical properties in terms of length, water absorption, maturity which makes it suitable for spinning. However, in case of strength and fineness it showed ordinary value compared to cotton fiber. Areca/cotton 50:50 blend 48tex ring and rotor yarn has been produced and yarns showed tenacity 7.1cN/tex and 6.88 cN/tex accompanied by 6.81% and 6.35% elongation, respectively. The water absorption of areca/cotton blend yarn showed 4.8 times higher value than 100% cotton yarn. All over the world people are now thinking about better utilization of natural resources. Areca fiber is a sustainable source of natural fibers which is also biodegradable, highly water absorbent and eco-friendly. In this research, the physical, mechanical and chemical properties of fine areca fiber have been analyzed and it was found that areca fiber has sufficient characters, which guarantees to manufacture yarn by both ring and rotor spinning system using cotton processing line. The length property of areca fiber is comparably high and excellent. The maximum length of areca fiber is near about 35mm where the effective length is 28mm and short fiber percentage is only 15%, which makes its suitable to manufacture spun yarn by cotton processing line. The water absorption is more than 200% which is very high compared to other natural fibers. Treatment with acid and alkali shows normal behaviour like other vegetable fibers. This fiber shows the properties which are suitable for the application of breathable, absorbable medical and hygienic textiles that can bring humanity one forward step toward Green environment.

### Audience Take Away:

- The audience will be able to gain knowledge about areca fibres and extend it in their area of research.
- The audience will benefit from this presentation and use it in their job by way of carrying out research in the field and attempt to develop new products from the fibre.
- Diversified products could be developed that have functional applications and are eco-friendly.

### Biography

Dr.N.Gokarneshan was born in 1964. He has work experience in academic institutions and industry as well. He has had a stint of over a decade with the textile industry and rose to the position of General Manager. He has experience in academic institutions spanning over 25 years. He has held various positions like professor, head of department and principal. Presently he is working as Dean of the department of costume design and fashion, Dr.SNS Rajalakshmi College of arts and science. His contributions in teaching include authorship of 15 books, contribution of many book chapters for edited books, publication of over 200 papers in various leading scientific journals, paper presentation in conferences. Besides, he holds various portfolios like peer reviewer and editorial board member in journals. He has also been organizing committee member in many conferences. His areas of interest are fabric formation, Textile science, textile wet processing, technical textiles and nano technology in textiles. He is a recipient of many awards and recognitions for contributions in his field.



**Sweta Kumari\*, Om Prakash Gupta, Sandeep Kumar, Minnu Sasi, Arpitha S R, D Amirtham, Chandra Bhushan Mishra, Vinutha Thimmegowda, Veda Krishnan, Archana Sachdev, Rajeev Ranjan Kumar, Shelly Praveen, Anil Dahuja**

ICAR- Indian Agricultural Research Institute (IARI ) India

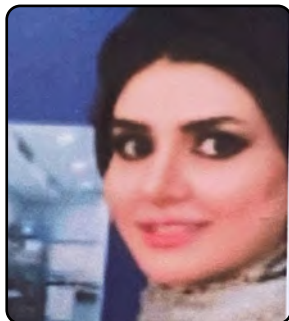
## **A novel continuous enzyme coupled colorimetric assay for phospholipase a<sub>2</sub> and its application in the determination of catalytic activity of oil body- associated oleosin protein**

The present work reports a novel, continuous, specific and colorimetric coupled method for the assay of phospholipase A<sub>2</sub> (PLA<sub>2</sub>), which involves use of acyl-CoA synthetase (ACS) as coupling enzyme and Dilinoleoyl Phosphatidylcholine (DLPC) as substrate. This method is based on the principle that free fatty acids (FFA) produced by PLA<sub>2</sub> are acted upon by ACS, which requires Coenzyme A (CoA) as co-substrate. The PLA<sub>2</sub> activity was measured in terms of amount of CoA utilized in the coupled reaction, determined indirectly by measuring unreacted CoA using 5,5'-dithiobis (2-nitrobenzoate). The PLA<sub>2</sub> assay was in agreement with Michaelis–Menten equation ( $V_m = 11.9$  nmole/min/mg),  $K_m = 5.3$  nmole,  $V_m/K_m = 2.2$  min<sup>-1</sup>mg<sup>-1</sup>). Compared to other available methods, this method provides an exact measure of PLA<sub>2</sub> as natural PLs are used as substrate in place of PL analogues. The embedded advantages of this method would have wider acceptability and applicability.

**Keywords:** Phospholipase A<sub>2</sub>, Acyl-CoA synthetase, Soybean, Oleosin, Dilinoleoyl Phosphatidylcholine.

### **Biography**

Dr. Sweta Kumari Holding the Position of Scientist at ICAR- Indian Agricultural Research Institute (IARI), New Delhi. She Graduated in Agricultural Science from Banaras Hindu University (BHU), Varanasi and Post Graduates (Master's and Ph.D.) in Biochemistry from ICAR- IARI, New Delhi. She is a Life Member of Society of Journal of plant Biochemistry and Biotechnology, New Delhi and Society of Indian Journal of Plant Physiology, New Delhi. She received much recognition in terms of awards and fellowship. She awarded two times with ICAR- NET by Agricultural Scientist Recruitment Board (ASRB), New Delhi, two times with JRF-NET by Council of Scientific and Industrial Research (CSIR) New Delhi, IARI –SRF by ICAR- Indian Agricultural Research Institute (IARI), New Delhi, ICAR-JRF (Junior Research Fellowship) for M.Sc by Indian Council of Agricultural Research (ICAR), New Delhi and UG-NTS (Undergraduate National Talent Scholarship) for B.Sc (Agri) by Indian Council of Agricultural Research (ICAR), New Delhi. She published several articles in the area of enhancement of nutrition and flavor quality of crop plants as plant food for improved human nutrition and health in different national and international journals and magazines.



**Anfal M. Alkandari\***, Yasser M. Alsayed, Atallah M. El-Hanbaly  
Mansoura University, Egypt

## Effect of chemical properties on liposomal encapsulation of radiopharmaceutical tracers

Drug loading in liposomes can be performed either passively (during liposome formation) or actively (after liposome formation). Thus, the trapping efficiency of hydrophilic drugs in passive liposome encapsulation is relatively low (around 30%) due to the limited volume of the encapsulated aqueous component in the liposome core. By using active loading methods, such as pH gradient entrapment, the trapping efficiency of hydrophilic drugs can be increased to 100%. This study aimed to reach the maximum encapsulation efficiency to upload drugs and radioisotopes by using different types of chemical agent and a different loading technique (the pH gradient technique). The  $^{99m}\text{Tc}$ -radiopharmaceutical kit has a pH range of 8.3–9.1, if prepared without the admission of air, and a shelf life of 8 hours. However, the addition of 2 ml of air changes the final pH range to 7.5–9.0.

In this study, the liposomes had an extra-liposomal pH of 7.2 and an interior pH of 5.0 in order to ensure better drug encapsulation. Many trials were performed, and the formula with the smallest particle size possible was selected. Trisodium citrate and ammonium sulfate were tested individually as hydration buffers with different concentrations. The pH gradient technique and drug encapsulation during liposome formation both offer advantages over using drugs without liposomes. Furthermore, the ammonium sulfate manifested the smallest particle size when compared to the other buffers. By adding cationic particles, the targeting efficiency was enhanced and the biodistribution of the radiopharmaceutical increased. The target-non-target ratio produce interesting results, as the uptake and specificity were enhanced.

### Audience Take Away:

- Audience will be able recognize the advantages of using nanoparticles encapsulation for drug delivery.
- They will know the chemicals and techniques that affect the nanoparticle sizes and charge in order to enhance the drug loading as well as the biodistribution of the drug.

### Biography

Nuclear medicine specialist. Anfal M. Alkandari from Kuwait has dual bachelor degrees in nuclear medicine, from Kuwait university, and the second major in medical biophysics, then completed her master degree at the age of 32 from Helwan university-Alkasr Alaini in Egypt. She is a PhD candidate from Mansoura University in Egypt.



## Anna Lagunas\*, Christine Belloir, Loic Briand, Pau Gorostiza, Josep Samitier

University of Barcelona, Spain

### The nanoscale effects of ligand binding on the electrical properties of olfactory receptors

Olfactory receptors (ORs) comprise the largest multigene family in the vertebrates. They belong to the class A (rhodopsin-like) family of G protein-coupled receptors (GPCRs), which are the most abundant membrane proteins, having widespread, significant roles in signal transduction in cells, and therefore, they are a major pharmacological target. Moreover, ORs displayed high selectivity and sensitivity towards odorant detection, a characteristic that raised the interest for developing biohybrid sensors based on ORs for the detection of volatile compounds. The transduction of odorant binding into cellular signaling by ORs is not well understood and knowing its mechanism would enable developing new pharmacology and high performance biohybrid electronic sensors. Recent findings suggest that ligand recognition by ORs is determined by the nanoscale alterations of charge distribution in the receptor structure. However, the electrical characterization of ORs and their response towards ligand binding in bulk experiments is subjected to microscopic models and assumptions. Here, we have directly determined the nanoscale electrical properties of ORs with unprecedented control over the receptor orientation, and their change upon odorant binding, using electrochemical scanning tunneling microscopy (EC-STM) in near-physiological conditions. Recordings of current versus time, distance, and electrochemical potential allows determining the OR impedance parameters and their dependence with odorant binding. The simultaneous measurement of RC equivalent by means of the open-circuit voltage ( $V_{oc}$ ) allows increasing the electrical sensitivity at the single receptor level for biosensing applications. Our results allow validating OR structural-electrostatic models and their functional activation processes.

