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Group

3RD EDITION OF

CHEMISTRY WORLD CONFERENCE

VIRTUAL EVENT

14-15
JUNE 2023

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BOOK OF ABSTRACTS

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14-15 JUNE

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ABSTRACTS

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CHEMISTRY WORLD CONFERENCE

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Welcome Message

Prof Dr Thomas J Webster, Boston, USA

Dear congress visitors,

Chemistry is everywhere. From designing new nanoparticles that can treat COVID-19 to improved solar panels for alternative energy, chemistry has been solving old problems for centuries and is well positioned to conquer our latest problems from the environment to medicine. Chemistry has provided wonderful fascinating materials from bucky balls (C60) to drugs that kill cancer. I am pleased to welcome everyone to the 3rd Edition of the Chemistry World Conference in Rome. As a diverse conference focused in chemistry, it is destined to spark conversations, scientific debate, and new ideas for some of our most persistent problems in society. I am positive new chemistries and materials will be presented for the first time, and you don't want to miss it. As a multidisciplinary conference, all scientists will find a forum for their research and be able to generate new ideas and find new materials to solve your specific problems. At a time when we continue to emerge from COVID, I strongly encourage everyone to take advantage of this conference where we must make up for lost time.

I hope to see you all in Rome where we will discuss and develop solutions to our most pressing chemistry problems!

Thomas J Webster, Ph.D

Welcome Message

Dear Distinguished Scholars, Engineers and Colleagues!

It is my great honour and pleasure as a Committee Member to invite you to join with a contribution to the 3rd Edition of Chemistry World Congress (**CHEMISTRY 2023**), which is all set to take place in Hybrid Format the magnificent city of Rome, Italy, during June 14-15, 2023. The Conference will include Plenary and Keynote Speeches and Invited Talks which will be given by Distinguished Scholars and Experts from academic institutions and industry, and oral presentation by delegates and poster presentations by young junior participants. Devoted to the rapid development of Chemistry and Chemical Engineering, this conference will provide excellent opportunity to meet distinguished scholars and experts and to exchange new ideas and application experiences, to establish research relations and collaborations for future research and projects. The conference has a wide variety of Chemistry and Chemical Engineering from Nano science and Materials Chemistry, Environmental and Green Chemistry to Physical Chemistry and Theoretical Chemistry and Nuclear and Radio Chemistry. International scientific activities are big scientific platforms for the scientists, colleagues, young academicians, and participants from all over the world, to interact and communicate with each other. I believe that 3rd Edition of Chemistry World Congress (CHEMISTRY 2023) will provide this opportunity for delegates from different cultures and countries. Also, this conference will be performed successfully, in favour of the qualified scholars, colleagues and experts and with their valuable and informative presentations. Also, the conference will be very beneficial for young delegates by encouraging them and improving their confidence of presenting research in an international platform. I am pleased to invite prospective scholars, academicians, engineers and other scientists to submit their original contributions to this important conference, where you are sure to have a meaningful experience with scholars and experts from different cultures and different countries from all around the World.

Yours truly,
Dr. Osman Adiguzel,
Firat University, Elazig, Turkey

Welcome Message

Prof Dr Kaushala P Mishra, Mumbai, India

Dear congress participants,

I am immensely happy to write a welcome note for the Chemistry 2023. Deeper chemical research holds a promise to unravel some unknown secrets of tumor cells/tissue aimed to achieve effective treatment of cancer patients. For example, level of reactive oxygen species (ROS) inside cells drives them from normal to transformed state and eventually the induction of cancer. In physiological conditions, living cells maintain a tight redox homeostasis necessary for the normal function of cells. In the situations of cell losing the redox balance, they experience oxidative stress, but adapt to survive by recruiting a variety of prooxidant molecules including upregulation of intracellular antioxidant enzymes such as SOD, GSH and other chemical species. In response to externally applied anticancer therapies such as chemo- and radiotherapy, the cytoplasmic level of ROS increases and after crossing the threshold barrier, they begin to eat tumor cells and result in tumor mass shrinkage. It is intriguing how ROS switch from life supporting to toxic threat to tumor cells. Evidently, the understanding of chemical switch would go a long way in designing effective cancer treatment strategies.

Keynote Speakers

Thomas J. Webster
Interstellar Therapeutics,
Boston, MA, USA

Osman Adiguzel
Department of Physics, Firat
University, Elazig, Turkey

Kaushala P. Mishra
Bhabha Atomic Research
Center, Mumbai, India

Thank You
All...

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 conferences 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 2023

Building on the success of previous editions, Magnus Group is delighted to announce the upcoming 3rd Edition of Chemistry World Conference (Chemistry 2023), a highly successful event that brings together chemistry professionals, researchers, scientists, and pharma industries. This year, the conference will be held virtually from June 14-15, 2023. The central theme of the summit is " Modifying Chemistry with the Novelties that Accomplish Future Goals."

Chemistry 2023 aims to provide a unique platform for academia, clinicians, and industry representatives to explore disruptive technologies, novel platforms, and discuss strategies to enhance productivity and reduce costs. The meticulously curated agenda features an array of stimulating activities, including Chemistry poster presentations, interactive panel discussions, and visionary keynote sessions.

By fostering collaboration and innovation, the two-day colloquium seeks to enable attendees to broaden their horizons in the field of chemistry. Magnus Group is confident that Chemistry 2023 will offer an incredible opportunity to discover new avenues of research and development. Join us in this global summit and be a part of shaping the future of chemistry. We look forward to welcoming you to Chemistry 2023.

Journal Collaboration

Open Chemistry is a peer-reviewed, open access journal that publishes original research, reviews, and communications in the fields of chemistry in an on-going way. Our central goal is to provide a hub for researchers working across all subjects to present their discoveries, and to be a forum for the discussion of the important issues in the field. There are no submission charges. In order to sustain the production of our fully-refereed open access journal, each article accepted for publication in Open Chemistry is subject to Article Processing Charges (APC).

Note: We offer 30% discount on APC for the CHEMISTRY 2023 conference participants.

For more details about the journal,
please visit: https://www.degruyter.com/journal/key/chem/html

BOOK OF ABSTRACTS

14-15 JUNE

DAY 01

KEYNOTE FORUM

3RD EDITION OF

CHEMISTRY WORLD CONFERENCE

Reactive oxygen species (ROS) act as chemical switch from supporting survival to death of cancer cells

Reactive oxygen species (ROS) are a group of highly reactive oxygen centred free radical chemical species in normal and cancer cells. In normal cells, ROS are maintained in tight control of level of the antioxidants. On the other hand, the level of ROS is generally elevated in cancer cells, due partly to metabolic activities and cell divisions, which are believed to play a critical role in the process of tumorigenesis and cancer progression. It is further known that ROS can act as cancer suppressors depending on the varying antioxidant capacities of different types of cancers. These results suggest existence of a complex redox state in cancer cells, and they are regarded as intracellularly stressed. In this talk, I will discuss the mechanisms of involvement of ROS and their functions in the initiation, signaling and proliferation of cancer cells. It is pointed out that the delicate balance of ROS and antioxidants levels determine their role in survival and death processes of cancer cells. This redox situation offers novel anticancer therapy strategies to achieve the goal of greater cancer cell killing by increasing the ROS level in response to anticancer therapies such as chemotherapy and radiotherapy. It is concluded that ROS acts as a chemical switch from favouring survival to destruction of cancer cells improving radiotherapy in clinic.

Kaushala P. Mishra

Bhabha Atomic Research Center,
Mumbai, India

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).

Are you harming the environment with your research ? Introducing novel environmentally friendly chemistries

Many scientists blame large industries for harming the environment, such as the oil and petroleum, automobile, airline, construction, etc. industries. This presentation will highlight how through our own research in our own laboratories we too are harming the environment. Whether we are conducting in vitro tests for new biomaterials, making novel nanoparticles, or simply conducting chemical research, the materials we use are not environmentally friendly and harm the environment. Furthermore, this presentation will give solutions to this problem where one can use environmentally friendly plastics, petri dishes, pipettes, etc. Moreover, it will introduce several environmentally friendly ways to make nanoparticles that do not rely on toxic catalysts or other chemicals that can harm our environment. Furthermore, this invited talk will highlight the improved properties of materials, such as nanoparticles, when synthesizing them in environmentally friendly ways. In summary, this talk will highlight that we all can play a role in using new chemistries that are environmentally friendly in our research and stop harming the environment ourselves.

Audience Take Away Notes

- How everyday scientists are harming the environment
- How new chemistries can be used by researchers to reduce our impact on the environment
- How new environmentally friendly nanoparticle synthesis methods can be used
- How materials with improved properties can be made while reducing an impact on the environment

Thomas J. Webster

Interstellar Therapeutics, Boston, MA, USA

Biography

Thomas J. Webster's (H index: 111; 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.

14-15 JUNE

DAY 01

SPEAKERS

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Wen-Yong Han
Key Laboratory of Biocatalysis & Chiral Drug Synthesis of Guizhou Province, School of Pharmacy, Zunyi, China

Domino annulations based on chromonyl -norbornyl-palladacycle intermediate

The close relationships between biological activity, molecular complexity, and structural diversity stimulate synthetic chemists and pharmaceutical chemists to develop novel strategies to access significant structures inspired from natural products or bioactive molecules. Chromone has particularly emerged as a privileged unit owning to its wide distribution in drugs and natural products. Therefore, exploring novel approaches for the construction of diverse chromone derivatives has been the focus of intensive efforts, and numerous significant advances have been made in the field of catalysis. Transition metal-catalyzed domino reaction has been proven as an effective approach to assemble complex molecules by forging two or more new chemical bonds from readily available substrates in one single operation. In this context, the Catellani-type annulation cooperatively catalyzed by palladium and norbornene (NBE), which was originally discovered by Lautens in 2000 and further developed by the groups of Catellani, Malacria, Liang, Luan, Zhou, et al., represents a powerful tool for the construction of complex arenes. It is notable that an aryl-NBE-palladacycle (ANP) generated via successive oxidative addition of palladium(0) into the aryl-iodide, *syn*-migratory insertion into NBE and C(sp^2)–H activation was a key intermediate for these transformations. Given that the importance of chromone scaffold in medicinal chemistry, we recently found that the chromonyl-norbornyl-palladacycle (CNP) intermediate derived from 3-iodochromone, norbornene, and Pd(0) catalyst was an active Pd(II) species, which could further react with different kinds of electrophilic reagent, such as α-bromoacetophenones, benzyl bromides, cyclopropenones, aziridines, dimethyl squarate and o-bromobenzoic acid, to construct various chromone-containing polycyclic compounds, wherein the corresponding [2+3+1], [2+2+1] and [2+2+2] domino annulations were involved

(Figure 1).

