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Posters



Comparative evaluation of chemical mass balance and multivariate receptor models using synthetic data

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In the field of atmospheric sciences, the term receptor models is customarily used to describe top-down approaches for air-pollution assessment, i.e. methods that begin by sampling air in a given area, in order to match common chemical and physical characteristics between source and air pollution samples. Source identification and quantification is realized by employing statistical analyses, widely known, under the term Multiple Linear Regression (MLR). There are two fundamental categories of RMs, Chemical Mass Balance (CMB) models, which assume full knowledge of the compositions of emissions, and multivariate models, which apportion sources on the basis of observations at the receptor site, alone. One of the first documented uses of RMs for air-quality management was by the United States Environmental Protection Agency (EPA), back in the early 80s. Since then, RMs have gradually become familiar to policy-makers all over the world, as there were vast improvements, not only in the MLR methods that can now be performed by modern computers but also in the chemical speciation techniques that provide RMs with input data. Nevertheless, there are still major concerns regarding RMs, such as the influence of personal judgment to model results, as well as the lack of a standard methodology for quantifying uncertainty levels, since, in the real world, one cannot check the model output, against the actual values of source contributions. This study presents a comparative

evaluation of RMs, using synthetic input datasets, i.e. where the values of source contributions are already known. Synthetic data were generated by inducing random variations to reference values, with the use of deterministic procedures, widely known as “pseudo-random number generators”. Virtual receptors have been set to match conditions that can actually hinder model performance, such as large measurement errors, collinearity between source profiles, strong correlations between the temporal variations of source contributions etc. The simulation includes the newest versions of CMB and multivariate receptor models, as well as some of the previous ones that are still in use, by the scientific community. Particular emphasis has been placed on a recently developed computational procedure, the so-called Robotic Chemical Mass Balance (RCMB), which has been considered to be a mathematical optimization of previous CMB models, minimizing personal judgment. Preliminary results indeed confirm the superiority of RCMB over the human modeler, if the latter one has under or overdetermined source profile input data.

Biography

Georgios Argyropoulos is a postdoctoral researcher in the Department of Chemistry, at the Aristotle University of Thessaloniki (AUTH), Greece. His educational background includes an MSc degree in Chemical Engineering, an MSc degree in Environmental Chemistry, and a PhD degree in Receptor Modeling, all received from AUTH. One of his major research interests is the use of statistical techniques, such as multivariate analysis, for source apportionment of atmospheric pollutants. He has participated in numerous research projects, including the LIFE Environment programme, funded by the European Commission. Recently, he also received a Fellowship of Excellence for Postgraduate Studies in Greece, from the State Scholarships Foundation (IKY) of Greece, in the framework of the Hellenic Republic – Siemens Settlement Agreement.

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 Notes:

Development of nature-inspired conjugated materials for plastic electronics

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Innovative developments of organic conjugated polymers have been reported to present future potential alternatives to supply photovoltaic energy. Present-day solar energy production is costly due to requiring the expensively processed crystalline silicon, therefore, we are working on developing nanostructured materials that would be low-cost. There have been some recent ongoing advances of using solar cells that are based on the earth-abundant, cheap, non-toxic organic active materials that also are light weight, flexible and its layers makes it versatile. Our research group aims to prepare efficient organic solar energy materials, which can absorb light and transfer to electric energy. This project was inspired by the natural dye, indigo, for its narrow

energy band gap, intensive color (high absorbance), and planar structure. Indigo has been accepted among various optoelectronic devices for decades. Its isomer, isoindigo, has better properties, it is fully conjugated, providing more space to be functionalized and the ability to install side groups for better solubility. Our target is the synthesis of thienoisindigo, which provides even a coplanar structure via the S-O interaction and a lower band gap, with maximum absorbance at a higher wavelength. Our aim in this research, is to test and reach optimum results to develop new organic materials containing isoindigo, thienoisindigo, or their derivatives units for use in plastic electronic and solar energy applications.