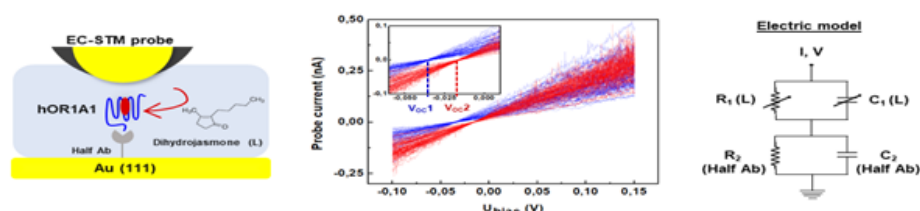


Fig.1. Dihydrojasnone binding to hOR1A1 caused a shift of VOC to lower potentials (absolute values), measured through current-voltage (I-V) recordings in the EC-STM. The electrical behavior of hOR1A1 is modeled as an RC parallel circuit and empiric impedance values were directly determined both in the presence/absence of dihydrojasnone.

#### Audience Take Away:

- As dealing with EC-STM, which is not a widely available technique, we think the audience could learn about the benefits and information that can be provided by this technique applied to biological systems.
- Although a large part of the results refers to EC-STM recordings, we also conducted cyclic voltammetry (CV) measurements in bulk, thus highlighting their implications at the macroscopic scale, and demonstrating a device that can be widely used by researchers in biology and materials. We extended our single-protein conductance measurements to large-area current recordings, which are widely accessible. Results obtained show an excellent match with the impedance parameters of olfactory receptors at the nanoscale (EC-STM) including their dependence with odorant binding. Thus, they demonstrate the application of our setup to sensing an extreme diversity of analytes whose biological functions remain largely unknown.

- Our results constitute a proof of concept of capacitance-operated odorant biosensors, which offer a significant increase in sensitivity and integration paving the way towards the next generation of biohybrid odorant sensors to detect volatile analytes, and to the study of the intriguing physiology of nasal and extra-nasal olfactory receptors. Capacitance-operated odorant biosensors constitute an alternative and a reliable way of sensing, which we think could be of interest to the audience of Chemistry World Conference.

### Biography

Dr. Anna Lagunas obtained her PhD in organic chemistry in 2007 from the University of Barcelona (UB). Her thesis was performed in the Institute for Research in Biomedicine (IRB) and in the Institute of Chemical Research of Catalonia (ICIQ). She worked on nanoparticles synthesis, functionalization, and characterization for asymmetric catalysis. Following her research interests in the nanotechnology field applied to biomedicine, she joined the Institute for Bioengineering of Catalonia (IBEC) where she is a CIBER-BBN Senior Researcher at the Nanobioengineering Group. Her research focuses on the design and fabrication of functional materials that together with high resolution techniques allow the interrogation of cells at the nanoscale, thereby revealing signatures of the spatio-temporal regulation of complex biological mechanisms. She has published more than 30 research articles in SCI(E) journals.



**D. A. Giraldo, P. Almodóvar\*, I. Álvarez-Serrano, J. Chacón,  
M.L. López**

Universidad Complutense de Madrid, Spain

## Dimensionality of $\text{MnO}_2$ cathodes as a key factor governing kinetics in aluminium-ion batteries

Along with the non-stopping technological expansion, modern societies are in need of a constant energetic supply. Equipment with a stationary and non-stationary objective must have battery or capacitor devices adapted to its requirements, where energy storage has to be efficient. The Lithium-ion technology remains the most demanded system. However, the high cost and limited amount of lithium available has led to research for alternative systems: Na, K, Mg, Al, Ca and Zn. One of the most promising alternative among next-generation energy storage system is the aluminium-ion battery (AIB) which has a higher theoretical volumetric ( $8046 \text{ mA h cm}^{-3}$ ) and gravimetric ( $2980 \text{ mA h g}^{-1}$ ) capacity, but also due to its low cost, sustainability and low flammability.

Electrochemical activity of different  $\text{MnO}_2$  phases as electrodes of aluminium-ion batteries (AIBs) is studied. For this purpose, different simple synthesis routes have been carried out to obtain on the one hand,  $\text{MnO}_2$  rod-like with tunnelled structure ( $\alpha\text{-MnO}_2$ ) and on the other  $\text{MnO}_2$  hexagonal micro-pellets with lamellar structure ( $\delta\text{-MnO}_2$ ).  $\alpha\text{-MnO}_2$  showed an outstanding capacity (Q) of  $120 \text{ mA h g}^{-1}$  at current densities of  $100 \text{ mA g}^{-1}$ , which remains stable after 100 cycles with efficiencies over 90%.  $\delta\text{-MnO}_2$  showed a good capacity of  $80 \text{ mA h g}^{-1}$  at current densities of  $50 \text{ mA g}^{-1}$  after 50 cycles and with efficiencies over 95%. Moreover, cyclic voltammetry (CV) measurements at different rates allowed for a better understanding of the electrochemical behaviour and revealed the contribution relation of diffusive and capacitive-controlled mechanisms in the corresponding AIB system. Further cyclic voltammetry (CV) measurements at different rates allowed a kinetic study of the diffusive and capacitive-controlled mechanisms. The results were interpreted concerning the influence of dimensionality (1D and 2D) of the  $\text{MnO}_2$  phases obtained.

### Audience Take Away:

- New battery technologies
- Learn about rechargeable aluminium batteries
- Understand the importance of the chemical and physical structure of materials in their electrochemical behaviour

### Biography

She have developed research career in the field of materials science, evolving from the most basic science in the initial stage to their final applications in different fields, highlighting energy storage devices. She obtained PhD in physics at the Complutense University of Madrid in 2019. During PhD She collaborated with different groups to develop new batteries, such as zinc-air electrodes or composite materials for lithium-ion battery anodes. Since September 2019 She have been working at Albufera Energy Storage, where She have been researching on the development of advanced materials and improved electrolytes for aluminium batteries technology.



## Domokos Gero

Semmelweis University, Hungary

### Cell-based screening for anti-inflammatory drugs with the premise of innate immune tolerance induction

Inflammation is a poorly regulated reaction to pathogens or tissue injury that often requires medical therapy to prevent further tissue damage and to reduce the associated symptoms. Excessive inflammatory response may be triggered by evolutionarily conserved molecular determinants, termed pathogen- or damage-associated molecular patterns (PAMPs, DAMPs) that stimulate macrophages to produce inflammatory cytokines, including tumor necrosis factor-alpha (TNF- $\alpha$ ), which in turn activates the inflammatory cascade. Current anti-inflammatory medications poorly block the early steps of inflammatory pathways and mainly act on downstream targets. To find compounds that mimic innate immune tolerance and inhibit the initial steps of innate immune cell activation, we performed a cell-based screening campaign on a monocyte-macrophage cell-line. RAW264.7 cells were pre-exposed to biologically active drugs (Tocriscreen Plus Screening Library, 1280 compounds) and treated subsequently with the prototypical PAMP lipopolysaccharide (LPS). Inflammatory response was evaluated by measuring the TNF- $\alpha$  secretion with simultaneous assessment of cellular viability.

Test compounds induced a marked effect on cytokine production while hardly affected the cellular viability: 12.8% of drugs blocked the production of TNF- $\alpha$  by 50% or more. Our target-agnostic approach identified 20 clinical drugs that suppressed the inflammatory response (hit ratio of 1.5%) including steroids and the lipid-lowering atorvastatin, the  $\beta$ 2-agonist salmeterol and the antidepressant escitalopram. In conclusion, the initial steps of PAMP-induced inflammation may be modified by pharmacological interventions using currently available clinical drugs. Further testing of these compounds may be considered in experimental models of sepsis with a drug repurposing approach to test the translational potential of these findings.

#### Audience Take Away:

- A novel, target-agnostic approach to target inflammation.
- A cell-based drug screening effort with a drug repurposing concept to target inflammation.
- A summary of the results with approachable graphic representation of data giving an example of cell-based screen results.

#### Biography

Dr. Domokos Gero graduated as an MD at the Semmelweis University Medical School in 2000 and also received his PhD degree at the Semmelweis University. In 2000, he started transgenic mouse research in Dr. Mozes' laboratory focusing on gene therapeutic approaches against renal fibrosis at the Pathophysiology Department of Semmelweis University, then from 2006 he has started working on cell-based drug screening projects after he joined the CellScreen Research Center at the University. In 2010, he was invited to lead the cell-based drug screening group in Dr. Csaba Szabo's lab and became a faculty of the Department of Anesthesiology, University of Texas Medical Branch (UTMB), USA and continued his work there on early drug discovery projects. In 2015 he moved to the UK, receiving a Marie Curie fellowship and joined the University of Exeter Medical School, Devon, UK for 2 years working with Dr. Matt Whiteman on further characterization of mitochondrial hydrogen-sulfide donors. Since 2017, he has been teaching at the Institute of Translational Medicine, Semmelweis University Medical School, Hungary and stated his own cell-based screening laboratory. He has published over 50 research papers.

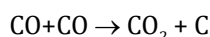


**Luca Vattuone**

University of Genoa, Italy

## Boudouard reaction under graphene cover

Ni is known to be a catalyst for the Boudouard reaction



This reaction is favoured by high pressure and it thus escaped so far direct investigation under operando conditions. We report here about a Near Ambient Pressure XPS study performed at Soleil (Tempo Beamline). Exposing bare Ni(111) to CO at a pressure  $P_{\text{CO}} \sim 2$  mbar we observed indeed graphene growth already at 550 K, a temperature significantly lower than the one (670 K) at which growth of graphene by segregation of dissolved carbon occurs. It was recently shown that the space between graphene and the substrate can act as a nano-reactor where the activation barrier for CO oxidation is effectively reduced. We show here that this is the case also for the Boudouard reaction. Exposing single layer Graphene on Ni(111) to CO at 3.7 mbar, CO intercalates under the graphene layer causing its detachment from the substrate. The so obtained high local CO coverage under graphene cover enables the formation of  $\text{CO}_2$  via the Boudouard reaction catalysed by the Ni(111) surface already at 340 K. The carbon produced by the reaction is used to transform carbide into graphene. Moreover under such conditions a chemisorbed CO species above graphene is observed, thus paving the use of graphene as an active support in catalysis.