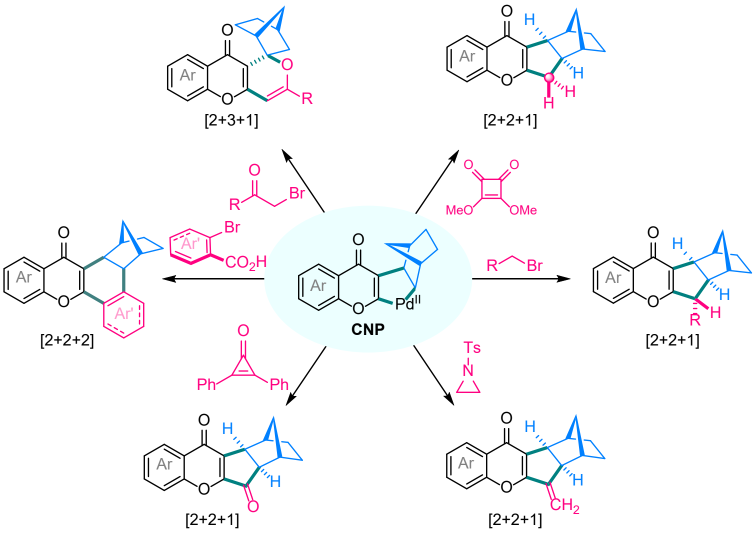


Figure 1. Domino annulations based on CNP intermediate.

Audience Take Away Notes

We revealed some highlights, including:

1. The 2, 2-bifunctionalization of NBE was firstly realized in palladium catalyzed [2+3+1] annulation;
2. The carbonylation with cyclopropenones as the sole CO surrogate can be firstly realized through a palladium-catalyzed [2+2+1] annulation;
3. The aziridine was firstly employed as a vinylidene unit in a unique manner by cleavage of two C−N bonds via palladium-catalyzed [2+2+1] annulation;
4. Dimethyl squarate was firstly utilized as solid C1 source in the [2+2+1] annulation. The novel characteristics of substrates will provide inspirations for organic chemists to design other reactions.
    - We developed the novel [2+m+n] domino annulations based on the CNP intermediate to synthesis of various chromone-containing polycyclic compounds, which will be interested from pharmaceutical chemists
    - These findings open a new venue for the properties of NBE, the synthesis of polycyclics as well as will be of interest to a broad audience — in addition to organic/organometallic chemists who can appreciate the conceptually novel nature of these reports, we anticipate that the chemical transformation based on chromone will be of use to researchers working on drug discovery and chemical biology

Biography

Wen-Yong Han received his B.Sc. degree from Xi'an Polytechnic University in 2007, an M.Sc. degree from Shaanxi Normal University with Prof. Dong Xue and Zun-Ting Zhang in 2010, and his Ph.D. degree from Chengdu Institute of Organic Chemistry, Chinese Academy of Sciences with Prof. Wei-Cheng Yuan and Xiao-Mei Zhang in 2013. Then he performed postdoctoral research at Colorado State University with Prof. Yian Shi. In 2014, he began his independent academic career at Zunyi Medical University, where he was promoted to a full professor in 2019. He has published more than 30 research articles in SCI(E) journals.

Stefan Nettesheim
Relyon plasma GmbH a TDK group company, Osterhofener Regensburg, Germany

Mediplas: More than a simple ozone generator

Dielectric barrier discharge flow reactors are among the most efficient technologies to produce ozone based on oxygen. If ambient air is used the chemistry gets much more complex and involves many competing reaction pathways and yields a mixture of ozone with nitric oxide components, nitric acids, and peroxides. The process parameters that determine to a certain degree the composition of the output are: Inlet gas composition and humidity, power density of the dielectric barrier discharge, amplitude of the electric excitation, and process temperature. We have designed a reactor for typical flow rates of 0-10 slm with integrated active Peltier cooling that offers a high control over process temperature. The specially adapted driving circuit can adjust power density (via PWM) and amplitude of the excitation voltage. The driver also includes a feedback signal that is proportional to the discharge intensity. A well-defined output including very high ozone concentrations of more than 30.000 ppm can be achieved with very high stability. However, for some sterilization and medical applications we were able to show that the sweet spot for killing germs is not necessarily the operating point of highest ozone concentration, but that the nitrogen oxide species in combination with humidity and peroxides play a decisive role. The components described in this contribution are easy to integrate into a wide range of systems and can be specifically controlled to optimize the desired effects.

Audience Take Away Notes

- Basic and practical properties of an ozone generator using a dielectric barrier discharge will be discussed
- The design of a specific small-scale high-performance ozone generator will be described
- Practical application examples including microbiological efficiency will be highlighted
- The research includes interdisciplinary topics of electronics, physics, chemistry, and microbiology
- The presented system can tune the output chemical composition using a given input gas composition e.g., humid air
- The described components are easy to integrate into different applications such as disinfection processes

Biography

Stefan Nettesheim studied physics at the TU Berlin and the University of Konstanz. He received his PhD in 1993 from the Fritz Haber Institute of the Max Planck Society in Berlin. Until 1998, he worked as a postdoc at the Universidad del Pais Vasco in San Sebastian and at the Swiss Federal Institute of Technology Zurich (ETHZ). He then worked as a development engineer at SIG Pack Systems in Beringen, Switzerland and as division manager at Sachsenring AG in Zwickau, Germany. From 2002, he was founder and general manager of Ekpro GmbH for fuel cells in Berlin. Currently, Dr. Nettesheim is managing director of relyon plasma GmbH, a TDK Group company.

Ruaraidh Wells[1]*, Dr William Davies[1] and Prof Xiong-Wei Ni[2]
[1]NiTech Solutions Ltd, Unit 39, 4-5 Lochside Way, Edinburgh Park, Edinburgh, EH12 9DT, UK
[2]Centre for Oscillatory Baffled Reactor Advancement (COBRA), School of Engineering and Physical Sciences, Heriot-Watt University, Edinburgh EH14 4AS, UK

Continuous crystallization of energetic materials using continuous oscillatory baffled crystalliser

Energetic materials such as explosives and solid propellants are typically manufactured in batch processes. Poor heat and mass transfers in batch vessels can lead to products produced with significant batch-to-batch variations, including inconsistent purity and wide particle size distributions, limiting final product performance. Reshoring or upgrading production capability presents unique opportunities to adopt continuous flow manufacturing methods which are safer, greener, more efficient, use less energy, and have lower cost. Crystallisation is a critical purification and isolation step in energetics manufacture as it influences solid purity, morphology, particle shape and crystal size, all of which have a direct impact on the performance and functionality of the explosive or propellant. In this presentation, we report the first successful demonstrations of continuous crystallisation of two energetic materials, ammonium perchlorate (AP) and nitrotriazolone (NTO), using NiTech's continuous oscillatory baffled crystalliser (COBC) technology. It has been demonstrated that AP and NTO can be continuously crystallised and product properties can be manipulated through varying processing conditions, giving consistent and tuneable particle size. High throughput has also been demonstrated with multiple kilograms of dry material produced per hour in a small footprint system. The feasibility, capability and benefits of continuous crystallisation in energetic materials manufacturing have been demonstrated and are ready to be scaled up to production operations, as well as to incorporate continuous synthesis prior to crystallisation using one continuous system.

Audience Take Away Notes:

- Crystallisation is a critical step in the manufacturing of energetic materials, controls crystal purity, morphology, shape, size and its functionality. Traditional batch systems suffer batch to batch variations, with significant challenges in scaling up, safety and waste generation. Continuous crystallisation of energetics is an elegant solution in comparison to traditional operations, delivering consistent crystal properties, reducing factory space, energy/solvent utilizations, waste generation and making the process much safer and greener. The audience would be able to learn from our work and apply continuous crystallisation in energetics.
- This research also offers a new tool for expanding audience's research, manufacturing as well as teaching. This work provides a practical solution to a problem in chemical, pharmaceutical and food industries, making crystallisation processes more efficient, safer, greener and cheaper.
- The continuous crystallizer is a new device, helps the design, operation and maintenance of traditional crystallisers.

Biography

Ruaraidh completed his master's degree in chemistry at the University of Glasgow. Since graduating he has gained 5 years' experience in product and process development roles in industrial chemistry. As a Process Development Chemist at NiTech Solutions, Ruaraidh has been involved in R&D project management and execution, as well as client technology transfer projects. Through this experience he has in-depth knowledge in the application of NiTech reactors and crystallizers specifically for energetic materials manufacturing, as well as within the fine chemical and pharmaceutical sectors.

Eva Falomir* and Raquel Gil-Edo

Inorganic and Organic Chemistry Department, ESTCE/ Jaume I University, Castellón, Spain

Aryl triazole-scaffold for multitarget anticancer immunomodulating drug discovery

A small library of aryl triazole-scaffold derivatives have been developed using click chemistry synthetic strategies. Docking studies using PD-L1 and VEGFR-2 crystallographic data confirmed their potential targeted action. The antiproliferative activity on monocultures of several tumour cell lines (HT-29, A-549 and MCF-7), and on the non-tumour cell line HEK-293 has been studied. Also, the effect on anticancer targets (PD-L1, VEGFR-2 and c-Myc) has been evaluated. Finally, the effect on cancer cell viability when co-cultured with immune cells (Jurkat T cells or THP-1) has been also studied together with their effect on IL-6 secretion to cell media.

Audience Take Away Notes:

- The audience will learn more about multitarget anticancer drug discovery for oncoimmunomodulating therapies.
- Those people in the audience involved in Drug Discovery research could use most of the information we are going to provide.
- This is a multidisciplinary and interdisciplinary work so people from research fields involved in Medicinal Chemistry, Biochemistry, Organic Chemistry, Cell biology, Immunology could be interested.

Biography

Dr. Eva Falomir studied Chemistry at the Valencia University, Spain and graduated as MS in 1994. She then joined the research group of Prof. Carda at Jaume I University (UJI). She received her PhD degree in 1998 at the same institution. After two years postdoctoral fellowship supervised by Dr A. Fürstner at Max-Planck Institute, Germany she obtained the position of an Associate Professor at UJI. In 2022, se got a Full Professor position in the same university. She has published more than 100 research articles in SCI(E) journals.

Rosangela Elliani, Antonio Tagarelli, Attilio Naccarato*

Dipartimento di Chimica e Tecnologie Chimiche, Università della Calabria, Via P. Bucci Cubo Arcavacata di Rende (CS), Italy

Quantification of target compounds in environmental waters by the combination of MEPS and PTV-GC-MS/MS, optimized through experimental design- PCA approaches: A case study with benzothiazoles, benzotriazoles and benzenesulfonamides

This study proposes a new method for the fast quantification of benzothiazoles (BTs), benzotriazoles (BTRs), and benzenesul fonamides (BSAs) in tap water, river water, and wastewater. The presented approach is based on the use of microextraction by packed sorbent (MEPS) combined with programmed temperature vaporization-gas chromatography-triple quadrupole mass spectrometry (PTV-GC-QqQ-MS) operating in tandem mass spectrometry. After the evaluation of different sorbent/solvent pairs, the variables influencing both PTV technique and MEPS procedure were simultaneously optimized by "Experimental design". Indeed, since some of the variables affecting PTV can be related to factors influencing MEPS extraction, comprehensive designs were used for evaluating at the same time all factors involved pointing out any synergistic effects between variables. Instead of the traditionally used Derringer's desirability function to convert a multi-response problem into a single-response one, we choose to apply the principal component analysis (PCA) to use the score on the first PC as a "comprehensive" response of the results of the experimental designs. Furthermore, this optimization strategy offered to the analyst response surfaces which, in compliance with the principles of Green Sample Preparation (GSP) [3] allow an informed choice of experimental conditions according to the required analytical performance.