Biography

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 Notes:

Copper-guanidine catalyzed asymmetric allylic alkylation under phase transfer conditions

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Forging a more intense link between transition metal catalysis and asymmetric ion-pairing catalysis are recently purchased by us. Enantiopure skipped 1, 4-enynes are useful building blocks due to its transformability. In this work, enantioselective alkylation of cyclic allylic bromides was achieved due to an in situ-generated guanidinium cuprate ion pair. Thus, enantiopure cyclic 1,4-enynes were obtained by the first time through a proposed distinct dynamic kinetic pathway, not common SN2' pathway. In the presence of catalytic amount of copper(I) salt and cyclic-guanidinium(CG), the asymmetric Csp-Csp3 bonds were formed via alkylation of racemic cyclic bromides with aid of K₂CO₃ as a base at room temperature. Various terminal

alkynes with different substituents on an aryl group and different functional groups such as ester, amide, silyl, amine, hydroxyl, and thioether are all suitable under the standard reaction condition. The enantiospecific derivatization of products demonstrated the practicability of this methodology. The mechanism study revealed that alkynide in this Cu-catalyzed reaction behaves as 'hard' nucleophile; a model ion-pairing catalysis which was characterized by X-ray analysis and 1H-NMR and; meanwhile, in situ CSI-MS and 1H-NMR spectra recognized several guanidinium cuprates ion-pairs and copper-alkynide complex which is a complementary to the current Cu-catalyzed asymmetric allylic alkylation mechanistic study.

Biography

Xi-Yang Cui is working as a assistant professor at Nanyang Technological University at Singapore. He belongs to chemistry department

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 Notes:

Determination of Some Antidiabetics by High Performance Liquid Chromatography

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Diabetes is a disorder of the metabolism mostly seen as a combination of inherited or environmental factors and resulted with over increase of blood glucose level (hyperglycemia), the prevalence is increasing day by day in Turkey and in the world. Dipeptidyl peptidase-4 inhibitors (DPP-4s), gliptins, are a new class of drugs for oral hypoglycemic and use for the treatment of type 2 Diabetes. Sitagliptin, vildagliptin and saxagliptin are the members of the gliptin drugs which are available in the market in Turkey. The advantages of gliptin drugs are differ from oral hypoglycemic drugs used in the treatment of type 2 diabetes like sulphonylureas, biguanids, α -glucosidase inhibitors and meglinids by oral implementation due to its non-peptide structure, and less side effects to the gastrointestinal system since the incretin receptors are not affected directly. In

this study a fast and simultaneous HPLC method was developed for the determination of sitagliptin, vildagliptin and saxagliptin in tablets. A Thermo Ultimate 3000 HPLC was used for the chromatographic method development. Separation was achieved on a Gemini C18 (4.6x250mm, 5 μ) HPLC column with a mobile phase combination of methanol: ortho phosphoric acid, in gradient elution. Analytes were detected both on 225 and 212 nm wavelengths. The developed method was validated and will be applied to biological samples. This work was carried out at Istanbul University, Faculty of Pharmacy as an undergraduate research project.

Biography

Sena Caglar Andac has completed her PhD from Istanbul University and Postdoctoral studies from Medical Center of Munich University, Laboratory of Bio-Separation. Currently, she is working as an Associate Professor at Istanbul University, Faculty of Pharmacy. She has researches published in liquid chromatography mass spectrometry for biological fluid analysis of drugs, on-line solid phase extraction coupled liquid chromatography, determination of drugs and degradation studies by high performance liquid chromatography, spectrophotometry and spectrofluorimetry.