### Audience Take Away:

- Brief overview about chemistry under graphene cover.
- Near Ambient pressure XPS study of the Boudouard reaction.
- Growth of graphene by the Boudouard reaction using Ni as catalyst.
- Graphene as an active support for catalysis.

### Biography

Luca Vattuone got his PhD from the university of Genoa. After a post-doctoral position at the University of Cambridge (UK) he came back to Genoa firstly as a post-doc and then as an Assistant Professor (1999). In 2012 he became Associate Professor of Condensed Matter Physics. His research activity focused on experimental investigation of gas-surface interaction using vibrational spectroscopy, photoemission, supersonic molecular beams and calorimetry. He also investigated surface plasmon dispersion. He published to date 135 papers and is a member of the Editorial Board of Coatings and of 4 Open.

**Ana I. Faustino**

University of Évora, Portugal

## **N-methyl-N-nitrosourea as a carcinogenic agent: What is its potential?**

Animal models are essential for biomedical research. Using them, the researchers are able to better understand the diseases, and search for more effective prophylactic and therapeutic approaches. Rodents are among the most frequently used species for scientific purposes. Chemical carcinogens' administration is one of the most frequently used methods to establish animal models of cancer. Indeed, these chemicals have the ability to induce cancer development in several organs. The carcinogen *N*-methyl-*N*-nitrosourea (MNU) is the oldest member of the nitroso compounds with the ability to alkylate DNA. So, MNU is classified as a complete, potent, and direct alkylating agent. Depending on the animals' species and strain, dose, route, and age at the administration, MNU may induce cancer development in several organs, like breast, ovary, uterus, prostate, liver, spleen, kidney, stomach, small intestine, colon, hematopoietic system, lung, skin, retina, and urinary bladder. This work intended to review the experimental conditions to the chemical induction of cancer development in several organs with this carcinogen agent, with a special emphasis in the mammary carcinogenesis.

### **Audience Take Away:**

- Future implementation of animal models of disease.
- Selection of animal models of disease.

### **Biography**

Ana Faustino is Professor at Department of Zootechnics of University of Évora and Researcher at CITAB/UTAD. She holds a Master in Veterinary Medicine and a European PhD in Veterinary Sciences. Animal models of cancer, tumoral angiogenesis and imaging are her main areas of interest. She has collaborating in several Financed Research projects. The results of her works were published in more than 250 publications in several formats. She received several prizes of scientific merit, and highlights and press honors. She has experience in supervising graduate and post-graduate students. She participated in several courses, workshops, international and national meetings. She is editorial member of several scientific journals and reviewer of more than 300 manuscripts. She is Guest Editor of two special issues in *Veterinary Animals* and in *Life*.

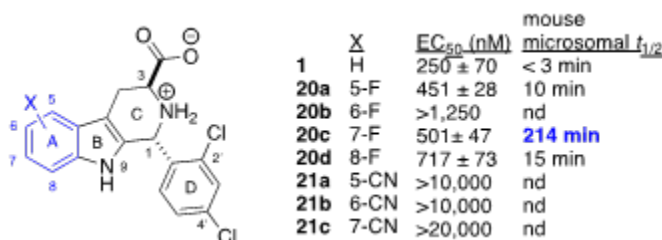


Maryam Ghamavi, Haibo Li\*, Lixuan Liu, Joshua H. Butler, Reagan Haney, Carla Slebodnick, Emilio F. Merino, Maxim Totrov, Maria B. Cassera, Paul R. Carlie

Virginia Tech, United States

## A-ring modification on MMV008138: effects on antimalarial potency and microsomal stability, implications for mode of inhibition

Tetrahydro- $\beta$ -carboline 1 (MMV008138)<sup>1,2</sup> controls growth of blood-stage *Plasmodium falciparum* by inhibiting a critical metabolic enzyme (IspD). It has a very specific D-ring structure-activity relationship, requiring halogen-disubstitution at the 2'- and 4'-positions.<sup>2,5</sup> It also cannot tolerate methyl substitution at positions 1-3 of the C-ring or 9 of the B-ring.<sup>6</sup> In this study we report the synthesis and evaluation of 19 A-ring variants of 1. Interestingly, extreme sensitivity to substitution is also seen in the A-ring, and only three derivatives had EC<sub>50</sub> within 3-fold of the parent (20a, c, d). 7-Fluoro analog 20c showed a marked improvement in microsomal stability. However, this improvement did not improve oral efficacy in a mouse model of malaria. Finally, we use X-ray crystallography of ( $\pm$ )-21a and <sup>1</sup>H NMR spectroscopy of 1 and 21a to address the equilibrium aqueous conformation of 1, and reevaluate a literature proposal for the binding pose of 1 in PfIspD.



### Audience Take Away:

- Audience will know how to do the modification of the lead compound to improve the growth inhibition and metabolism stability.
- We will show a good chemistry to synthesize our analogs and how we tested these analogs. Moreover, we will introduce how to deal with these problems.

### Biography

Haibo Li has been obtained his bachelor's degree in Shandong Normal Unveristy, China in 2014. He then graduated in University of Denver with a master's degree, USA in 2017. He is a Ph.D candidate in Virginia Tech, USA.

**Madhurima Chattopadhyay\*, Emilia Krok, Hanna Orlikowska and Lukasz Piatkowski**

Poznań University of Technology, Poland

**Hydration layer of few molecules controls lateral diffusion of lipids in biomembranes**

The cellular membranes are chemically highly heterogeneous structures, whose components work in a concerted manner, facilitating a broad range of important cell functions. The organization of the cell membrane involves not only assembly into microstructure, but also intricate interactions with the hydrating water. Since defects in membrane organization translate into dysregulation in their activity, understanding the interactions of membrane components with their hydration layer is of utmost importance. As lipid bilayers curl up to form vesicles and aggregates during dehydration, preparation of membranes with decreased hydration has been very challenging. We established an unprecedented method of obtaining desiccation-tolerant supported lipid bilayer (SLB) by a slow and gradual decrease of relative humidity (RH) of the sample, which enabled us to study lipid dynamics at varying hydration conditions. Using confocal imaging and fluorescence recovery after photobleaching (FRAP) technique, we studied single component as well as phase-separated SLBs prepared in 10 mM HEPES-150 mM NaCl buffer at varying local hydration states. Our study showed that the lateral mobility of PC lipids varies accordingly with the change in local hydration state reversibly and repeatably during dehydration and rehydration cycles. A six-fold decrease in diffusion coefficient values was observed from a fully hydrated membrane to a membrane equilibrated to 0% relative humidity condition.

The diffusion coefficient of PC lipid decreases steadily in the range of 90-50% RH, whereas, below ~50% RH, lipid mobility remains almost constant. The break at ~50% RH is related to the breaking of the water clathrate cage around the phosphocholine moiety of the lipid head groups which facilitates lateral diffusion of lipids acting as a lubricant. Arrhenius plots for fully hydrated and dehydrated samples revealed almost a twofold increase in activation energy of diffusion as a result of dehydration indicating the role of water molecules in the clathrate cage screening the electrostatic repulsion between the adjacent lipid head groups. Moreover, as the measured diffusion coefficient at different hydration conditions can be precisely correlated to the number of water molecules per lipid, the strong correlation between the lateral diffusion of lipids and the availability of water molecules per lipid can be used as a novel method of sensing the local hydration state of lipids in biomembranes down to 2-3 water molecules per lipid. Thus our study not only provides a clear picture of the dehydration process of lipid membranes, but the hydration dependence of lipid mobility possesses a huge potential to be utilized to investigate local hydration heterogeneity on a molecular level in biomimetic systems.

**Audience Take Away:**

- Explain the importance of investigating the water-lipid interactions at lower hydration conditions. There are several biological phenomena including cell fusion, adsorption of macromolecules, viral entry, fertilization etc., where local and transient dehydration is an important intermediate step. Understanding how lipids behave at low water availability is essential to understand the mechanism of such processes. Knowing about this motivation of my work, the audience may conceptualize their own research projects related to this.
- Preparation of desiccation-tolerant membrane has been very challenging as lipid bilayer curls up when water is removed. I shall discuss how slow and gradual dehydration keeps the structure of the membrane intact at lower hydration condition. Understanding this procedure of successful preparation of a dehydrated lipid bilayer will offer the audience huge possibilities for performing various experiments on lipid membranes at dehydrated condition.
- I shall also explain how lateral diffusion of lipid is controlled by the hydration level of the membrane. A clear molecular picture of hydration dependence of lipid mobility will help the audience to understand the chemistry behind such behavior of PC lipids. I believe that it will be very interesting for any membrane scientist.