Very good linearities were achieved in the tested calibration ranges for all analytes achieving determination coefficient values >0.99. Intra-day and inter-day accuracies and RSD values tested at three concentrations were in the range of 79% to 132%, and from 1 to 18%, respectively. The LODs obtained can be considered good, ranging between 0.005 to 0.85 μg/L. The Analytical Eco-Scale, Green Analytical Procedure Index (GAPI), and Analytical Greenness metric for sample Preparation (AGREEprep) approaches were applied to evaluate the "green" character of the procedure. The satisfactory results achieved from the testing with real water samples demonstrate its applicability for monitoring campaigns and exposome studies.

Audience Take Away Notes

- A new method for benzothiazoles, benzotriazoles, and benzenesulfonamides quantitation in waters is presented, using commercially available equipment
- The "Experimental design" was used to achieve the simultaneous optimization of MEPS extraction and PTV technique and to provide an in-depth understanding of the whole analytical system
- The "green" character of the procedure described in this study was evaluated by the use of greenness metrics
- The new high throughput protocol is reliable, fast, and automatable. It can potentially be used for monitoring purposes of the target compounds in environmental waters

Biography

Dr. Attilio Naccarato is an Assistant Professor at the University of Calabria. He is involved in National and European projects aimed at the monitoring of persistent and emerging pollutants in the environmental compartments. Besides, his research activity focuses on method development for the analysis of pollutants in environmental, food, and clinical matrices using different analytical strategies such as microextraction approaches, mass spectrometry-based techniques, and multivariate optimization. He also serves as an Associate Editor on the editorial board of Chemical Papers (Springer), Frontiers in Analytical Science, and Separations (MDPI).

Theodosios Geo Douvropoulos

Hellenic Naval Academy/Physical Sciences Sector, Piraeus Greece

Electrostatic control of inversion frequency for a model potential of the ammonia molecule

In the current work, we analytically study the possibility of electrostatic control of a model potential corresponding to the ammonia molecule. The model is described by a one-dimensional double-well potential as far as the relative position of the nitrogen atom to the hydrogen level is concerned. In particular, we study how the presence of electric fields affects the inversion frequency of the model potential. We use the semi-classical path-integral technique to construct the system's Green function. The latter receives a fractional form corresponding to the perturbed energy poles of the system. Thus we reveal the complex energy spectrum of the system. The evolution of the molecule is then described in detail. The frequency of oscillation between the potential wells, known as the inversion frequency, is of particular interest to us. We specifically link the oscillation rate to the decoherence time. The latter corresponds to the gradual dissociation of the molecule into the continuum set of states through the applied field barriers. Since our findings are analytic, they can be established experimentally with the help of appropriate parameter fitting. In addition, we can equally well apply our results in a variety of systems that the same model, such as coupled quantum dots in quantum computing or charge transport in nanostructures can describe.

Audience Take Away Notes

- Someone can actually apply the method described here, to realistic physical systems and calculate various time scales concerning the system's dynamics
- As mentioned in the abstract, the model concerned, can equally well describe systems serving Quantum Computation or charge transport in Nanostructures. In addition someone can learn about path integrals and think about expanding his teaching in Chemistry by incorporating the method
- Since the findings of the current work come in analytic form, a designer may vary the parameters included, (such as the barrier height or the well depth), to succeed the desirable time-control of the system
- In this work, we introduce and define quantities, such as the similarity factor between the potential well and the potential barrier, that play a crucial role in the system's evolution. These quantities provide new information to assist in the model's design, to improve control

Biography

Theodosios Geo Douvropoulos studied Physics at Patra University, Greece (1996). He then joined the research group of Prof. C.A. Nicolaides at the National Hellenic Research Foundation (Theoretical Physics and Chemistry Institute), where he received a Master's degree in Physics (2001) and his Ph.D. degree (2005) in Quantum Dynamics. His main research activity is about the quantum evolution of low-dimensional physical and chemical systems. He has published 13 research articles and has obtained the position of Lecturer at the Hellenic Naval Academy of Greece since November 2022.

Donghee Lee
Saint Petersburg Mining University, Dept of Transport and storage of oil and gas, Saint Petersburg, Russia

A study on the possibility and optimization of SMR cycle natural gas liquefaction process for LNG -FPSO using polar seawater temperature

Recently, as the demand for natural gas has increased, the global liquefied natural gas (LNG) market has also expanded significantly. Consequently, several new LNG production projects are currently under development worldwide. The Arctic region is believed to contain significant deposits of natural gas. According to estimates from the US Geological Survey, the Arctic region may hold up to 1,669 trillion cubic feet of technically recoverable natural gas resources, accounting for approximately 25% of the world's total. Nowadays, several LNG projects are being planned or developed in the Arctic region.

However, accessing and developing most other potential natural gas deposits in the Arctic region is challenging due to the region's specific characteristics. Mining natural gas and employing LNG production methods using LNG-FPSO are expected to offer significant advantages in developing various small and medium-sized gas fields located in the sea and along the coast of the Arctic region.

The LNG-FPSO is an innovative solution for offshore natural gas liquefaction, providing flexibility and cost-effectiveness in remote locations. However, compared to the existing Cascade method, the liquefaction of natural gas in LNG-FPSO requires a significant amount of power and refrigerant consumption. This is because LNG-FPSO aims to minimize the need for liquefaction facilities, and SMR (Single Mixed Refrigerant) refrigeration cycles with simple structures are generally utilized for natural gas liquefaction.

Therefore, this study focuses on the following objectives to enhance the overall efficiency and sustainability of LNG-FPSO operations while reducing harmful emissions:

1. Reducing the total refrigerant usage required for the SMR refrigeration cycle
2. Decreasing compressor power consumption, which is the primary contributor to power consumption in SMR refrigeration cycles
3. Substituting environmentally harmful or expensive refrigerants with environmentally friendly and cost-effective alternatives

To achieve these goals, this study presents the concept and feasibility of the SMR liquefaction process using polar seawater temperature and optimizes it using HYSYS, a process simulation program

In this study, natural gas liquefaction was conducted by mixing propane, ethylene-based (R-1150), methane, and nitrogen refrigerants. Taking Sakhalin-3, a representative medium-scale natural gas production project, as a reference, LNG production was assumed to be 6,741 kg/hour. Additionally, the average seawater temperature in the Arctic region, -2℃, was utilized as the temperature of the polar seawater used for cooling. As a result, the total refrigerant flow rate used in the entire SMR refrigeration cycle was reduced by approximately 8.66%, from 37,114 kg/hour to 33,900 kg/hour. Among them, the flow rate of the hydrocarbon refrigerant, which was 12,434 kg/hour, was replaced by a more environmentally friendly and cost-effective nitrogen refrigerant with a flow rate of 7,038 kg/hour. Furthermore, the compressor power consumption of the SMR liquefaction process could be reduced from 4,335 kW to 2,182 kW, representing a decrease of about 49.67%. This study demonstrates the potential of utilizing polar seawater temperature in the SMR cycle of the natural gas liquefaction process for LNG-FPSO. Further research and development are needed to refine the optimization strategies and validate the feasibility on a larger scale.

Audience Take Away Notes

- The audience can gain knowledge about the design of the SMR cycle LNG liquefaction process and the natural gas cooling system that utilizes the ocean temperature difference. This information can be used to conduct in-depth research on the LNG industry in the polar region
- The utilization of a natural gas cooling system that employs cold seawater in the polar region is expected to assist the audience in determining the power consumption and flow rate of propane, ethylene, and methane refrigerants required for the SMR natural gas liquefaction process facility in the polar region The design of the SMR LNG liquefaction process can serve as a basis for lectures on its fundamental concepts
- The process itself utilizes a cooling system that takes advantage of the temperature difference in the polar region, resulting in high efficiency through a design method that employs simple ideas and variables. This applied concept is beneficial for both lectures and research
- The natural characteristics of the polar region can be utilized to increase the efficiency of natural gas liquefaction, as opposed to using power, without requiring complicated additional processes
- This solution may simplify the designer's job, making the process more efficient

Biography

Mr. Donghee Lee studied Oil and Gas Engineering at St. Petersburg Mining University, Russia graduated as MS in 2018. In 2021, he completed the LNG design expert training course supervised by Gyeongnam Techno Park in Republic of Korea, and in 2022, he completed the chemical engineering course for plant experts supervised by the Education Institute Construction in Republic of Korea. He is currently pursuing his doctorate at St. Petersburg Mining University in Russia, and at the same time, he is conducting research on non-destructive testing of lubricating oil and pipes in a research team at HAEJIN LS, an official partner of Shell Korea.

Vladimir Voronov
Irkutsk National Research Technical University, Irkutsk, Russia

Structural features of substituted azoles bearing a biologically active heterocycle and their complexes: NMR study

The research work, carried out with the participation of this competition applicant, was devoted to, first of all, the structural analysis of molecular (multi-electron) systems using ^{1}H and ^{13}C nuclear magnetic resonance (NMR) spectra. In a number of cases, other NMR spectra (apart from ^{1}H and ^{13}C) were also employed in the studies. In some works, quantum-chemical calculations were performed. The spatial and electronic structure of various molecules bearing heteroatoms (such as nitrogen, oxygen, sulfur, silicon, and phosphorus) as well as diverse functional groups was investigated. The special research was devoted to the coordination (diamagnetic and paramagnetic) and complex compounds of the donor-acceptor type. Conformational transitions and tautomerism of molecular systems, intramolecular hydrogen bonds, rotational isomerism, competitive coordination, nature of metal–ligand bonds, and mechanisms of chemical transformations were discussed. Almost all studied compounds and their complexes are new (synthesized or isolated from natural feedstock for the first time). Among the investigated compounds there are more than fifty derivatives of the azole series.

1. High-resolution NMR spectra of several dozens of 1-substituted azole derivatives were recorded and analyzed. The values of chemical shifts and spin-spin coupling constants (including those of long-range spin-spin coupling), characteristic of the azole ring and the most well-known functional groups contained in substituted imidazoles and pyrazoles, were determined. It is shown that these parameters can be used to establish the spatial and electronic structure of novel compounds bearing an azole heterocycle.

2. The ^{1}H and ^{13}C NMR spectra of the solutions of 1-vinylimidazole complexes with manganese, cobalt, nickel, and copper chlorides as well as with organylhalostannanes $(C_2H_5)SnX$ were analyzed. It is found that in a solution of paramagnetic complexes of 1-vinylimidazole with chlorides of the first transition group elements, the coordinating atom has an octahedral environment, and four ligand molecules occupy the equatorial position. It is established that in the complexes of cobalt, nickel, and copper, 1-vinylimidazole molecules are coordinated to the central ion by the pyridine nitrogen atom N-3. In the paramagnetic complex of manganese, the molecules of this azole can also be coordinated by the pyrrole nitrogen atom N-1 in a certain temperature range. Structurally, the diamagnetic complexes of this azole with organylhalostannanes represent a trigonal bipyramid.

3. A method for the study of molecular structure using the NMR phenomenon in paramagnetic systems has been developed. On the example of 1-substituted azoles, it is shown that this method can be successfully employed to address some issues related to the structure and intramolecular dynamics of multi-electron systems.