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 Notes:

Catalytic hydrogenation of biomass derived levulinic acid using zero valent non-precious metal Fe catalysts based on N-triphos ligand

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The global concern on declining crude oil resources and efforts to reduce the anthropogenic emission of CO₂ has led to an intensified search for renewable and environmentally benign alternative sources of carbon for the production of transportation fuels and chemical. Biomass remains the most suitable and sustainable alternative that meets both the demand for clean energy and the production of liquid transportation fuels and chemicals.¹ Levulinic acid (LA) is an important biomass derived platform molecule that can be transformed to more valuable chemicals and fuels, with catalysis playing a key role in its transformations. Ru-triphosphine complexes have recently proven to be excellent homogeneous catalysts for effecting the hydrogenation of LA to gamma-valerolactone (GVL), 1, 4-pentanediol (1, 4-PDO) and 2-methyltetrahydrofuran (2-MTHF), however, there are few reports on non-precious based metal catalyst for this transformation.^{2,3}

Herein we explore the catalytic hydrogenation of LA to GVL, 1, 4-PDO and 2-MTHF using more sustainable non-precious metal Fe complexes as catalysts (fig.1). The Fe metal precursors Fe₃CO₁₂ and FeCO₅ were chosen because of their previously reported catalytic activity and commercial availability. The novel bimetallic [Fe(CO)₃(K²-NP3^{Ph})(μ-PPH₂)Fe(CO)₄] and monometallic Fe(CO)₃(K²-NP3^{Ph}) Fe⁰ complexes were synthesized from

the reaction of N, N, N- tris(diphenylphosphinomethyl) amine (N-triphosPh) ligand with Fe₃CO₁₂ and Fe(C₈H₈)(CO)₃ precursors respectively. Catalysis of LA was performed in a high pressure autoclave under the conditions of 150o C and 50 bar H₂. Near quantitative conversion of LA was observed in most cases, yields were determined by GC.



Fig. 1 Hydrogenation pathway of levulinic acid (LA)

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Biography

Uwaila Omoruyi obtained her BSc (2006) and MSc (2013) in industrial chemistry from the University of Benin, Nigeria. She then proceeded to United Kingdom in 2014 to pursue a PhD in the Department of Chemistry, Imperial College London under the supervision of Dr. Philip Miller. She is currently in the final year of her PhD and her research is focused on the catalytic hydrogenation of biogenic acids using novel phosphine complexes. Uwaila is a recipient of a scholarship award from the Nigerian Petroleum Technology Development Fund (PTDF)

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Abstracts



Cu(II) complexes of hydrazone Schiff base ligands: synthesis, characterization, DNA and topoisomerase I enzyme interactions

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Small inorganic complexes that can interact with DNA or other biological molecules have tremendous conservation. Because such compounds can pass the inhibitions that large molecules cannot pass through to show desired activities. It is a known phenomenon that transition metal complexes oxidize or bind to DNA in the presence or absence of reductants. Therefore, it is important to understand the structure activity relationship especially in the antitumor action mechanism of metal complexes that can bind to DNA under physiological conditions and specifically cleave DNA. In particular, Cu(II) complexes containing Schiff base are much more attractive as they can enter into the bases of DNA. The interaction of DNA with metal complexes is closely related to the design of synthetic restorative enzymes and chemotherapeutic drugs. Transitional metal complexes play a key role in the formation of newly bound complexes in the DNA domain, although structural flexibility and variable dimensionality are

taken into consideration. In recent years, the use of certain chemotherapy drugs by interfering with topoisomerases in cancer cells has focused on the enzyme topoisomerase I in the development of anticancer drugs. In this study, new cationic hydrazone Schiff bases and their coordination compounds with Cu(II) have been synthesized and characterized. Firstly, various p-substituted benzohydrazine derivatives were reacted with cationic acetophenone derivatives, which were served as a chelating bridge, in order to prepare hydrazone Schiff base ligands. In the second step of this study, coordination compounds of the synthesized ligands with biologically important transition metal Cu(II) were isolated and characterized. Then, inhibitory activities of topoisomerase I enzyme and DNA binding and cleavage activities was examined for the compounds. The effect of the factors such as ligand and geometry tetrahedral square-planar, octahedral, etc. on the activity where be defined. That the synthesis of some Schiff base derivatives bearing functional groups such as -OH and -NH₂ increasing the pharmacological activities was discussed in this study. Consequently, novel and effective agents interacting with DNA, showing topoisomerase inhibitions activity have been revealed.