- From my presentation, the audience will also learn about our novel approach of using the diffusion coefficient of lipids as a local hydration sensing tool in biomembranes. Scientists working on cell fusion or other biological processes where two lipid bilayer merge, will find it very helpful as they can try to use this approach in their research.
- Presentation will provide a deep insight on the hydration dependence of lipid mobility in phase-separated supported lipid bilayer. Understanding the chemistry behind hydration dependence of lipid mobility, many scientists may get interested in this topic, formulate new research questions and plan to start their own research projects on related topics. Moreover, they might be interested to collaborate with us. Faculty members can also use this knowledge for teaching their students. Dehydrating a lipid membrane while keeping its structure intact is very challenging. Knowing about our method of slow and gradual membrane dehydration, the audience will be able to prepare a dehydrated membrane without the addition of any external chemical and physical modifications. This will solve the problem of membrane dehydration and allow them to perform various interesting experiments on dehydrated lipid bilayers.
- It will enable the audience to use the diffusion coefficient of lipids to sense the hydration level in their biomembrane samples down to 2-3 water molecules per lipid. The audience may design new research experiments using the hydration sensing approach to solve their research problems.

### Biography

Madhurima Chattopadhyay is a doctoral student at Poznan University of Technology, Poland working on membrane biophysics. She finished her Master's studies in Chemistry from Banaras Hindu University, India in 2018. Her research focuses on the role of biological water on lipid dynamics and molecular interactions. She works with biomimetic cell membranes using fluorescence microscopy and fluorescence recovery after photobleaching (FRAP) technique. Her research provided new insights on the molecular basis of hydration-dependence of lateral diffusion of lipids. Being a freshman researcher, she has already published in high-impact peer-reviewed journals and filed a few patent applications.

**Seongwoo Woo**

Ethiopian Technical University, Ethiopia

## Improving the reliability design of mechanical systems such as refrigerator

To enhance the lifetime of mechanical system such as automobile, new reliability methodology – parametric Accelerated Life Testing (ALT) – suggests producing the reliability quantitative (RQ) specifications — missioning cycle— for identifying the design defects and modifying them. It incorporates: (1) a parametric ALT plan formed on system BX lifetime that will be X percent of the cumulated failure, (2) a load examination for ALT, (3) a customized parametric ALTs with the design alternatives, and (4) an assessment if the system design(s) fulfill the objective BX lifetime. So we suggest a BX life concept, life-stress (LS) model with a new effort idea, accelerated factor, and sample size equation. This new parametric ALT should help an engineer to discover the missing design parameters of the mechanical system influencing reliability in the design process. As the improper designs are experimentally identified, the mechanical system can recognize the reliability as computed by the growth in lifetime, LB, and the decrease in failure rate,  $\lambda$ . Consequently, companies can escape recalls due to the product failures from the marketplace. As an experiment instance, two cases were investigated: 1) problematic reciprocating compressors in the French-door refrigerators returned from the marketplace and 2) the redesign of hinge kit system (HKS) in a domestic refrigerator. After a customized parametric ALT, the mechanical systems such as compressor and HKS with design alternatives were anticipated to fulfill the lifetime – B1 life 10 years.

### Audience Take Away:

- Reliability test plans of multi-module product based on its BX life definition.
- Acceleration method of mechanical system.
- Derivation of sample size equation combined with targeted BX lifetime and accelerated factor.
- Accelerated life testing with reproduction of design problems and its action plans.
- Evaluation of the final product design to ensure the BX lifetime are satisfied.

### Biography

Dr Woo has a BS and MS in Mechanical Engineering, and he has obtained PhD in Mechanical Engineering from Texas A&M. He major in energy system such as HVAC and its heat transfer, optimal design and control of refrigerator, reliability design of thermal components, and failure Analysis of thermal components in marketplace using the Non-destructive such as SEM & XRAY. In 1992.03–1997 he worked in Agency for Defense Development, Chinhae, South Korea, where he has researcher in charge of Development of Naval weapon System. He was working as a Senior Reliability Engineer in Refrigerator Division, Digital Appliance, and SAMSUNG Electronics. Now he is working as associate professor in mechanical department, Ethiopian Technical University.

**Azhar Hajri\*, Dhouha Alimi and Hichem Sebai**

Institute of Biotechnology of Beja, Jendouba University, Tunisia

**Synthesis, characterization and *in vitro* acaricidal activity of new [1, 2, 4] triazolo [4,3-b] [1,2,4,6] thiatriazine-1,1-dioxides against cattle tick : *Hyalomma scupense***

A new series of [1,2,4]triazolo[4,3-b][1,2,4,6]thiatriazine-1,1-dioxides (2a-f) were synthesized, characterized and evaluated for their acaricidal activity against larvae and adults of *H. scupense*. The synthesis of triazolothiatriazine-1,1-dioxides (2a-f) was carried out. The approach involves a reaction between *N*-alkyl/aryl-*N'*-(4*H*-1,2,4-triazol-3-yl) amidines 1 and Sulfuryl chloride in the presence of pyridine. The structure of the synthesized compounds was confirmed by FTIR spectroscopy, <sup>13</sup>CNMR, mass spectra and elemental analyses. Adult immersion test (AIT) was performed to determine the mortality of ticks, inhibition of oviposition and hatching, after synthetic compounds (2a-f) application. Larval packet test (LPT) was performed on larvae produced from collected ticks. All of the tested compounds displayed a potent acaricidal activity. Among the series, compound (2d) represented the most potent ixodicide activity with LC50 values of 0.19 mg/ml as compared to the standard drug amitraz 0.06 mg/ml. Furthermore, after 24h of exposure, the 2d compound caused a high mortality on *H. scupense* larvae, as it induced 100% mortality at the highest tested concentration (1 mg/ml) followed by (2c), (2b), (2f), (2a) and (2e) (84.27%, 82.67%, 71.10%, 62.78%, 57.44%, respectively) (P<0.001). New heterocyclic compounds [1,2,4]triazolo[4,3-b][1,2,4,6]thiatriazine-1,1-dioxides (2a-f) were synthesized successfully and displayed satisfactory acaricidal properties against larvae and adults of *H. scupense*.

**Audience Take Away:**

- Get an idea of the biological valorization of new sulfur heterocycles
- Makes it possible to solve the problem of resistance of certain veterinary parasites against classic treatments.
- The molecules synthesized can be valued by other researchers

**Biography**

Dr. Azhar Hajri studied organic chemistry at the carthage university, Tunisia and graduated as MS in 2007. He received her PhD degree in 2012 at the Faculty of sciences of Bizerte, carthage university. He obtained the position of an Assistant Professor at the ISB Béja, university of jendouba. She has published more than 20 research articles in SCI(E) journals.)



KEYNOTE FORUM

DAY 02



2<sup>ND</sup> EDITION OF

CHEMISTRY

WORLD CONFERENCE

13-14 JUNE



**Valeriy Chernyak\*, Igor Fedirchyk, Vitalii Iukhymenko, Olexander Tsimbaliuk, Kostiantyn Iukhymenko. Volodymyr Ninyovskij**

Taras Shevchenko National University of Kyiv, Ukraine

## **Reforming and synthesis of hydrocarbons activated by plasma of gliding discharges in rotating gas flows**

A series of original plasma-chemical systems with plasma sources based on rotating gliding discharge and designed for the reforming of hydrocarbons into syngas and synthesis of hydrocarbons will be presented. The principal design of these systems stems from considering the negative effect of chemical processes on plasma nonequilibrium. Experimental studies of syngas production during reforming were combined with the numerical modeling of the chemical reaction kinetics to determine the connections between the temperature of the reaction chamber, reactants injection methods, and hydrogen yield. In addition, the requirements for achieving the maximum hydrogen energy yield and hydrocarbon reforming efficiency were investigated.

Plasma parameters were investigated using optical emission spectroscopy, The composition of reforming products was analyzed by gas chromatography, IR adsorption spectroscopy, and mass spectrometry, products of synthesis were studied using polarimetry and luminescence analysis. BOLSIG+ and ZDPLASKIN codes were used combined with the database of more than 150 components and 1400 process rate constants.

Research has put special emphasis on 1) the study of the possibility of using CO<sub>2</sub> as a reactant during the reforming and hydrocarbon synthesis; 2) the differences between the optical activity of the products of the chemical and plasma-chemical synthesis from the reactants without optical activity. In addition, the physical model of the synthesis of optically-active substances using only reactants without optical activity using gas dynamic systems with rotating flows of reactants will be presented.

### **Biography**

Over the course of his career, Prof Chernyak has worked on development and investigations of nonequilibrium plasma systems. His current research interests are focused on complex heterophase plasma-liquid systems with secondary discharges and their applications in plasma-assisted material processing, air & water treatment, toxic chemicals destruction, bio-fuel reforming, hydrogen-enriched combustion and other technologies. Prof. Chernyak is the author of four books, has published over 100 articles in professional journals and conference proceedings, and made dozens of presentations at conferences, including at least ten plenary lectures/invited.



## Nickolas Rigopoulos

University of the Aegean, Greece

### Scanning probe microscopy in food science: A review

Scanning Probe Microscopy is a nanotechnology tool that allows imaging at the nanoscale. In food chemistry, molecules such as gelatin, casein, proteins as well as larger structures like polysaccharide gels, and starch are of paramount importance. In this talk a short review of the experimental techniques will be given followed by applications in science and propose some future research.

#### Audience Take Away:

- Keep up to date information on applications of Scanning Probe Microscopy in Food chemistry.
- Suggests new paths for research.
- Allows better understanding on processes related to food science at their natural environment.

#### Biography

Dr. Rigopoulos studied Physics at the University of Patras, Greece and graduated 1995. Then he joined the research group of Prof. Bruce Hamilton at the Department of Pure and Applied Physics, of University of Manchester Institute of Science and Technology, from which he was awarded a PhD degree in 2001. After a three year postdoctoral fellowship supervised by Prof Bruce Hamilton, he obtained a lecturer on contract position at the Department of Food Science and Nutrition, University of the Aegean, Greece (2014 – 2021), followed by a three year postdoctoral fellowship supervised by Dr Ioannou at the same institute.