Some publications on the topic of the report

Voronov V.K., Podoplelov A.V. Paramagnetic complexes in high resolution NMR spectroscopy. NOVA publishers: New York, 2015, 181 p.

Voronov V. K., Ushakov I.A., Funtikova E.A. NMR spectra of 1-vinylimidazole, transformed by paramagnetic complexes. Applied Magnetic Resonance, 2019, v. 50, № 4, p. 569 – 577.

Biography

Professor Vladimir Voronov's research interests are related to solving problems of molecular spectroscopy and physico-organic chemistry by methods of nuclear magnetic resonance and quantum chemistry. In addition, for the last twenty years or so, his research interests have included scientific and methodological issues related to cognitive barriers of university students. He is the author of more than three hundred publications in periodicals, including more than thirty books. He received a number of awards established by the Russian Academy of Natural Sciences, including the Gold Medal "For innovative work in the field of higher education". Member of the American Chemical Society.

Iliana Ivanova*, Yulia Kutzova, Lilia Petrova
Sofia University Saint Kliment Ohridsk, Bulgaria

Thin nanostructured films as food packaging

Nanoparticles included in food packaging could adsorb oxygen, produce reactive oxygen species and destroy microorganisms in food to prolong the food storage. Antimicrobial packaging is not still in the market, but copper, Zink and TiO^2 are reported as promising antimicrobial materials.Thin films obtained by magnetron sputtering of TiO^2: Cu:Ag as packaging of Yellow cheese and formed ham were investigated. Microbial quantity was determined during 3 months after the start of experiment. The metals in the thin slice of the food mass were determined using ICP AES. In both product the metal concentration raised from the first till the end of experiment. The results have shown that thin films obtained by magnetron sputtering are not stable on glass surface and cannot be used as food packaging that way.

Biography

Dr. Iliana Ivanova finished Medical college in Plovdiv in 1979. She finished her Biochemistry and Microbiology Master's degree at Sofia University " Saint Kliment Ohridski" in 1986 (diploma thesis on Aspergillus niger acid production) and her Ph.D. degree in Microbiology "Microflora of oil-field Tyulenovo and its application" in 1994. In 2009 Dr. Ivanova started to test the antimicrobial activity of ZnO thin films and now has more than 50 articles published in international journals and books. Her interests are in the antimicrobial activity of nanoparticles and nanocomposites and their medical application.

Brij Bhushan Tewari
Department of Chemistry, University of Guyana, Guyana

Implications of metal complexes in biology and medicine (The system cadmium (II) / iron (II) / zinc (II) – hydroxyproline)

The importance of metal ions to essential functions of living systems and for the wellbeing of living organisms is well known. Metal ions are fundamental elements for the maintenance of the life spans of the human, animals and plants. The stability constants of Cd^{2+}, Fe^{2+} and Zn^{2+} complexes with hydroxyproline were determined by Paper Electrophoretic Technique (PET). This method is based on the movement of a spot of metal ion in an electric field at various pH of background electrolyte. A graph of pH against mobility gives information about the formation of binary complexes and permit to calculate their stability constants. The stability constant of the ML (first) and ML2 (second) complexes of Cadmium (II) – hydroxyproline, iron (II) – hydroxyproline and zinc (II) – hydroxyproline, have been found to be (4.41 ± 0.01; 2.95 ± 0.06), (4.41 ± 0.01; 281 ± 0.11) and (4.83 ± 0.02; 3.28 ± 0.07) (logarithm stability constant values), respectively at ionic strength 0.1 mole L^{-1} (per chloric acid as background electrolyte) and a temperature of 35^{o} C. the first and second stability constants of metal complexes follow the order Zn (II) > Cd (II) > Fe (II). Metal complexes can offer their action such as anti-inflammatory, antimicrobial, antibiotic, anti-thyroid and anticancer compounds. Metal based drugs bioactivity can be increased by metal chelation, which in turn increase their absorbance and stability. Recent advances in inorganic chemistry have made possible formation of number of transition metal complexes with organic ligands of interest which can be use as therapeutic agents

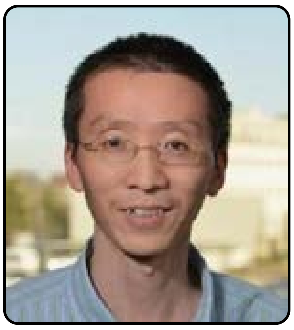
Audience Take Away Notes

- Audience can initiate to study in the same research area
- Audience can expand their research work of similar interest
- Audience can also prepare metal complexes of their interest and study their therapeutic applications
- Audience can teach their students the applications of simple paper electrophoretic technique in the determination of stability constants of complexes
- Audience also teach applications of stability constants in biological systems and medicine. The knowledge gained can be used to enhance their teaching and research
- Yes, any Faculty member can use this technique in their teaching and research
- Stability constants of metal complexes of interest can be determined
- Therapeutic applications of synthesized metal complexes can be attempt
- Yes. Present technique can be modified in following ways to make it more efficient
- By maintaining moisture of electrophoretic chamber constant
- By using glass plate below the paper strips
- Leaving the moisture paper strips by back ground electrolyte for long time (over 30 minutes) before running current for one hour
- Yes, Accuracy of results can be improved. In term of uncertainty in the results ± 5 % results are reliable

- Accuracy of results can be increase by improving the technique as mentioned in above item
- Simple Paper Electrophoretic Technique is useful in determining that metal complexes are formed or not if formed its stability constants can also be determined
- Technique is useful in chelation therapy
- Metal complexes can be prepared on a long scale and at a particular condition and study for their therapeutic applications

Biography

Dr. Brij Bhushan Tewari is a Professor of Chemistry in the Department of Chemistry at University of Guyana. Prof. Tewari obtained the Doctor of Philosophy degree in Science (Chemistry) 1985 from Allahabad University, India. He has taken teaching/research appointments at several universities in Asia, Europe, USA, Canada and Guyana. His major research interests are in the area of (i) Metal complexes in biology and medicine (ii) Astrobiology & chemical evolution and origins of life (iii) Environment, Microbiology and Agriculture. He has published 133 research papers in international journal, one book and seven book chapters.



Haibo Ge

Department of Chemistry & Biochemistry, Texas Tech University, Lubbock, TX, USA

Distal functionalization via transition metal catalysis

The ubiquitous presence of sp^3 C–H bonds in natural feedstock makes them inexpensive, easily accessible, and attractive synthons for the preparation of common and/or complex molecular frameworks in biologically active natural products, pharmaceutics, agrochemicals, and materials. However, the inertness of these bonds due to the high bond dissociation energies and low polarity difference between the carbon and hydrogen atoms makes them challenging reaction partners. Moreover, the desired site-selectivity is often an issue in reactions with multiple analogous sp^3 C–H bonds. To overcome these problems, transition metal-catalyzed C–H functionalization has been developed with the assistance of various well-designed directing groups which can coordinate to a metal center to deliver it on a targeted C–H bond through an appropriate spatial arrangement, enabling C–H activation via the formation of a cyclometalated species. However, the requirement of often additional steps for the construction of the directing groups and their subsequent removal after the desired operation severely hampers the efficacy and compatibility of the reactions. A promising solution would be the utilization of a transient ligand which can bind to the substrate and coordinate to the metal center in a reversible fashion. In this way, the directing group is installed, sp^3 C–H functionalization occurs, and the directing group is then removed in situ without affecting the substrate function after the catalysis is finished. Overall, the whole process occurs in a single reaction pot. Herein, we are presenting our studies on transition metal-catalyzed transient directing group-enabled C–H functionalization reaction.

Audience Take Away Notes

- This study could potentially be used for others to build small molecules in an efficient way
- This study could potentially be used for others to carry out late-stage functionalization of natural products or drug molecules
- This research could also be used by others to expand their research

Biography

Haibo Ge received his PhD degree in Medicinal Chemistry from The University of Kansas in 2006, and then moved to The Scripps Research Institute for postdoctoral study. In 2009, he began his independent academic career at the Indiana University – Purdue University Indianapolis and relocated to Texas Tech University in 2020. Research by his group is mainly focused on the development of novel methods for carbon–carbon and carbon–heteroatom bond formation through transition metal catalyzed C–H functionalization.

14-15 JUNE

DAY 01

POSTERS

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Dmitrijs Lubriks
OSPT laboratory, Latvian Institute of Organic Chemistry, Riga, Latvia

Design and development of novel apramycin antibiotics

Apramycin is an atypical 2-deoxystreptamine-type aminoglycoside antibiotic (AGA) isolated from *Streptomyces ribosidificus*. It is well known in veterinary and is used for treatment of many bacterial diseases. In our study it was chosen as a basis for the development of new antibiotics, because of its unique structure that evades the clinically widespread mechanisms of AGA resistance, that currently compromise the efficacy of other members in this drug class. As well, unlike other aminoglycosides, apramycin has reduced risks of ototoxicity and nephrotoxicity. There are already known examples of apramycin derivatives that contains apramycin as a scaffold and showed excellent target selectivity and exhibiting increased antibacterial activity for ESKAPE (*Enterococcus faecium*, *Staphylococcus aureus*, *Klebsiella pneumoniae*, *Acinetobacter baumannii*, *Pseudomonas aeruginosa*, and *Enterobacter spp.*) pathogens, as well LD50 values were significantly less than the parent in the ex vivo mouse cochlear explant model. Therefore, successful use of apramycin in the development and design of novel apramycin analogs (apralogs) would result in new potential antibiotics with excellent antibiotic activity against multidrug resistant pathogens.

In our quest to improve the antibacterial activity of apramycin, we based on the idea of developing apramycin's hybrids by installation of a substituted additional furanosyl ring into the 5-position of apramycin, in such a manner as to append substituents at the furanosyl ring 3-position so as to mimic of paromomycin scaffold. These novel derivatives carry activity-enhancing aminoalkyl substituents at the ribose 3-position via a carbon-carbon or nitrogen-carbon bonds. This modifications allow the retention of a hydroxy or amino group at the ribose 3-position with the potential to engage in adventitious hydrogen bonding interactions in the hydrated binding site and the consequent potential to further increase activity and selectivity.

Herein we report the design and synthesis of novel apralogs, both anomers of 5-O-(5-amino-3-C-d m thylaminopropyl-D-ribofuranosyl)apramycin, 5-O-[3-C-dimethylaminopropyl)-*β*-D-eryt rofuranosyl), 5-O-(5-amino-5-deoxy-3-amino-3-deoxy-D-ribofuranosyl) and 5-O-(5-amino-5-deoxy-3-N-dimethy aminopropyl-3-deoxy-D-ribofuranosyl)apramycins.

Audience Take Away Notes

- The audience will know how to properly design synthetic schemes of novel apralogs, how to improve the antibacterial activity of apramycin and to form the glycosidic bond at the 5-position of apramycin
- It will provide a practical solution to solve problems with glycosidic bond formation in the presence of basic amino substituent, installation of substituents in the different positions of the ribose (furanosyl ring)
- It will help to improve the accuracy of a synthetic scheme design and practical choice of protection groups

Biography

Dmitrijs Lubriks has completed his PhD at the age of 32 years from Riga Technical University. He is the Principial Scientist at Latvian Institute of Organic Chemistry. He has published 7 papers in reputed journals.