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MIP nanoparticles in diagnostics and bioimaging

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Two years ago we have made a major breakthrough in MIP technology developing solid-phase approach for preparation of soluble molecularly imprinted nanoparticles (nanoMIPs) with exquisite affinity and selectivity for their templates¹. The success came from combining controlled radical polymerisation² with an affinity separation step performed on surface-immobilised template³. This approach represents the state-of-the-art in nanoMIP synthesis: not only are soluble particles with defined size (20-200 nm) and a narrow size distribution produced in one hour, they possess subnanomolar dissociation constants for their respective targets, they can be easily functionalised with fluorescent, electrochemical or magnetic labels, and the immobilised template can be re-

used. High affinity nanoMIPs were made for small molecules, proteins, membrane proteins and virus particles⁴.

The main practical niches for application of synthesised nanoMIPs are diagnostics, imaging and drug delivery. Particularly exciting is an opportunity to use MIP sensors in companion diagnostics. Members of our team have used nanoMIPs successfully as a replacement for antibodies in ELISA-type assays, electrochemical and optical sensors⁵. The exciting examples of our work with in vivo application potential are targeting membrane receptors, enzymes and quorum sensing molecules⁶. Very encouraging facts that enables practical applications of MIPs in vivo are lack of polymer toxicity, ability of nanoMIPs to penetrate into cells and to pass blood barrier. Current paper discusses challenges and opportunities that are faced by MIP technology in the light of these developments.

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Chemical ensuring subnanostructures formation in densely crosslinked organic-inorganic hybrid polymer networks

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Cyanate Ester Resins are known to form polymer networks through reaction of polycyclotrimerization of cyanate groups. Cyanate groups are highly reactive towards active hydrogen containing organic groups as well. The high crosslink density organic-inorganic hybrid polymer networks have been synthesized from the mixture of tetraethoxysilane (TEOS), 3-aminopropyltrimethoxysilane (APTMS) and 1,1-Bis(4-cyanophenyl)ethane (DBCE). First, acid hydrolysis of the silanes followed by polycondensation reaction of the hydrolysis products was fulfilled in situ, and then reaction of DBCE cyanate groups with amino and hydroxyl groups of silica units formed was carried out under mild conditions. As a result, some DCBE molecules appeared to be chemically grafted to the silica network units. Then, polycyclotrimerization of DCBE free and grafted (by one

side) molecules was performed at high temperatures. The composites with silica contents from 0.01 to 10 wt. % were prepared. The state of silica in the composites has been characterized by means of FTIR, high-angle annular dark-field scanning transmission electron microscope (STEM) combined with Energy-dispersive X-ray spectroscopy (EDXS). For the composites with ultralow silica contents ($\ll 1$ wt. %), the structures without nano- or microclusters but with silica units distributed quasi-regularly within the amorphous polymer matrix have been formed. The data obtained imply the existence only in this case of subnanometer-sized silica nodes connected covalently with the matrix, i.e., the formation of the hybrid subnanocomposites. The Far-IR spectroscopy, DMA (Dynamic Mechanical Analysis) and DSC (Differential Scanning Calorimetry) data showed that these subnanocomposites manifest the largest “constrained dynamics” effect and superiority in thermal and mechanical properties compared to those of the nanocomposites with higher silica contents containing nanoclusters and their aggregates.