**K.P.Mishra**

Ex Radiation Biology and Health Sciences Division, India

## Promise of new thermosensitive liposomes loaded with chemotherapeutic drugs for targeted cancer radiotherapy

The challenge and obstacle in chemotherapeutic strategy to cancer treatment consists mainly in the inadequate drug concentration at the tumor site in the body. Radiotherapy is the most common modality for cancer treatment but undesirable drug toxicity to normal tissues and unavailability of adequate drug concentration at the local tumor site results in sub-optimum treatment outcome in the clinic. Recent progress in research on the use of liposomes to encapsulate and deliver anticancer drugs to the tumor environment have offered new strategy to achieve the desired greater therapeutic outcomes. Our research group at Bhabha Atomic Research Center, Mumbai has undertaken to develop strategies for optimizing the tumor toxicities by designing liposomes which are long surviving and stable in the body circulation after administration and are capable of releasing the loaded anticancer drug to the intended organ site in response to local hyperthermia (thermosensitive liposomes) and open the new vistas to achieve targeted cancer radiotherapy.

The talk will highlight the design and development of long surviving surface engineered liposomes and optimization of loading the anticancer drug, doxorubicin (DOX), in the new nanosized vesicles capable to release the cargo in response to hyperthermia. Subsequent delivery of therapeutic radiation dose to the site with adequate level of released chemo- drug is anticipated to help realize the dream of targeted cancer radiotherapy. Experimental results from our laboratory will be presented together with the relevant developments elsewhere in the world on the design and development of multi-stimuli responsive liposomes for targeted cancer radiotherapy.

**Keywords:** New long surviving liposomes, Thermosensitive liposomes, Anticancer Drug Loading, Hyperthermia, Targeted Cancer Radiotherapy.

### Biography

Dr. Kaushala Prasad Mishra studied Chemistry at the University of Allahabad, India and graduated as MSc. in 1968. He then joined as Scientific Officer, a permanent position in the reputed nuclear research institute, Bhabha Atomic Research Center (BARC), Govt of India, Mumbai. He received his PhD degree in 1979 from the University of Gujarat, Ahmedabad, India. He grew upward in the career from position to position in Radiobiology Division of the same Center. He was visiting Professor at several universities, namely, Kyoto University, Japan, University of Bielefeld, Germany, University of Sydney, Australia, Institute of Biochemistry, France, University of Rome, Italy, University of New York, USA, Tokyo Institute of Technology, Japan, Nagoya University, Japan and others. He became the Head of Radiation Biology and Health Sciences Division, BARC. He has published more than 250 research papers and has received citations more than 4000 (Google Scholar).

**SPEAKERS**

**DAY 02**



**2<sup>ND</sup> EDITION OF**

**CHEMISTRY**

**WORLD CONFERENCE**

**13-14** **JUNE**



**Noor Ul Afsar\*, Xingya Li , Yanran Zhu, Zijuan Ge, Yue Zhou, Zhang Zhao, Arif Hussain, Liang Ge, Rongqiang Fu, Zhaoming Liu and Tongwen Xu**

University of Science and Technology of China, PR China

## **In-situ interfacial polymerization endows surface enrichment of -COOH groups on anion exchange membranes for efficient Cl<sup>-</sup>/SO<sub>4</sub><sup>2-</sup> separation**

In-situ interfacial polymerization (ISIP) technique is developed to prepare monovalent anion-permselective membranes (MAPMs). The introduction of multi-hydroxyl (-OH) and cationic groups in the base membrane provide suitable routes towards the monovalent anion transport. Only trimesoyl chloride (TMC) is employed to generate a crosslinked polyester layer on membrane surface. The ISIP transforms the surface of anion exchange membranes into a dense and negatively charged layer to promote the ion permselectivity. The modified membranes show a high limiting current density and low membrane resistance of 4.7 Ω.cm<sup>2</sup>. The resultant membranes exhibit a high Cl<sup>-</sup> flux of 6.3 × 10<sup>-8</sup> mol cm<sup>-2</sup> s<sup>-1</sup> and a high permselectivity of ~60 for Cl<sup>-</sup>/SO<sub>4</sub><sup>2-</sup>. The findings demonstrate the ISIP technique having great potentials for the fabrication of highly permselective MAPMs.

**Keywords:** Monovalent anion permselective membranes, In-situ interfacial polymerization, Anion separation, Permselectivity, Ionic flux, Electrodialysis.

### **Biography**

Noor Ul Afsar (born 1984) is a Pakistani physical and applied chemist and a postdoc fellow with prof. Wu Liang at the department of chemistry University of Science and Technology of China, Hefei, Anhui Province PR China. Noor obtained his MS and Ph.D. from the University of Science and Technology of China (USTC) under the supervision of prof. Xu Tongwen. Noor's research focuses on synthesizing ion-selective membranes for efficient ion separations. His main academic accomplishments are; developing cost-effective membranes for acid-base recovery by utilizing environment-friendly materials. He has established a facile protocol for ion-exchange membranes and is used for acid-base and lithium recovery via diffusing dialysis and electrodialysis processes.





## Ankush Gupta

DAV University, India

### Aggregation-induced emission enhancement (AIEE) phenomenon: A smart phenomenon for sensing applications

Recently, there has been a lot of activity in the development of fluorescent self-assembled aggregates due to their potential applications in nanostructure templating, light harvesting and energy transfer, chiral amplification and tuning, hole transportation, drug delivery, nanodevices, as photoswitches, logic gates, stimuli responsive materials, and sensors. Self-assembly of fluorescent molecules are known to exhibit significant changes in their photophysical properties as a result of intermolecular interactions. In most of the cases, such interactions lead to the fluorescence quenching. However, for many applications it is necessary to retain the fluorescence emission during the self-assembly of the molecules. Thus, it is important to develop a fluorescent material in which fluorescence of the molecules during the self-assembly does not quench. In this context, aggregation-induced emission enhancement (AIEE) phenomenon and fluorescent organogelation are the powerful tools to synthesize fluorescent aggregates.

Organic materials with aggregation-induced emission (AIE) and aggregation-induced emission enhancement (AIEE) have become a versatile tool for the construction of fluorescent self-assembled aggregates. The fluorescent aggregates formed by this AIE(E) strategy played an important role for the development of sensitive and selective fluorescent chemosensors. Further, fluorescent nanofibers formed from self-assembled aggregates have been found to be good sensing materials for the detection of nitroaromatic explosives. In the presentation, we have focused on the highlights of the fluorescent self-assembled aggregates based probes having sensing applications. The discussion comprises of structural designing for generating fluorescent aggregates for sensitive sensing of various analytes. Discussion on fluorescent self-assembled aggregates for detection of molecules will provide a new design strategy for the development of novel sensing systems.

#### Audience Take Away:

- Aggregation-Induced Emission Enhancement phenomenon mechanism.
- How fluorescent self-assembled aggregates are useful in sensing applications.
- Other researchers can use the AIEE phenomenon to expand their research.
- Yes, AIEE phenomenon provides practical solution to the problem and simplifies the designer's job more efficient.

#### Biography

Dr. Ankush Gupta was born in small town Dhuri, Punjab, India in 1985. He received his B. Sc. (Hons. School) and M. Sc. (Hons. School) degree in Chemistry from Guru Nanak Dev University, Amritsar, India. After completing his masters, he received his Ph.D. degree in 2013 from the same institute under the supervision of Dr. Vandana Bhalla and Prof. Manoj Kumar. He also served as Post-doctoral fellow in the Dong-A University Busan, South Korea. Currently, he is working as Assistant Professor in Department of Chemistry, DAV University, Jalandhar. He has published 21 research articles in SCI(E) journals of high impact like Chem Comm, Organic Letters, J. Org. Chem., Appl. Mater. and Interface, etc. His research interests include the design, synthesis of optical chemosensors and nanomaterials.





## Dr. Prateeti Chakraborty\* and Debasis Das

Bangabasi College, India

### Chemistry of Zn complexes with different non covalent interactions

Study of non-covalent interactions is the main pillar of supramolecular chemistry. Mostly it plays an important role in controlling the physical property as well as structural topology. In order to explore that role a series of four mononuclear Schiff-base complexes, namely,  $[\text{Zn}(\text{L})(\text{NCS})_2]$  (1),  $[\text{Zn}(\text{L})(\text{N}_3)_2]$  (2),  $[\text{Cu}(\text{L})(\text{NCS})_2]$  (3) and  $[\text{Ni}(\text{L})(2\text{bpy})(\text{NCS})](\text{ClO}_4)$  (4), [where L = N,N-dimethyl-N'-(phenyl-pyridin-2-yl-methylene)-ethane-1,2-diamine and 2bpy = 2-benzoylpyridine] were synthesized and the role of different non-covalent weak interactions responsible for the crystal packing of the complexes were thoroughly investigated. All of them were structurally characterised by X-ray diffraction analysis. In addition to conventional  $\text{CH}_3 \cdots \pi$  and  $\pi \cdots \pi$  interactions, the importance of unconventional C-H  $\cdots \pi$  interactions in the crystal packing of compounds 1–4 was investigated by means of Hirshfeld surface analysis and DFT calculations. In these unconventional C-H  $\cdots \pi$  interactions, the  $\pi$ -system (electron donor) is provided by the pseudohalide coligands.

The interactions formed by the  $\pi$ -system depend on the nature of the pseudohalide ( $\text{N}_3$ , NCO, NCS or NCSe) as demonstrated by molecular electrostatic potential calculations. Additionally, we have explored the photophysical properties of these complexes. Finally, we have combined a search in the Cambridge Structural Database and DFT energy calculations to analyse the rare ambidentate behaviour of SCN within the same complex.