Nina Belotserkovets
Department of Physical Chemistry, Tver State University, Russian Federation

Quantum chemical study of the molecular structure of utyltrimethyl ammonium cation

Salts containing alkyltrimethylammonium cautions are widely studied as ionic liquids (ILs). The structure of the caution significantly affects the properties of ionic liquids and the possibility of their use for various purposes. In this work, in order to systematically study the relationship between the structure and properties of alkyltrimethylammonium compounds, geometry optimization, calculation of the total energy, dipole moments, partial charges of atoms, and harmonic vibration frequencies of various rotational isomers of the butyltrimethylammonium cation were carried out in the framework of the second-order Möller-Plesset perturbation theory in the MP2/6-31G(d,p) approximation. According to the results of quantum chemical calculations four stable conformational states of the butyltrimethylammonium cation corresponding to the local minima on the potential energy surface were found. For these conformations after full geometry optimization the total energy, the partial atomic charges, dipole moments, the energy frontier molecular orbitals are calculated.

Biography

Nina Belotserkovets, Chemistry Doctor (Ph.D. – Chemistry) now is an Associate professor of Chemistry of the Department of Physical Chemistry of the Tver State University. Education: Lomonosov Moscow State U., 1971; Insignia "Inventor of the USSR" (1983). Recipient Cert. of Honour, Ministry of Education of Russian Federation, 2003. Laureate of the Russian competition "Engineer of the Year" in the nomination "Chemistry (research)" (2011). She has published more than 70 research articles.

Anderi Sumich*, V. Shevchuk

Department of mineral fertilizers, Institute of General and Inorganic Chemistry of the National Academy of Sciences of Belarus, Belarus

Synthesis of macrodisperse silica as a filler for rubber technical goods

In this work m acrodisperse silica was synthesized by the hydrolysis of diluted liquid glass (≈15w.% of SiO_2, molar $SiO_2/Na_2O \approx 3.0$) with 1N H_2SO_4. The liquid glass was added to the solution of sulfuric acid while continuous mixing until the pH of the reaction mixture achieved 3±0.2. Then the synthesized gel was washed with distilled water, dried at 100°C and milled. A part of the synthesized silica gel was modified. For this purpose, the silica gel was mixed with 0.6N CH_3COOH and held in these conditions for 3 days. The determination of particle size distribution was defined via the laser diffraction method using a laser particle sizer “Analysette 22” (Fritsch GmbH, Germany).According to the obtained results, the differential curve of the particle size of the modified and unmodified silica gel corresponds to the normal distribution along a bell curve. The main (about 75%) size of the particles of the unmodified silica gel ranges from 14 to 70 μm. The content of the particles with the size of less than 14 μm is about 15% and the content of the particles with the size of more than 70 μm is around 10%. Modifying the silica gel using CH_3COOH allowed us to obtain a sample with a narrower particle size distribution. In accordance with the results of the laser diffraction method about 75% of the particles correspond to the size 15–60 μm. The content of the particles with the size of less than 15 μm is about 15% and the particles with the size of more than 60 μm – 10%. This modifying influence of acetic acid can be caused by dispersing effect of the CH_3COOH on the macrostructure of the silica gel when the decreasing of the size of globules occurs. It is shown that synthesized macrodisperse silica gel can be used as a filler for rubber materials.

Audience Take Away Notes

- The found relation between the dispersity of silica gels and the conditions of their synthesis and modifying can be used in physical, colloidal and applied chemistry
- This knowledge is also of interest for technology of rubber technical goods
- The results of the work have a practical importance and can be used in the production of rubber technical goods
- The obtained knowledge can be used in teaching physical and colloidal chemistry

Biography

Andrei Sumich studied chemical engineering and scientific foundations of inorganic technology at the Belarusian State Technological University, Belarus and graduated with an MS in 2009. He received his PhD degree in 2017 at the same university. He taught chemical engineering and the scientific foundations of inorganic technology at the department of inorganic materials technology and general chemical technology at the Belarusian State Technological University. Now he is working as the leading researcher of the department of mineral fertilizers at the Institute of General and Inorganic Chemistry of the National Academy of Sciences of Belarus. He has published more than 20 papers in reputed journals.

Habiba Amira-Guebailia[1]*, Hanane Messiad[1,2], Fatima Zahra Hamamdia[1], Karima Belguidoum[1], Nadjet Lemouari[3, 4]

[1]Laboratoire de Chimie Appliquée -LCA, Université 8 Mai 1945 Guelma, BP 401, Guelma 24000, Algeria.
[2]Université de Constantine 3, Algeria.
[3]Centre de Recherche Scientifique et Technique en Analyses Physico – Chimiques, CRAPC, Bousmail, Tipaza, Algeria.
[4]Laboratoire de N-corps & structure de la matière, École Normale Supérieure de Kouba, Algeria.

Donor-acceptor interaction between biologically active hesperetin 7-rhamnoglucoside and π-acceptors DDQ and TCNE

The interactions between a biologically active flavonoid, Hesperetin 7-rhamnoglucoside (HESP) and two of the most known π- acceptors DDQ and TCNE were investigated leading to two new charge transfer complexes (CTC). UV- Visible spectrophotometry was used to follow the reactions in solution in methanol and ethanol as sol- vents. Infrared and NMR spectrophotometry was used to characterize the products formed in the solid state reactions. The1:1 stoichiometry of formed charge transfer complexes (HESP-DDQ and HESP-TCNE) was con- firmed by Molar ratio method and Benesi-Hildbrand equation was used to calculate the formation constants K CT and the molar extinction coefficient ε CT of the formed CTC. CTC formed in the reaction of Hesperetin 7-rhamnoglucoside with π-acceptors DDQ and TCNE showed high formation constants K CT. K CT values for both CTC formed in ethanol are higher than those formed in methanol and those found for the HESP-DDQ CTC were higher than those of HESP-TCNE. Our results suggest the formation of stable CT complexes of Hesperetin 7-O-rhamnoglucoside with π-acceptors DDQ and TCNE which could enhance biological properties of this phytochemical and accelerates its use a full-fledged medicine.

Audience Take Away Notes:

- Improvement of bioavailability of plant metabolites through charge transfer complexation
- Use of plant polyphenols as full-fledged medicines

Biography

Dr. Amira-Guebailia studied Chemistry at the Guelma University, Algeria and graduated as Chemical engineer in 1991 and got a Magister degree in 1994. She then joined the research group of Prof. Jean-Michel Mérillon at Bordeaux II University in France and she received her PhD degree in 2007 at Guelma University, Algeria in collaboration with Bordeaux II University in France. She obtained the position of an Associate Professor, lecturer then professor of chemistry at Guelma University. She has published more than 14 research articles in SCI(E) journals and supervised 7 PhD theses.

Evangelia Stathi[2], Alexandra Bakratsa[1], Vasiliki Zacharopoulou[1], Georgia Kastrinaki[1], George Karagiannakis[1]*, Vasileios Zaspalis[1,2]

[1]Chemical Process & Energy Resources Institute, CERTH, Greece
[2]Department of Chemical Engineering, Aristotle University of Thessaloniki, University campus, Greece

Synthesis and characterization of iron oxide nanoparticles

The constantly rising carbon dioxide (CO_2) emissions at the earth's atmosphere highlight the necessity of implementing mitigation strategies to restore carbon balance. In this direction, CO_2 is captured and then used as feedstock to produce high added value products, such as chemicals or light fuels (CCU technologies). One common approach refers to CO_2 hydrogenation through the combination of the Reverse Water-Shift (RWGS) reaction (CO_2 is converted into CO) and the Fischer – Tropsch (FTS) like reactions (CO hydrogenation). The properties of the catalytic materials that catalyze the above reaction pathways are crucial for the desired product distribution and CO_2 conversion, hence, they have attracted researchers' interest throughout the years. Iron oxide nanoparticles with alkali additives or/and secondary metals catalyze both RWGS and FTS reactions and were synthesized through co-precipitation. The synthesized nanoparticles were dispersed on substrates (alumina, zeolite) with acid/basic sites that promote the effective CO_2 conversion. All the produced materials were extensively characterized regarding their physicochemical properties. BET and XRD analysis, FTIR and Raman spectroscopies, as well as Temperature Programmed Desorption measurements (TPD-NH_3, TPD-CO_2) were employed to elucidate the proper physicochemical characteristics that promote CO_2 hydrogenation to the desired products. FTIR and Raman analysis indicated the coexistence of different iron oxide phases such as hematite, maghemite and magnetite. TPD-CO_2 analysis showed that the iron oxide nanoparticles supported on alumina have weak basic sites, while TPD-NH3 revealed that the surface of nanoparticles supported on zeolite contains weak and medium acid sites. Preliminary experiments were conducted in a continuous flow reactor under $H_2/CO_2=3:1$ ratio, 320°C and 30 bar temperature and pressure conditions, accordingly. The output gas stream was analyzed online employing GC Chromatography. The catalytic materials were previously reduced under pure hydrogen flow at 350°C for four hours. C_1-C_3 deoxygenated hydrocarbons, such as methane, ethane, propene and propane were produced. However, further investigation regarding the correlation of the catalysts' attained physicochemical characteristics to the product distribution is necessary.

Acknowledgements

We acknowledge support of this work by the project "PROMETHEUS: A Research Infrastructure for the Integrated Energy Chain" (MIS 5002704) which is implemented under the Action "Reinforcement of the Research and Innovation Infrastructure", funded by the Operational Programme "Competitiveness, Entrepreneurship and Innovation" (NSRF 2014-2020) and co-financed by Greece and the European Union (European Regional Development Fund).

Audience Take Away Notes

- Catalytic carbon dioxide valorization aspects
- Effect of specific catalytic properties on the reaction product distribution

Biography

George Karagiannakis (MEng ChE, MSc, PhD) is principal researcher and head of the newly established ARTEMIS Laboratory (ARTEMIS stands for LAboratory of novel mateRials & Technologies for sustainable Energy & environMental Integrated applicationS) of the Chemical Process and Energy Resources Institute (CPERI) of CERTH, Greece. His main research focuses on materials and subsystems for the production of energy carriers from solar-thermal/thermochemical processes, as well as on technologies using alternative fuels in gasification and fuel cell systems.

G. Karagiannakis[1]*, E. Daskalos[1], M. Karani[1], N. Vlahos[1], G. Kastrinaki[1], A. Zygogianni[1], D. Zarvalis[1]

[1]Chemical Process & Energy Resources Institute, CERTH, Greece

Li-ion battery materials: Advanced characterization tools

Batteries constitute one promising solution regarding the ongoing transition towards a low-carbon economy. Electrochemical energy storage will enable the decarbonisation of both the transport and power sector. The complexity of physico-chemical processes inside batteries renders any development strongly dependent on the proper description and monitoring of the inherent evolution and interaction of all materials inside an electrochemical cell. Advanced characterization techniques that are non-destructive, highly sensitive and selective, fast or real-time, cost effective, and more generally capable to assess materials in their overall diversity and complexity as well as in operando environments, will address the critical mechanisms in chemical reactions and material structures during and after battery cycling and will provide in-depth information for optimization. Raman spectroscopy, with advanced instruments (Qontor inVia Renishaw), can perform 2D and 3D mapping of materials and in combination with an operando electrochemical cell (EL-CELL) can contribute to study in high resolution (0.5 μm) chemical reactions and material structure on the Cathode (CEI) and Anode (SEI) Electrolyte Interface. X-ray tomography allows having not just a cross-section but information about the whole volume of the sample. It allows the 3D reconstruction from cross-sectional images, enabling the possibility to analyze the whole volume of the sample and visualize the cross-section at any desired depth in any direction. The understanding of multi-physics processes that are taking place during battery charging and discharging in combination with additional characterization tools can contribute to multi-scale validation of battery systems and effective optimization of next generation energy storage materials.