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Hybrid nanocarbons encapsulating redox and magnetically active nanoswitches

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The electrical coupling of nanocarbons with redox and magnetically active nanoscale objects has attracted a great deal of attention for achieving functional hybrid nanostructures with a wide range of exploitable properties. This is especially important for designing next-generation electronic or spintronic devices that will be based on nanoscale functional materials such as isolated spin centres or single-molecule magnets. In order to harness the magnetic bistability, quantum tunnelling of magnetization, and quantum coherence of nanometer-sized magnetic objects, the coupling to the macroscopic world that is essential for read and write purposes has become a key challenge. Hollow carbon nanostructures with one macroscopic and two nanoscopic

dimensions can act as bridges to achieve this coupling, through the encapsulation and confinement of magnetic species, while maintaining their structural integrity and properties that would otherwise induce decoherence (–a major obstacle for quantum applications). Another important challenge facing the humankind today is the production of clean and sustainable energy where electrochemical technologies have shown to play an important role. However, the market potential of electrochemical devices based on electrocatalyst containing precious metals, such as Pt, is currently hindered by their short-term durability. As these precious elements are rapidly diminishing, the research community is forced to urgently address this major issue until more abundant efficient electrocatalysts are put forward. In this respect, high-aspect ratio carbon nanostructures can provide an excellent mean for the fabrication of highly durable electrocatalyst materials through platinum encapsulation, allowing their sustainable use in fuel cells technology.

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Electrode-modified with nanoparticles composed of 4,4'-bipyridine-silver coordination polymer for sensitive determination of Hg(II), Cu(II) and Pb(II)

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A glassy carbon electrode modified with nanoparticles of 4,4'-bipyridine-silver coordination polymer was used for highly sensitive analysis of heavy metals (Hg(II), Cu(II) and Pb(II)) by differential pulse voltammetry. The coordination polymers were immobilized on the glassy carbon electrode surface via an organic layer that contains phenylmethyl-4,4'-bipyridinium and coordinated silver ions. The modification method is rapid (an electrode is produced in less than 30 min); electrodes are stable and can be used for the analysis of at least 70 real samples. A glassy carbon electrode (GCE)

modified with nanoparticles composed of a 4,4'-bipyridine silver coordination polymer (CP) were applied to the sensitive differential pulse voltammetric analysis of the ions Hg(II), Cu(II) and Pb(II). The coordination polymer was prepared by mixing a solution of silver nitrate and 4,4'-bipyridine at room temperature. The surface of the GCE was modified with an organic layer of synthesized 1-[(4-nitrophenyl)methyl]-4,4'-bipyridinium and silver ions, which caused the binding of the added Ag-bipy-CP. Anodic (oxidative) peaks of the electrode were at +300 mV for Hg(II), -70 mV for Cu(II), and at -540 mV for Pb(II) [versus Ag/AgCl]. The detection limits were 0.09 mg/L Hg(II), 0.71 mg/L Cu(II) and 2.3 mg/L Pb(II). Relative standard deviation was 3.2% at a level of 4 mg/L of Hg(II) for n=10. Importantly, the sensitivity and stability of the developed modified electrodes allowed their use for determination of Hg(II) in spiked fish samples and Cu(II), Pb(II), and Hg(II) in spiked plant samples with good recovery 90 to 108%. This study demonstrates the utility of coordination polymers for the development of electrochemical sensors and opens a new area of applications for these versatile materials.

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An array of semiconducting metal oxide heterojunction sensors used for explosive detection

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Terrorists frequently use explosives and they represent an imminent threat to national and global security. Recent events highlight the necessity of explosive detection, demonstrating the need for developing and applying new sensors for explosive gas detection. Semiconducting metal oxide gas sensors can be incorporated into electronic noses, which provide a cheap, portable and highly sensitive device, therefore making them a reliable method when detecting explosives. Using unmodified, admixed and 2-layered sensors consisting of WO₃ and CTO (chromium titanium oxide) an array of seven heterojunction semiconducting metal oxide sensors was produced. All seven sensors were tested

against gases associated with explosive materials at a range of temperatures 300°C, 400°C and 500°C. All sensors produced underwent X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM), Energy-Dispersive X-ray Spectroscopy (EDX) and Raman spectroscopy, in order to establish if any structural changes occurred to the array due to the exposure of the gases or temperatures. Both the admixtures and the 2-layered semiconducting metal oxide gas sensors have been shown to enhance sensor response when detecting explosives. The data collected was processed against a support vector machine in order to comprehend the sensors application into an electronic nose. The technique produced a high data classification when classifying the gases used within the study. Therefore, the array produced has successfully discriminated the tests gases from one another, consequently showing the potential use of the array implemented into an electronic nose for the use of explosive detection to be an effective method.