#### Audience Take Away:

- By explaining different weak interactions present in the complexes audience will be able to learn the behavior of different pseudohalide moiety in formation of the complexes.
- The audience will learn the synthetic methodology of above mentioned coordination complexes.
- This research will help to understand the interactive behavior of pseudo halide chemistry.
- The simple synthetic strategy will help researchers to develop such coordination complexes in no time.

#### Biography

Dr. Prateeti Chakraborty studied Chemistry at Bethune College affiliated to University of Calcutta and graduated in 2007. She then did her master's from the same university in the year of 2009. After completing her post graduate study she joined the research group of Prof. Das at University of Calcutta and received her PhD degree in 2015. After 1 years of postdoctoral research in the same lab on Zn Chemistry, Catalysis she Joined Sharda University, Greater Noida as an Assistant Professor presently, she is working as an Assistant Professor in Chemistry at Bangabasi College. She has published 4 book chapters with an International Publisher and more than 35 research articles in journals of International repute.

**S. Girish Kumar**

CMR University, India

## Understand the doping mechanism in co-doped TiO<sub>2</sub>: A case study of C-N-S- TiO<sub>2</sub>

The multi non-metal doping of TiO<sub>2</sub> finds promising for the design and development of solar light harvesting photocatalyst and also for overcoming the drawbacks associated with conventional metal ion substitution. In particular, tridoping of C-N-S into TiO<sub>2</sub> has garnered major interests because of its mesmerizing features like simultaneous and relatively low energy substitution of carbon, nitrogen and sulfur from the cheaply available precursors (thiourea, L-cystine and L-cysteine), stabilization of the anatase crystal structure, red shift in the band gap response towards the solar spectrum, cooperative interactions with these codopants, and the absence of any impure phase formation even at elevated temperature and with high doping density during the substitution process.

Despite these unique merits, accessible reports on C-N-S-TiO<sub>2</sub> are not extensive and the discussions presented are far from the relevant aspects of the doping mechanism. With the intention of shedding light on the pros and cons of C-N-S-TiO<sub>2</sub>, this presentation review is framed to understand the beneficial effects multiple doping photocatalysis, doping mode of each dopant in the codoped system with respect to the reaction conditions and contradictions about the doping states of each dopant in the codoped system with reference to the previous literature. The concepts like modifications of defect structures, dopant distribution, doping mode and mutual interferences among will be dealt. It would be emphasized that the codoping process involving carbon, nitrogen and sulfur is quite obfuscated as several doping modes are witnessed for each dopant, which are coupled to other factors like dopant diffusivity and solubility, extent of doping, dopant segregation at the surface, nature of the dopant precursor, unpredictable interactions of the dopant states, and interactive reactions between the dopant and titania precursor together with the annealing conditions.

### Audience Take Away:

- As the research interests on non-metal doped titania is widespread, the presentation appeals to the wider audience working on the semiconductor photocatalysis. It would definitely provide a deeper understanding on the relationship between the precursor chemistry and the doping process.
- Draw meaningful conclusion on the optimization of the preparation conditions including the annealing temperature, time, and ambience and also on the precursor's concentration.
- The lowering of annealing temperature provides a way to fabricate the materials in the larger scale.
- The choice of the precursors may be conveniently selected which will help to reduce the economy involved in the preparation method.
- A photocatalyst with larger red shift in the band gap can be obtained by altering the reaction conditions.
- The strategy can be expanded to other widespread oxide photo catalysts.

### Biography

Girish is active in the interdisciplinary area of scientific research associated with materials chemistry and physics. He has published 44 research articles which have received more than 6300 citations. He is serving as Associate Editor for 'Chemical Papers-SPRINGER' and 'Applied Surface Science Advances- ELSEVIER' along with potential member in the Reviewer Panel Committee, RSC Advances. He has reviewed more than 1600 manuscripts from 175 journals. He has been recognized as 'Top 2% world scientist' by the survey conducted by 'Stanford University, USA (2019 and 2021) and 'Top 1% reviewer' by the Publons (2018 and 2019).



## Najam ul Hassan\*, Ishfaq Ahmad Shah

University of Education, Pakistan

### Composition dependent structural, martensitic and magnetic properties of NiMnCoTi ferromagnetic shape memory alloys

Ni-Mn based ferromagnetic Heusler alloys have gained much attention because they have applications in many areas such as magnetic refrigeration, sensors, magneto-mechanical devices and energy-harvesting devices. In present work we investigate the structural, martensitic and magnetic properties of  $\text{Mn}_{35+x}\text{Ni}_{35-x}\text{Co}_{15}\text{Ti}_{15}$  ( $x=0, 1, 2$  and  $3$ ) alloys using X-ray diffraction (XRD), Scanning electron microscopy (SEM), Differential scanning calorimetry (DSC) and magnetic measurements. XRD analysis shows two sets of diffraction patterns, with increase in values of  $x$ : the proportion of cubic B2 type increases while 5M modulated structure decreases. Large endothermic/exothermic peaks with distinct thermal hysteresis in DSC measurement indicate the martensitic/reverse martensitic transformations and martensitic transformation temperature decreases with increase in  $x$ . Thermal magnetization (M-T) curves show an abrupt change of magnetization from paramagnetic martensite to ferromagnetic austenite near MT temperature. Isothermal magnetization (M-B) curves for  $\text{Mn}_{35+x}\text{Ni}_{35-x}\text{Co}_{15}\text{Ti}_{15}$  show that magnetic field can induce the magnetostructural transformation. A magnetic entropy change of 12 is observed at room temperature (290 K) in  $\text{Mn}_{35+x}\text{Ni}_{35-x}\text{Co}_{15}\text{Ti}_{15}$ .

#### Audience Take Away:

- Martensitic Transformation, Magnetocaloric effect, Magnetic refrigeration.
- The materials showing martensitic transformation (MT) exhibit various multifunctional phenomena such as magnetocaloric effect (MCE), exchange bias (EB), magnetothermal conductivity (MC) and magnetoresistance (MR). This coupled transition is obtained around the MT temperature.
- The MCE is a magneto-thermodynamic phenomenon in which temperature is changed in the material when exposed to the external-non-constant magnetic field.
- Magnetic refrigeration is a best alternate conventional gas cooling technology, showing many, such as environment friendly, high refrigerant efficiency, low cost, occupying less space, low mechanical vibration, and harmlessness.

#### Biography

Dr. Hassan is working as Assistant Professor at Department of Physics, Division of Science & Technology, University of Education, Lahore, Pakistan. Before this he has worked as Assistant Professor of Physics at department of Physics, University of Central Punjab, Lahore, Pakistan. He has published more than 25 research papers in well-known International journals of Physics & Materials Science. He has also served as committee member, reviewer and keynote speaker in various International Conferences/Symposiums. Dr. Hassan did his Ph.D. in Materials Science & Engineering from Nanjing University of Science & Technology, Nanjing, China. Before commencing his doctoral degree, he has worked as subject specialist in Higher Education Department, Punjab Province, Pakistan.



## Saima Farooq\*, Asima Siddiq, Marium Mushtaq, Shabnam Shahida

University of Nizwa, Oman

### Visible-light photocatalysis for wastewater treatment

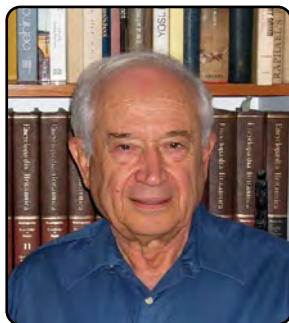
Photocatalysis is considered as one of the potential advanced oxidation processes for the de-pollution of wastewater. In particular, dye-contaminated wastewater is not only polluting the environment but causes serious health risks to both human and aquatic biota. This necessitates the development of efficient methods to remove dyes from contaminated effluents before their release in the environment. Titanium dioxide is the most widely used catalyst for the dye's degradation in photocatalysis due to its low cost, thermal stability, chemical stability, huge surface area and non-toxicity. The present work reports a one-pot synthesis of non-metal/transition metal co-doped  $\text{TiO}_2$  nanocomposites for photocatalytic degradation of reactive azo dye from aqueous solution. Various derivatives of  $\text{TiO}_2$  nano photocatalysts as  $\text{S@TiO}_2$  (singly-doped), and  $\text{Mn/S@co-doped TiO}_2$  with different weight percent were successfully synthesized and analyzed for detailed material characterization. The results revealed that  $\text{S/Mn co-doped TiO}_2$  nanocomposite exhibited high surface area, large pore volume and enhanced optical properties than undoped and  $\text{S-doped TiO}_2$ . Furthermore, the photoactivity of  $\text{TiO}_2$  nanoparticles was tested for Reactive Blue photocatalytic degradation. The co-doped nanocomposites ( $\text{Mn/S@TiO}_2$ ) manifested remarkable photocatalytic activity for the degradation of Reactive Blue dye under visible-light irradiation. The optimum degradation efficiency attained for reactive blue with  $\text{Mn/S@TiO}_2$  nanocomposites was 92% in a short time of  $\sim 70$  min. The significant degradation values and kinetic rate constant values strongly suggested that co-doped  $\text{TiO}_2$  degraded Reactive Blue at a higher rate than did undoped and  $\text{S-doped TiO}_2$ . In addition,  $\text{Mn/S@TiO}_2$  catalyst can be effectively employed for the degradation of emerging contaminants from industrial wastewater.