Acknowledgements

We acknowledge the support of this work by the project “PROMETHEUS: A Research Infrastructure for the Integrated Energy Chain” (MIS 5002704) which is implemented under the Action “Reinforcement of the Research and Innovation Infrastructure”, funded by the Operational Programme "Competitiveness, Entrepreneurship and Innovation" (NSRF 2014-2020) and co-financed by Greece and the European Union (European Regional Development Fund).

Biography

George Karagiannakis (MEng ChE, MSc, PhD) is principal researcher and head of the newly established ARTEMIS Laboratory (ARTEMIS stands for LAboratory of novel mateRials & Technologies for sustainable Energy & environMental Integrated applicationS) of the Chemical Process and Energy Resources Institute (CPERI) of CERTH, Greece. His main research focuses on materials and subsystems for production of energy carriers from solar-thermal/thermochemical processes, as well as on technologies using alternative fuels in gasification and fuel cell systems.

14-15 JUNE

DAY 02

KEYNOTE FORUM

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Lattice vibrations and atomic reactions governing reversible behaviour of shape memory alloys

Metals and alloy systems have different phases at different temperatures and these phases are described in phase diagrams depending on the alloy composition. A series of alloy systems, shape memory alloys exhibit a peculiar property called shape memory effect at the β-phase region with chemical compositions. These alloys are very sensitive to external conditions, and crystal structures turn into other crystal structures with the movement of atoms with variation of temperature and stressing. Lattice vibrations (phonons), atomic bonds and interatomic interactions play an important role in the processing of transformation. Shape memory effect is initiated on cooling and deformation, and performed thermally on heating and cooling, with which shape of the materials cycles original and deformed shapes in reversible way. Therefore, this behavior can be called thermoelasticity. This deformation is plastic deformation, and strain energy is stored in material and released on heating, by recovering the original shape. This phenomenon is governed by the stimulus-induced crystallographic transformations, thermal and stress induced martensitic transformations. Thermal induced martensitic transformations occur on cooling with cooperative movements of atoms in <110 > -type directions on the {110} -type planes of austenite matrix, by means of lattice invariant shear, along with lattice twinning reactions, and ordered parent phase structures turn into twinned martensite structures. The twinned structures turn into detwinned martensite structures by means of stress induced transformation by stressing the material in the low temperature condition. These alloys exhibit another property called superelasticity, which is performed in only mechanical manner by stressing material in elasticity limit in parent phase region just over austenite finish temperature, and recover the original shape upon releasing, by exhibiting elastic material behavior. Stress-strain profile exhibits nonlinear behavior, stressing and releasing paths are different, and hysteresis loops refer to energy dissipation. Superelasticity is also result of stress induced martensitic transformation and ordered parent phase of the alloy turns into the detwinned martensitic structure with stressing. Copper based alloys exhibit this property in metastable β-phase region. Lattice invariant shear and twinning is not uniform in these alloys, and gives rise to the formation of layered structures, like 3R, 9R or 18R depending on the stacking sequences on the close-packed planes of the ordered lattice. In the present contribution, x-ray diffraction and transmission electron microscopy (TEM) studies were carried out on copper based CuZnAl and CuAlMn alloys. X-ray diffractograms and electron diffraction patterns exhibit super lattice reflection. X-ray diffractograms taken in a long-time interval show that locations and intensities of diffraction peaks

Osman Adiguzel

Department of Physics, Firat University, Elazig, Turkey

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 change with the aging time at room temperature, and this result refers to the rearrangement of atoms in diffusive manner.

Keywords: Shape memory effect, martensitic transformation, superelasticity, twinning, detwinning, and lattice invariant shear.

Audience Take Away Notes

- 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.

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.

14-15 JUNE

DAY 02

SPEAKERS

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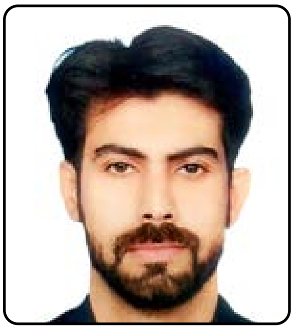

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Ammonia induced anomalous ion transport in covalent organic framework nano channels

More anomalous transport behaviors have been observed with the rapid progress in nanofabrication technology and characterization tools. The ions/molecules inside nanochannels can act dramatically different from the bulk systems and exhibit novel mechanisms. Here, we have reported the fabrication of a nanodevice, covalent organic frameworks covered theta pipette (CTP), that combine the advantages of theta pipette (TP), nanochannels framework, and field-effect transistors (FET) for controlling and modulating the anomalous transport. Our results show that ammonia, a weak base, causes a continuous supply of ions inside COF nanochannels, leading to an abnormally high current depending on the ionic/molecular size and the pore size of the nanochannel. Furthermore, CTP can distinguish different concentrations of ammonia and have all the qualities of a nano-sensor.

Audience Take Away Notes

- Mass transport of ions and molecules in nanochannels has attracted much attention due to the emergence of anomalous transport behavior, which is distinctive from the bulk systems. In the hope of controlling and modulating the anomalous transport, efforts have been made to understand its mechanism and the affecting factors to help explore and develop further applications. Exploring the anomalous transport behavior will also pave the way for imitating biological systems' ionic and molecular transport processes. Therefore, transport phenomena in nanochannels are critical research topics requiring in-depth study
- Theta pipette (TP) or dual-channel pipette has two barrels separated by a band of glass. TP have often been utilized for gas sensing, probing ionic reactions by creating a liquid-liquid interface between aqueous-organic solutions, and field-effect transistor (FET) sensor for single-molecule detection. However, the above-mentioned applications require an interface to limit the movement of ions between barrels or use one of the barrels as a gating electrode, therefore limiting the potential of TP. Furthermore, there is a lack of study to create a nanoconfinement that connects both barrels and the bulk for sensing. So yes, our design can help utilize the full potential of the TP
- List all other benefits
- The findings of this work can help understand and manipulate the anomalous ion transport behavior in nanochannels, which is essential for biological systems and the field of energy. Furthermore, the findings of this work can also help in designing FET nanodevices for label-free sensing in the bulk solution

Biography

Saud Asif Ahmed obtained his Ph.D. degree in Analytical Chemistry from Nanjing University, Nanjing, China, in 2020, under the supervision of Prof. Xing-Hua Xia and Prof Kang Wang. Later, he worked as a post-doctoral fellow in the same research group till 2022. He has joined Prof. Ping Yu and Prof. Lan-Qun Mao's research group as a Junior Research Fellow of the Beijing National Laboratory for Molecular Sciences (BNLMS) at the Institute of Chemistry, Chinese Academy of Sciences, Beijing, China. His research mainly focuses on electroanalytical chemistry, electrochemical sensing, and the mass transport of ions through porous materials using single and double-barrel nanopipettes. He has published more than 14 research articles in SCI journals.

Sunil Kumar[1, 2]
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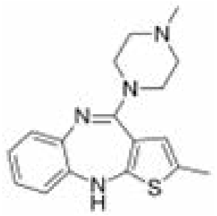
Novelty determination in the design of drug molecules chemical formula

The primary motivation behind choosing the topic is to analyze the novelty criteria for Active Pharmaceutical Ingredients (API) products and process patents. As a pharma chemist specializing in organic chemistry, the genuine concern is whether a general Markush structure could destroy the novelty of a drug molecule. It was argued in *Dr. Reddy (UK) Limited vs. Eli Lilly* case that a general formula can cover the patented compound olanzapine (Fig. 1a). However, to interpret each compound from a general formula, it needs length and breadth of knowledge of organic/medicinal chemistry. One general formula can produce trillions of drug molecules, which indicates that unless a single compound has not been synthesized, it might not be possible to prepare in the laboratory. For instance, if only R^1 (Fig. 1b) is substituted and other variables are kept constant, it may give thousands of compounds. Another aspect is the biological activity of chemical compounds, which shows that one molecule might have one or more activities against many diseases. Therefore, based only on the theoretical aspect of the general formula, it is improbable that a person skilled in art can guess the actual pharmacological activity of a predicted compound.



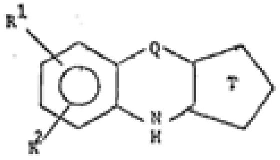


Fig 1a Olanzapine Fig 1b General Formula of compound

Where R^1, R^2, Q, and T are variables

Audience Take Away Notes

- Audiences in medicinal chemistry will learn to establish novelty to discover patented inventions
- This presentation will help the researcher to open their capacity to work towards patents rather than just journal publications
- A presentation about the novelty of drug molecules will be helpful for academic and industry research
- Yes this provide a practical solution to a problem that could simplify or make a designer's
- Yes it improve the accuracy of a design, or provide new information to assist

Biography

Sunil Kumar received his Ph.D. in Pharmacy from India in 2012. He worked as a scientist-IPR (Intellectual Property Rights) at pharmaceutical R&D. He was employed as an Assistant professor at ISF College of Pharmacy, Moga, India. He was awarded a postdoctoral fellowship by National Science Council (NSC), Taiwan. His research is mainly based on medicinal and natural product chemistry, specializing in anti-inflammatory and anti-cancer drug design. Dr. Kumar has more than 20 publications in reputed journals like PloS One, the Journal of Natural products, the European Journal of Medicinal Chemistry, etc. To understand drug discovery's novelty and patent aspect, he pursued LLM-IPR from Nottingham Trent University in 2021-2022.

Sejallon- Cipolla Mylene[1], Devel Laurent[2], Subra Gilles[1], Cantel Sonia[1*]

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Targeting out of range biomolecules: Chemical labeling strategies for qualitative and quantitative MS-based detection

In health sciences and particularly in –omics approaches, Mass spectrometry is of strategic importance for the detection and identification of specific molecules involved in biological processes, leading to a better understanding of physiological and physiopathological processes and consequently for diagnosis purposes. However, a large number of these relevant biomarkers remain undetectable due to several parameters, a low molecular weight, a weak abundance, their ionization potential or their localization in a complex environment. To overcome these limitations, labeling strategies have been developed. MS labeling require the development of diverse tags as versatile as possible, involving innovative chemistry, and targeting different functional groups such as amine, hydroxy groups or carboxylic acids. Specific probes, such as ABP have been designed to selectively label biomolecules of interest and to match the current need for in vivo labeling methods following the development of imaging techniques.