#### Audience Take Away:

- Facile synthesis methodology for nanocomposite preparation, their structure-property relationship and catalytic behavior can be utilized in water de-pollution processes.
- Nanomaterial synthesis strategies and material characterization is an applied advanced level subject that could phenomenally shape the graduate level curricula.
- The learned ideas can equally be effective for audience in their job/teaching because the said-topic have potential both in applied research and teaching, as mentioned above.
- The progressive depletion of fresh water resources has surged the development of wastewater treatment strategies. The presented topic is providing viable solution to wastewater treatment which can be effectively applied for decontamination of a wide range of organic and inorganic emerging contaminants from wastewater. It will further be beneficial for adopting (i) one-pot synthesis of nanocomposites at possibly low temperature (ii) visible-light active photocatalyst varieties.

#### Biography

Dr. Saima Farooq has been working as Assistant Professor of Physical Chemistry at the University of Nizwa, Oman since 2013. She received her PhD degree in Physical Chemistry at the Quaid-i-Azam University, Pakistan in 2012 and did short-term post doc supervised by Prof. Chedly Tizaoui in 2019 at the Water and Resources Recovery Research Laboratory, Swansea University, UK. She has published more than 28 research articles in SCI(E) journals, 2 book chapters with total citations 628; h-index 14. Her research interests are wastewater treatment, advanced oxidation processes, adsorption and heterogenous catalysis.



## Raphael Mechoulam

Institute of Drug Research, the Hebrew University of Jerusalem Israel

### The endocannabinoids – looking back and ahead

Over the last few decades research on the cannabinoids has gone through several distinct phases: 1) research on the plant cannabinoids, mostly on tetrahydrocannabinol (THC) and cannabidiol (CBD); 2) research on the endogenous cannabinoids, mostly on anandamide and 2-arachidonoyl glycerol (2-AG); and 3) research on anandamide-like endogenous fatty acid amides with amino acids and ethanol amines. Thousands of publications have been published on the cannabinoids and some of them are already in use as therapeutic drugs. Of particular interest is the non-psychotropic plant cannabinoid, CBD; it is an approved anti-epileptic drug and is being evaluated in many other therapeutic areas (for example, inflammation, cancer, bone fractures and auto-immune diseases). Similarly, cannabidiolic acid methyl ester, a stable synthetic derivative of cannabidiolic acid (CBDA), a major constituent of *Cannabis sativa*, proved to be effective in suppressing nausea and anxiety in rats and reducing depression-like behavior in animal models of depression.

Endogenous fatty acid – amino acid amides have been shown to be of major importance in a large spectrum of biological functions and diseases. Thus, oleoyl serine, is an anti-osteoporotic molecule, anandamide and arachidonoyl serine possess antimicrobial activity against methicillin resistant *S. aureus* strains, arachidonoyl serine exerts neuroprotective effects following traumatic brain injury and oleoyl glycine prevents both nicotine conditioned place preference – an addiction animal model - and nicotine withdrawal-associated behaviors in mice and thus may possess efficacy in treating nicotine addiction. We can expect therapeutic advances in all areas.

#### Biography

Mechoulam was born in Sofia, Bulgaria in 1930, He gained his first research experience in the Israeli Army working on insecticides. He received his M.Sc. in biochemistry from the Hebrew University of Jerusalem (1952), and his Ph.D. at the Weizmann Institute, Rehovot (1958), with a thesis on the chemistry of steroids. After postdoctoral studies at the Rockefeller Institute, New York (1959–60), he was on the scientific staff of the Weizmann Institute (1960–65), before moving to the Hebrew University of Jerusalem, where he became professor (1972) and Lionel Jacobson Professor of Medicinal Chemistry from 1975. He was rector (1979–82) and pro-rector (1983–85). In 1994 he was elected a member of the Israel Academy of Sciences. Mechoulam is one of the founding members of the International Association for Cannabinoid Medicines.



## Manar Ahmed Fouad\*, Francesco Ferretti, Simone Galie, Fabio Ragaini

Università degli Studi di Milano, Italy

### CO From Our Worst Enemy to Our Best Friend: Pd-Catalyzed Reductive Cyclization of $\beta$ -Nitrostyrenes Using Phenyl Formate as a CO Surrogate

The reduction of suitably substituted organic nitro compounds by CO, catalyzed by palladium-complexes, is a valuable method for the preparation of a variety of *N*-heterocyclic compounds. Despite the high efficiency of many of these reactions, the use of pressurized CO is a drawback since it requires the use of high-pressure equipment and CO lines and the presence of the corresponding safety measures. This limits the application of this kind of reactions as practical synthetic methods. In the aim of turning this kind of reaction into a “general tool” for the synthetic chemist, we developed a procedure based on the use of phenyl formate as an efficient *in-situ* CO surrogate.

Recently, our group employed phenyl formate in the palladium-catalyzed reductive cyclization of 2-nitrostyrenes to afford indoles and in the reduction of nitroarenes in the presence of conjugated dienes to give oxazines. It was found that phenyl formate is the most effective CO source and the desired products were obtained with selectivities and yields that in most cases are higher than those previously reported using pressurized CO. The reaction can be performed in a glass pressure tube, a cheap equipment accessible to every laboratory. Here, we report our results regarding the use of phenyl formate as a CO surrogate in the synthesis of indoles by reductive cyclization of  $\beta$ -nitrostyrenes, catalyzed by  $\text{PdCl}_2(\text{MeCN})_2$  + 1,10-phenanthroline. It has been found that satisfactory results are obtained when the starting nitrostyrene has an aryl substituent at the *alpha* position. On the other hand, in the absence of such substituents, only moderate yields of indole have been achieved since the base required to degrade the formate can also catalyze the oligo-polymerization of the starting styrene.

#### Audience Take Away:

- This work presents a one-step reaction to get indoles in excellent yields through the reductive cyclization reaction of  $\beta$ -Nitrostyrenes without the need of CO lines.
- The same reaction was used before to synthesize different heterocycles and fine chemicals which considered as a building block for valuable pharmaceutical and industrial compounds.
- The reaction can be performed in a single glass pressure tube, a cheap and easily available piece of equipment, so, we can avoid the use of autoclaves.

#### Biography

Manar Ahmed Fouad graduated from Faculty of Science, Alexandria University (Egypt) in 2016 after receiving a chemistry honor degree, and in 2019 she received a master's degree in science from the same university. She is currently a lecturer at Alexandria University (Egypt). In 2020, she received a PhD scholarship from University of Milan (Italy) to develop her research under the supervision of Prof. Fabio Ragaini. Her research interests include homogeneous and heterogeneous catalysis, heterocyclic compounds chemistry, organic synthesis, multicomponent reactions and bio-organic chemistry.





## Alaa Adawy

University of Oviedo, Spain

### Functionalizing metal phosphates to synthesise antimicrobial biomaterials

**M**etal phosphates are an important group of materials with established technological and industrial applications that are still attracting special scientific interest, owing to their outstanding physical and chemical properties. Most of the conducted research regarding metal phosphates as biomaterials focuses on calcium phosphate compounds (CPCs). To date, CPCs are among the most widely studied, and thus, accepted compounds for biomaterial applications together with less famous phosphates compounds, such as magnesium phosphates. In particular, resorbable phases have gained particular attention in recent years, owing to the revolution that has been encountered in this research field and the increased consideration of the bioreactivity (bio-functionality) of biomaterials side by side to their biocompatibility. Therefore, increased interest has been gained in brushite and its anhydrous form monetite that are among the most interesting resorbable CPCs that can be applied as cements and for *in situ* fabrication of three-dimensional (3D) implants. However, according to our recent investigations we found that there are other promising metal phosphates, Based on titanium and zirconium, that can provide alternative materials to the heavily studied calcium-based metal phosphates. In this talk, recent developments in this context will be discussed. In addition, the different polymorphs of titanium and zirconium phosphates will be highlighted focusing on their relatively easy synthetic routes and the possibilities they can provide in the biomaterials field if they are doped, enriched or intercalated with antimicrobial agents.

#### Audience Take Away:

- This is an old-but-gold field of research with continuous progress and possibilities owing to the advancing characterization possibilities at the nanoscale and its increasing interest in the medical field.
- The talk will provide a highlight to the recent advancements and their future perspectives.
- This field is interdisciplinary and thus provides different possibilities for researchers involved from the chemical, physical, biological and medical fields.

#### Biography

Dr. Adawy, B.Sc. in Biophysics, cum laude; M.Sc. in Biomaterials is the staff scientist responsible for the Electron Microscopy facilities at the University of Oviedo, Spain. Since her graduation she has been extensively involved in academic teaching and scientific research in multidisciplinary projects in which scientists from different disciplines collaborate to develop new scientific insights. Finishing her PhD on creating a new protein crystallisation at Radboud University, the Netherlands in the research groups of Professors Elias Vlieg (IMM) and Wim de Grip (RIMLS), in 2014, she joined Prof. Jan van Hest's group at the same University to investigate nanoconfined crystallisation. In 2016, she moved to Groningen University to work on a Japanese-funded research project on the usage of SLS and microfluidics to study protein nucleation with Prof. Matthew Groves. However, in parallel, she has continued her research interests on biomaterials applications.