Audience Take Away Notes

- Chemical development in currently highly-relevant topic of chemical labeling, which allows overcoming the limitations of the MALDI MS, generally considered as a label-free technique. Different labeling strategies for MALDI-MS are presented
- MALDI-MS is a key technique for biomolecule gentle identification and proteomics
- This talk supplies a description of derivatization methods while putting into perspective the importance of MALDI labels in the bioresearch context by targeting out of range biomolecules in complex media
- Yes Is this research could use to expand their research or teaching
- Yes through chemical derivatization, compatible with biological media
- Yes by designing specific probes for detection of post translational modification hard to detect

Biography

Sonia Cantel obtained her PhD in 2004 in Chemistry of Biomolecules from the University of Montpellier, in the field of pseudo-peptide and solid phase organic synthesis. For the following two years as Post-doctoral Fellow in the Laboratory for Translational Research (Harvard Medical School, Boston, USA), she actively participated to biomedicinal projects and developed extensive skills in analytical techniques applied to peptide and protein engineering. She joined in 2007 the IBMM, taking advantage of her multidisciplinary experience to develop new projects at the interface of Chemistry, Biology and Analytical Sciences. She focuses her research on the development of chemical probes for specific and sensitive detection of peptides and proteins, and pharmacological studies (GPCR/ligand interaction) by MALDI Mass Spectrometry. Actively involved in peptide environment, she is currently at the directing board of the GFPP (French Group of peptides and proteins). She has published more than 50 research articles in SCI(E) journals h-index:16.

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Plasmonic effects and localized melting in gold nanoparticles systems

Plasmonic materials are subjects of great interest due to their potential for a wide range of applications such as: catalysis, optoelectronics, drug delivery, etc. One particularly intriguing aspect is the ability of metal nanoparticles (NPs) to exhibit localized surface plasmon resonances (LSPR), which lead to the concentration of electromagnetic fields near the nanoparticle surface. The localized heating and melting in gold nanoparticles can be attributed to the interaction between the LSPR and the incident electromagnetic field but also to the excitation of interband transition. When the particle is excited with light of a suitable energy, generally resonant with the energy of the LSPR or interband transition, the absorption of the radiation by the nanoparticle leads to different phenomena. Indeed, the excitation at the LSPR wavelength leads to the formation of electromagnetic hot spots, whereas the excitation at the interband energy produces hot electrons, which are more homogeneously dispersed in the NP volume. Such differences can be exploited to obtain control over the melting of nanoparticles and optimize the features of the nanoparticle for the specific application.

Femtosecond transient absorption spectroscopy (FTAS) is a powerful tool for characterizing the features of plasmonic nanoparticles. FTAS allows us to obtain information into the fundamental physical processes related to the optical properties of these nanoparticles, which has important implications for using these materials in a wide range of applications. Indeed, FTAS is a time-resolved pump and probe technique that can probe the dynamics of plasmonic nanoparticles with high temporal resolution. We have applied this technique to separate the contributions of non-thermal and thermal electrons to the transient spectrum of arrays of gold nanoparticles in the first picoseconds after excitation to gain insight into the ultrafast dynamics of the photoexcited electrons.

The ability to induce localized heating and melting in gold nanoparticles is a route for using plasmonic nanoparticles in a variety of applications. For example, plasmonic nanoparticles have been proposed for cancer photothermal therapy, where localized heating can selectively kill cancer cells. Gold nanoparticles have also been proposed as a platform for drug delivery, where plasmonic heating can be exploited to release drugs previously bonded with the nanoparticle.

Another promising application of plasmonic nanoparticles is in plasmon-enhanced photocatalysis. Indeed, plasmonic nanoparticles can be used to improve the efficiency of photocatalytic processes concentrating the light on the interface between the catalyst surface and gold nanoparticle and increasing the rate of electron transfer between the catalyst and the reactant.

In conclusion, plasmonic effects and localized melting in gold nanoparticle systems represent a fascinating area of research in plasmonics with many potential applications. This research aims to understand the mechanisms of the melting of gold nanoparticles promoted by the excitation of the LSPR or interband transition and to develop new approaches for controlling the morphological properties of plasmonic nanostructures.

Biography

Dr. Francesco Toschi is graduated in Materials Science at the University of Rome "Tor Vergata" (Italy) in 2005. He joined the Institute of Structure of Matter of the National Research Council of Italy (CNR – ISM) as a permanent researcher in 2019. Presently, his work is centered around the Ultrafast Laser Spectroscopies applied to innovative and nano materials for technological applications, such as plasmonic devices, new-generation photovoltaics, new materials for automotive, etc. His activities are carried out at the EuroFel Support Laboratory at CNR-ISM where state-of-the-art femtosecond laser instrumentation is available for Ultrafast Spectroscopies.

Orchidea Maria Lecian

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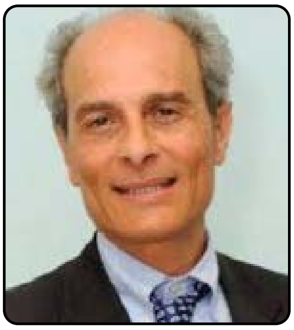
A new lemma of the optical equivalence theorem: Applications in theoretical chemistry and new challenges

The Optical Equivalence Theorem demonstrates the equivalence between the expectation value of an operator in the opportune Hilbert space and the expectation value of the pertinent functional representation in the phase space formulation with respect to a suitable distribution; for the purposes of this demonstration, a phase space reprenstation is chosen, which does not involve the Number operator. The Optical Equivalence Principle allows one to construct a sequence of the density operator. A new lemma of the Optical Equivalence Theorem is demonstrated, after which there is associated with the quasi-probability distribution and improved functional reprentation as far as the allowed expansion order is concerned; the construction is apt to codify almost-inifinite-momentum states. A compact-support control weighting function is introduced, to display the action of operators of high-intensity fields, whose states are determined. Applications in Theoretical chamistry are provided with. Applications are explained within molecular dynamics trajectories: the atomic coordinates at specific times are framed in the phase space, where the new improved reprentation of the quasi-probability distribution is used to improve the long-time-limit error calculation in the quantum fluctuations, quantum jumps (also in lasing), comparison of chemical shift with MNR spectroscopy for control of composition; Markovv modelisation: the long-timescale dynamics of molecular systems is analysed as consisting of probabilistic jumps between est of states, which are now newly issued as those which are the pertinent states of the new improved functional representation: quantum fluctuation, transition to lasing, carrier energy states, comparison with Monte-Carlo simulation; mocular chemistry: protein stability and folding kinetics, coordinate shift with determination of transition states, transmission probability, definition of entropic reaction coordinates; laser molecule activation; transition state spectroscopy: potential energy surfaces are newly established within the new representation of the phase space; molecular activation: the process of the molecular activation is framed within the new representation of the states within the new representation of the phase space obtained after the new improved representation of the probablity- distribution sequence. New challenges are envisaged.

Audience Take Away Notes:

- Aplications to molecular dynamics, quantum fluctuations, quantum jumps, molecule chemistry, protein folding, spectroscopy.
- Improvement of errors estimations from theoretical framework
- Yes
- Improvement in calculation of experiemtnal errors from theoretical framework
- Yes
- List all other benefits
- Further understanding of chemistry theory and statistics



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Synthesis and consolidation of high entropy ceramics

The synthesis and consolidation of High Entropy-Ultra-High Temperature Ceramics (HE-UHTCs) based on transition metal borides is addressed in this work. This emerging class of ceramics is based on the combination, in near equimolar proportions, of at least four constituents to generate single-phase crystalline solid solutions with maximum configuration alentropy, i.e.(Hf0.2Ti0.2Ta0.2Nb0.2Mo0.2)B2, (Hf0.2Ti0.2Ta0.2Zr0.2Mo0.2)B2, etc. The studies conducted so far evidenced that HE-UHTCs often exhibit superior oxidation resistance and mechanical properties, with respect to their individual constituents. Therefore, these materials have gained a significant interest for their high-temperature applications in several innovative and traditional industrial fields. Unfortunately, the obtainment of dense single phase HE-UHTCs represents quite a difficult goal. In this work, a two-steps process, consisting in the combination of the SHS technique with Spark Plasma Sintering (SPS), is successfully adopted for the preparation of various HE-UHTCs. In this regard, the use of the SHS method is found to highly promote the obtainment of the single-phase HE ceramic during the subsequent SPS stage. The introduction of different additives on SHS powder prior the SPS step is also considered.

Biography

Giacomo Cao got his Master Degree in Chemical Engineering at the University of Cagliari in February 1986 and his PhD also in Chemical Engineering at the University of Bologna in 1990. He became Assistant Professor in 1990, Associate Professor in 1992 and Full Professor in 2001. He has been a visiting scholar at the Department of Chemical Engineering, University of Notre Dame, USA, in 1988, 1991 and 1992 and research associate at the same University in 1993. He is co-author of 3 books, 1 edited book, more than 150 papers in refereed journals, 17 papers in refereed conference proceedings, 12 patents, 18 book chapters, 126 papers in conference proceedings. He has been the co-author of 239 presentations at national and international symposia.

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Study of dielectric and acoustic characterizations of alcohols with amide

The present paper explains the study of Static Permittivity, Density and Ultrasonic Velocity and derived properties for the binary mixtures of Dimethylacetamide (DMA) with four isomers of tertiary alcohols over the entire concentration range were measured at 300 K. Using Experimental parameters, Bruggeman factor, compressibility, and acoustic impedance, molecular free length, inverse relaxation time, Gibbs Free energy, Enthalpy of activation, Entropy and excess parameters were calculated. The values of excess properties afterward fitted with Redlich–Kister polynomial equation to estimate the standard deviation. The excess parameters were used to study the interactions between the molecules inside the binary mixtures. Results confirm that strong hydrogen-bonded intermolecular interaction occurs between due to contraction in the volume in DMA and isomers of tertiary alcohol. Results also confirm that branched-chain structured tert-alcohols + DMA shows the most potent interaction as compared to DMA+ other isomers of Butanol.

Keywords: Bruggeman factor, Compressibility, Excess dielectric constant, Excess inverse relaxation time

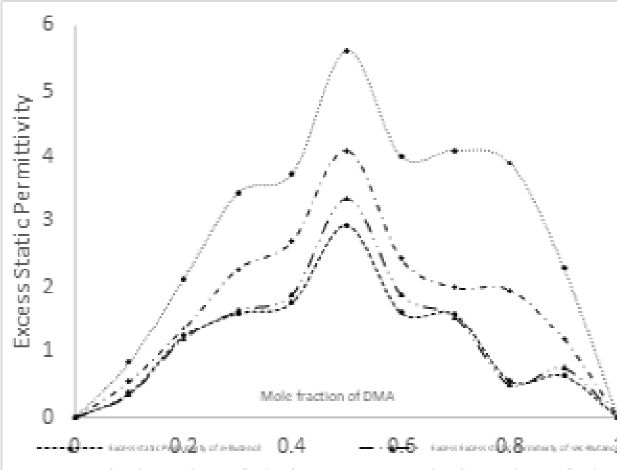


Fig:- Excess Static permittivity of isomers of alcohol with amide

Audience Take Away Notes

- Audience will get detailed regarding dielectric constant and relaxation time and its use to calculate other derived parameters and excess parameters. Further these parameters are also used to interpret type of intermolecular interactions, strength of bonding, dynamics of intermolecular interactions
- These intermolecular interactions study is very useful in chemical, medical, paint and material science
- Yes, this research that other faculty could use to expand their research or teaching with proper permission from author
- This study provides a solution to a problem that could simplify to reduce further efforts of drugs/ pharmaceuticals / chemical industry

- Yes, it improves the accuracy of a molecular design, or provide new bonding and molecular dynamics information to assist in a molecular design problem
- This study may be used in ceramic, chemical, agricultural study also

Biography

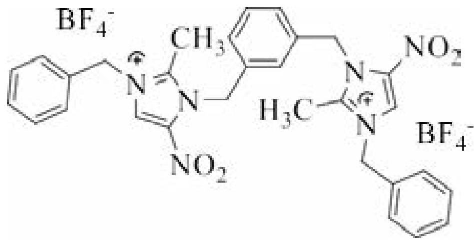
Aruna P. Maharolkar studied M. Sc. Physics at the Dr. BAM University, Aurangabad, India in 2007. She received her PhD degree in 2013 at the same institution. After completing her PhD Degree she has joined MIT Institution in 2013 and started her teaching career. She has published more than 40 research articles in SCI journals and international conferences. Two patents granted to her. She is working as reviewer for various international, national journals and conferences.