## Dr. Daniel Köster\*, Dr. Christiane Kaus

Institute for occupational safety and health of the German social accident insurance, Germany

### Measurement of aldehydes from ambient air and method validation and proficiency testing using a dynamic test gas facility

In the field of occupational health and safety, the measurement of hazardous substances is one of the cornerstones in the prevention of occupational diseases. Aldehydes are found in many workplaces mainly due to their use as disinfection agents and for the fixation of biological samples. As Formaldehyde is classified as carcinogenic to humans (IARC group 1), routine monitoring of aldehydes is of major importance for workplace safety. For method validation and regular proficiency testing for internal and external partners, the Institute for Occupational Safety and Health (IFA) provides proficiency testing schemes for various hazardous substances including selected aldehydes at its dynamic test gas facility. Currently, the setup of the test gas facility allows simultaneous sampling for up to 25 participants with a total test gas flow of up to 12 m<sup>3</sup>/h. The provided test gases must meet high requirements regarding correctness, homogeneity, precision, and stability. To ensure the quality of the test gas in real time, Selected Ion Flow Tube Mass Spectrometry (SIFT-MS) has been established to monitor the quantitative test gas compositions. With the help of this new technique, short-term changes in the test gas composition can be observed in real time in contrast to the previously utilized measurement of offline-control samples by HPLC. This made it possible to verify a newly designed dosing system for the test gas generation of substances with high vapor pressure such as acetaldehyde and propionaldehyde by SIFT-MS. The special challenge here is that the entire dosage must be carried out in a cooled environment to avoid vaporization of substances in the tubing of the dosing system. By combining three individual components, a novel system for generating test gases was developed. The system is modularly composed of a microfluidic pressure-based pump system, a high precision cooling unit and a modified gas chromatographic inlet system. The system is suitable to produce an aldehyde test gas with the required quality in the dynamic test gas facility of the IFA. The suitability of the system was successfully demonstrated by parallel investigations using SIFT-MS and classical offline-HPLC analysis.

#### Audience Take Away:

- Techniques for the air monitoring of aldehydes.
- Importance of method validation during method development for air sampling techniques.
- Advantages of selected ion flow tube mass spectrometry (SIFT-MS) for the monitoring of test gas in real time.
- Advanced generation of dynamic test gas atmospheres.

#### Biography

Dr. Daniel Köster studied Forensic Science (BSc.) at the University of Applied Sciences Bonn-Rhein-Sieg, Germany and Robert Gordon University (BSc. honours), Scotland. After a MSc. course in Water Science at the University of Duisburg-Essen in Germany he joined the research group for Instrumental Analytical Chemistry of Prof. Dr. Schmidt at University of Duisburg-Essen. He received his PhD degree in 2020 at the same institution. In 2020 he joined the Institute for occupational safety and health of the German social accident insurance where he works as a research chemist for HPLC applications in the department for Chemical and Biological Hazards.



## Dr. Ez-zouhra El Maaiden

African Sustainable Agriculture Research Institute, Morocco

### A comparative study between conventional and advanced extraction techniques: Pharmaceutical and cosmetic properties of plant extracts

Medicinal and aromatic plant (MAPs) extracts are attracting much attention because of their interesting phytochemical composition, leading to the development of new pharmacological and cosmetic drugs. Extraction represents a critical step in the itinerary of phytochemical discovery from MAPs. The type of extraction procedure used can substantially influence the final extract recovered. This study aimed to compare the influence of extraction methods on the pharmaceutical and cosmetic properties of medicinal and aromatic plants (MAPs). For this purpose, the dried plant materials were extracted using advanced (microwave (MAE), ultrasonic (UAE), and homogenizer (HAE) assisted extractions) and conventional techniques (maceration, percolation, decoction, infusion, and Soxhlet). The tyrosinase, elastase,  $\alpha$ -amylase, butyryl, and acetylcholinesterase inhibition were tested by using L-3,4 dihydroxy-phenylalanine, N-Succinyl-Ala-Ala-p-nitroanilide, butyryl, and acetylcholine as respective substrates. Antioxidant activities were studied by ABTS, DPPH, and FRAP.

In terms of extraction yield, advanced extraction techniques showed the highest values (MAE > UAE > HAE). Chemical profiles were dependent on the phenolic compounds tested, whereas the antioxidant activities were always higher, mainly in infusion and decoction as a conventional technique. In relation to the pharmaceutical and cosmetic properties, the highest inhibitory activities against  $\alpha$ -amylase and acetylcholinesterase were observed for Soxhlet and macerated extracts, whereas the highest activity against tyrosinase was obtained with MAE > maceration > Soxhlet. Elastase and butyrylcholinesterase inhibitory activities were in the order of Soxhlet > maceration > percolation, with no activities recorded for the other tested methods. In conclusion, advanced methods afford an extract with high yield, while conventional methods might be an adequate approach for minimal changes in the biological properties of the extract.

**Keywords:** Advanced extraction, conventional extraction, bioactive compounds, enzyme inhibition, oxidative stress, microwave-assisted extraction.

#### Biography

Dr. EL maaiden EZzouhra is a Postdoctoral Researcher at African Research Institute for Sustainable Agriculture (ASARI) of the Mohammed VI Polytechnic University (UM6P) in phytochemistry and Valorization of plant species by the production of high added value molecules for cosmetic and wellness. She earned his M.Sc. and Ph.D. degrees from the University of Hassan 1st University in Settat in 2016 and 2021, respectively. His ongoing research focuses on valorization of the biomass of medicinal and aromatic plants to discover and characterize new bioactive metabolites that could pave new avenues for cosmetics, nutraceutical, and pharmaceutical applications.

**V.O. Cheranovskii\* and V.V. Slavin**

National University, Ukraine

**Quantum phase transitions in frustrated two-leg spin ladder model for nanostructured complexes of transition metals**

The ground state properties of the frustrated two-leg spin ladder model for nanostructured magnetic materials on the base of transition metal complexes have been studied. Using perturbation theory and numerical methods we found the possibility of quantum phase transitions, mediated by the value of the interactions between neighbouring ladder rungs. These phase transitions are characterized by significant change of the spin ordering in the ground state and are central to potential applications in molecular spintronics.

**Audience Take Away:**

- It is shown, that the theoretical approach based on spin formalism of valence bond method of quantum chemistry is of interest for the explanation of the relationship between chemical structure and magnetic properties of nanomaterials.
- The results of above study will be useful for targeted design of the new magnetic materials on the base of transition metal complexes for needs of molecular spintronics. In particular, sensitivity of the spin ordering in the ground state of the proposed model nanomagnets to the chemical surrounding can be used for the design of new chemosensors.

**Biography**

Vladyslav Cheranovskii completed his Doctor of Sciences in the year 1994 at the age of 38 years from Institute for Single Crystal, National Academy of Sciences of Ukraine. He is a Professor of V.N.Karazin Kharkiv National University, department of Chemistry. He has published 61 papers recognized by Scopus database. He is working in field of solid state physics and quantum chemistry. Main subject of interest: strongly correlated electron systems, theoretical simulation of electron structure and thermodynamics of nanomagnets.



**Matías G. Rinaudo\***, Ana M. Beltrán, María A. Fernández, Luis E. Cadús, María R. Morales

National University of San Luis (UNSL), Argentina

## On the importance of supports when designing supported catalysts. The case of TiO<sub>2</sub> polymorphic mixes

Recent studies have reported the importance of supports in heterogeneous catalysis, since their role is not limited to act as carriers for metal particles. There is evidence that support's nature, crystalline phase and physicochemical properties could enhance catalytic performance during reaction. In this line, TiO<sub>2</sub> is a well-known reducible oxide in catalysis since it can be used as promoter, carrier for metals and catalyst itself. Furthermore, titania is particularly used as support due to its low-cost, strong oxidizing power and great metal-support interaction. Hence, we propose a rational design of TiO<sub>2</sub> mixtures for catalyst support application. We also present the high-energy ball milling as an effective technique to prepare tailored mixtures of titania phases, including anatase, rutile and high-pressure TiO<sub>2</sub> (II), as confirmed by X-ray Diffraction (XRD), Raman Spectroscopy and Transmission Electron Microscopy (TEM). Starting material could double its specific surface area due to particle fragmentation, as confirmed by surface area of Brunauer-Emmet-Teller ( $S_{\text{BET}}$ ) and Scanning Electron Microscopy (SEM). Defects introduced during milling process generated oxygen vacancies in the surface and bulk of supports, as evidenced by X-ray Photoelectron Spectroscopy (XPS) and Electron Paramagnetic Resonance (EPR). Moreover, longer milling time increased reducibility and oxygen mobility of supports, as observed by H<sub>2</sub> Temperature Programmed Reduction (H<sub>2</sub>-TPR) and O<sub>2</sub> Temperature Programmed Desorption (O<sub>2</sub>-TPD). Phase composition remained unchanged even under severe conditions, highlighting the stability of unusual TiO<sub>2</sub> (II) phase. Solids with enhanced physicochemical properties reported in this work could be successfully used as catalyst supports for oxidation reactions. Pd/TiO<sub>2</sub> catalysts prepared with these supports are being tested in glycerol selective oxidation in liquid phase to study its effects in metal-support interaction and catalytic performance.

### Audience Take Away:

- We present high-energy ball milling as a simple and eco-friendly method of synthesis and/or modification of materials.
- We also highlight the need of considering support's design when it comes to supported catalysts, since it could enhance catalytic performance under specific reactions.
- Defective structures and polymorphic mixes of anatase, rutile and TiO<sub>2</sub> (II), induced by milling, could change physicochemical and catalytic properties of solids affecting future metal-support interactions.
- Obtained materials with distinctive features could be suitable as catalytic supports in oxidation reactions.

### Biography

Matías Gastón Rinaudo graduated as Chemical Engineer at National University of San Luis (UNSL), Argentina in 2016. He then joined the research group of Prof. Dr. Luis Cadús at the Institute of Research in Chemical Technology (INTEQUI), National Scientific and Technical Research Council (CONICET) to pursue his PhD in Chemistry, studying the rational design of catalysts for glycerol valorization. In 2020 he obtained a scholarship to work for 6 months as Visiting Research Student at Prof. Dr. Robert Scott's group, University of Saskatchewan, Canada. At present, he is working as Teaching Assistant and concluding his doctoral thesis in heterogeneous catalysis at UNSL.

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