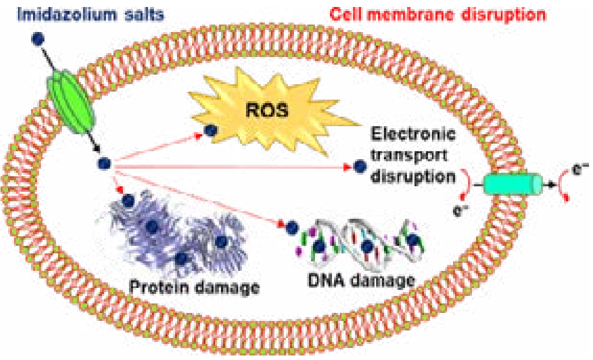
Kilivelu Ganesan

Assistant Professor, PG & Research Department of Chemistry, Presidency college, Tamilnadu, India

Solvent free synthesis of dimeric substituted imidazolium salts and its applications

Ionic liquids are an important and interesting application-oriented molecules. Ionic liquids consist of organic cationic segment which is pharmaceutically active and a simple inorganic anion which is easily soluble in water, hence ionic liquids are used in pharma industries. Dimeric substituted imidazolium ionic liquids under conventional and solvent free solid supported method and evaluate the hydrophilic and lipophilic segments containing dimeric substituted imidazolium salts as antibacterial agents against human pathogenic microorganism and docking analysis.





Audience Take Away Notes

- How the solvent free method is more advantageous than the conventional method
- How to achieve target molecules from environmentally safe and easy working procedure
- Researchers could minimize the toxic solvent during their synthesis
- Human pathogenic organism which shows effective binding with ionic liquids
- Inorganic counter anion plays a crucible role in antibacterial response

Biography

Ganesan received his Ph.D., degree in dendrimer chemistry from University of Madras, India. He has joined postdoctoral research associate at National Chaio-Tung University, Taiwan in combinatorial medicinal research group, then moved to University of Malaya, Malaysia as postdoctoral research associate in ionic liquids research group. Currently, he is working as an assistant professor chemistry in the Presidency college, India which has been fifth place national level and first place in state level college ranked by NIRF 2020. Current research area of ionic liquids, catalysis and bio-organic chemistry. He has received **Best Teacher award 2019** from **PARE FOUNDATION; Outstanding Faculty in Science 2019** received from **Venus International Foundation**; and **Teaching and research excellence national award** received from **Prestigious innovative research development and publishers (IRDP) award 2018.**

Mujtaba Ikram
Institute of Chemical Engineering and Technology (ICET), University of the Punjab, Lahore

Alumina- graphene hybrid for applied applications

In this invited lecture, enhanced physical properties of hybrids composed of γ-Al_2O_3 nanorods and reduced graphite oxide (RGO) platelets will be discussed which are prepared after calcination and hot-press processing. The hybrid processed at various calcination time shows an enhanced electrical conductivity, simultaneously with enhanced higher mechanical tensile strength and higher thermal conductivity, compared to the bare Al_2O_3. The dielectric constant of the hybrid is found much higher than that of the bare Al_2O_3. It is found that the oxygen-containing groups on graphene oxide benefit to the adsorption of aluminum Isopropoxide, leading to the uniform dispersion of RGO with Al_2O_3 which is hydrolyzed from aluminum Isopropoxide in solvothermal reactions. XRD characterizations show that the increase in calcination temperature and further hot-press processing at 900°C leads to the enhanced crystallinity of γ-Al_2O_3 nanorods in the hybrid, resulting in enhanced physical properties of the hybrids which are beneficial for applied applications.

Audience Take Away Notes

- Audience may learn about hot pressing and their impact on physical properties of hybrids
- This research proves beneficial to material scientists to expand their research or teaching
- New applications of graphene based hybrids may be developed in industry

Biography

Mujtaba Ikram has received his BS hons. (computational physics), MS (materials and surface engineering) and Ph.D. (material sciences and engineering), respectively. His research interests include nanotechnology, renewable energy, material science and engineering. His work has been cited by scientists from all over the world. He has authored/ co- authored number of publications in world prestigious journals as Advanced materials, Journal of Materials Chemistry C, ACS Omega, Nanoscale Research Letters, RSC advances, RSC New Journal of chemistry, Chemcatchem, Journal of alloys and compounds, Applied nanoscience, International Journal of hydrogen energy, Journal of physics and chemistry of solids, Journals of solid state chemistry and many others. He has represented his research in the USA, Italy, Egypt, Germany, Slovenia, China, Hong Kong, Malaysia, UAE and many other countries. He has attended various research training/conferences/workshops on industrial physics, renewable energy, advanced carbon materials and nanotechnology in various parts of the world. He is a frequent visiting scholar at the Abdus Salam International center for theoretical physics (ICTP)-Italy. He was selected among two young scientists from south Asia for TWAS science diplomacy, which was held in Trieste Italy, 2013. He has been invited many times as Invited lecturer by CAS-TWAS Beijing. In 2015, he was awarded with CAS-TWAS green technology award. In 2017, he was awarded with CAS-TWAS green chemistry and technology (GCT) award for his guest lectures. He has been awarded with various world prestigious fellowships in his academic and professional career.

Raghda A. El-Nagar* and Alaa Ghanem[2]

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Effect of different imidazolium ionic liquids on the dispersion of aggregated asphaltene in heavy crude oil

Due to the predicted increase in heavy oil production spurred on by energy problems, challenges relating to asphaltene are receiving increased attention. The formation of tough emulsions and blocked wellbores caused by asphaltene precipitation make production operations difficult and reduce the amount of recovered oil. Due to operational issues, safety concerns, and an oil production constraint, the petroleum industry suffers significant financial losses. In the extraction, production, and transportation operations, asphaltene dispersion in crude oil utilising green ionic liquid is being explored as a potential option. Ionic liquids (ILs) have the ability to break-down different types of crude oil emulsions such as water in oil emulsions (tough emulsions) and oil in water ones. ILs have many advantages such as they are eco-friendly and can be recycled. Herein in the presented study, the effect of the prepared ionic liquids on asphaltene aggregates has been investigated to determine the role of different structures of ILs on the dispersion of asphaltene molecules. Therefore, three different ILs containing different lengths of alkyl chains, Imi-C12, Imi-C8, and Imi-C4, were synthesized, characterized via FT-IR and 1HNMR. Moreover, the surface tension of ILs was measured to determine the critical micelle concentration. The prepared ILs were found to be thermally stable up to 380 °C after conducting the thermal gravimetric analysis. The dispersion activity of the ILs was investigated using the viscometric method, where n-heptane is used as a precipitant. It was found that using Imi-C12, Imi-C8, and Imi-C4 can delay the asphaltene onset precipitation from 30% to 55, 65, and 70 %, respectively. As a result of their interaction with asphaltene molecules and formation of steric stabilising layers surrounding them, ionic liquids with long alkyl tails (> eight carbon chains) are efficient asphaltene dispersants that lower oil viscosity and asphaltene aggregates. To avoid asphaltene aggregation in petroleum feed streams, ionic liquids can be used as an environmentally friendly chemical substitute for surfactants.

Keywords: Asphaltene, Ionic liquid, surface tension, onset precipitation, Heavy oil, viscosity.

Biography

Dr. Raghda El-Nagar studied Chemistry at the Zagazig University, Egypt and graduated in 2009. She then joined the research group at the Egyptian Petroleum Research Institute, Cairo, Egypt. She received her MSc degree in 2013 and his PhD degree in 2018 at Ain Shams University. Dr. Raghda El-Nagar is a Researcher - Oil Testing Lab - Analysis and Evaluation Department. Senior of Oil lab analysis in Central Lab Services Center with over 14 years of experience providing technical support concerning routine petrolieum studies to over 25 petroleum companies in Egypt, Sudan, South Africa and Chad. She has published more than 20 research articles in SCI(E) journals.

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Chemical composition, antioxidant activity, cholinesterase inhibitor and in vitro insecticidal potentiality of essential oils of lippie multiflora moldenke and eucalyptus globulus Labill. on the main carpophagous pests of cotton plant in côte d' ivoire

In the face of the abusive and repeated use of synthetic insecticides that are harmful to human health and to the viability of the cotton production system in Côte d'Ivoire, finding alternatives becomes imperative. Thus, the objective of this study was to study the chemical composition and biological activity of essential oils of Lippia multiflora (Verbenaceae) and Eucalyptus globulus (Myrtaceae) and to evaluate their insecticidal potential in the laboratory on three main carp pests of cotton. After extraction of essential oils by the chemical composition of these was determined. Also, their antioxidant and anti-acetylcholinerase activities were evaluated. Subsequently, different concentrations of the two essential oils were prepared and applied by contact on batches of insects constituted by ten. The essential oil of L. multiflora was the most toxic for the three pests tested. Indeed, the lethal concentrations (LC50) determined were 1.74 %, 1.39 and 7.20 % respectively on Pectinophora gossypiella, Thaumatotibia leucotreta and Helicoverpa armigera. In contrast, the values obtained with E. globulus EO were nine to two times greater (16.05 %, 10.23 % and 16.32 % respectively on these pests). With respect to the chemical composition of the essential oils, E. globulus EO was the richest in oxygenated monoterpenes (65 %) with 1,8-cineole or eucalyptol as the majority compound (61.6 %). The EO of L. multiflora was distinguished by a lower proportion of oxygenated monoterpenes (44.3 %), but it contained more terpene elements (24 against 15 for the EO of E. globulus). The EOs of L. multiflora and E. globulus also showed significant inhibitors of acetyl (2.13 and 2.16 mg GALAE/g, respectively) and butyryl cholinesterase (4.03 and 3.61 mg GALAE, respectively). L. multiflora was differentiated by its good inactivation of tyrosinases (163.46 versus 58.95 Mg KAE/g in E. globulus). Better antioxidant activity was observed with L. multiflora EO relative to DPPH (7.05±0.34 mg TE/g). Biopesticides based on L. multiflora essential oil could be developed for the phytosanitary protection of cotton plant.

Keywords : Essential oils, Carpophagous insects, Antioxidant activity, Antiacetylcholinesterase activity, insecticidal activity

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