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Whey biorefinery: sustainable strategies for added-value food manufacture – a bioeconomic approach

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Nowadays, enormous quantities of food waste are becoming a global concern. Specifically, dairy industry which is a major economical resource is generating a large volume of waste liquid effluent, namely whey. To address this persistent problem, sustainable interventions with green technologies are essential. Valuable products can be economically recovered from cheese whey using new biochemical processes. Thus, in the present study, whey was utilized initially as a substrate for the production of immobilised functional biocatalysts for the production of novel added-value food products. In parallel, after the biocatalysts removal the detergent liquid-whey was used as a raw material for manufacturing of functional beverages. Whey can be a valuable nutrient medium for cultivation of microorganisms and thus it was used as a substrate for the production of functional immobilised biocatalysts. Dried organic berries (*Hippophae rhamnoides* L.) were selected as supports for the immobilisation bioprocess of the probiotic bacterial strain *Lactobacillus casei* ATCC 393 due to their antioxidant

and antiproliferative activities along with their exceptional technological properties as natural immobilisation carriers. Whey protein and immobilised biocatalyst were removed from whey and used for the production of added value frozen desserts. Subsequently, valorization of the detergent whey was achieved by the incorporation of *Pistacia lentiscus* mastic gum added as a natural preservative. Mastic gum has been used in traditional Greek medicine for various gastrointestinal disorders from the ancient years and is well known for its antimicrobial properties. The incorporated freeze-dried mastic gum significantly reduced the initial high counts of yeasts and fungi of the produced beverages compared to initial whey used as a control sample during 30 days of storage at 4°C. The good texture and the exceptional mastic gum flavor & aroma, along with possible antimicrobial indicates the products high commercialization potential. Adapting biorefinery strategy with integrated approach can lead to the development of circular bioeconomy. Likewise, from the knowledge of environmental stress, proper treatment of whey is extremely necessary and thus the suggested bioprocess of whey valorization for the production of novel added value food products will explore many unfold issues in the field of food fortification, human nutrition and upgradation of dairy effluent whey.

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Intracellular delivery of biomacromolecules

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Efficient delivery of non-permeant therapeutic agents with intracellular therapeutic targets is challenging. Over the years, methods using viral and/or non-viral vectors have been developed. Synthetic polymers, often considered a safer alternative, may be tailored to improve cytoplasmic access and

modulate cell specific targeting. Poly(amidoamine)s (PAAs) are a family of synthetic functional polymers developed for use as polymer therapeutics. They are synthesized by Michael addition polymerization, are generally water soluble and display pH-dependent membrane activity. We will discuss the biological rationale for the development of these polymers and review their application for the delivery of macromolecular drugs (e.g. proteins, oligonucleotides).

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The concept of sustainable chemistry: key drivers for the transition towards sustainable development

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Producing, using, re-using, disposing, and eliminating chemicals with the least possible adverse effects on human health and the environment is the so-called 2020 goal which has been initially formulated 2002 by the Johannesburg World Summit for Sustainable Development. While rapidly approaching the initial target date, we face globally ongoing progression of production volumes, count, and uses of chemicals. Thus, the need for broad transformation to a sustainable chemistry becomes exigent. Moreover, as humankind has to rely on the chemicals sector for contributions to nearly all Sustainable Development Goals (SDG) of the Agenda 2030, it is even more essential to get the urgently needed sustainable solutions from a thoroughly sustainable chemistry. Sustainable development is a process to ensure the future as well as present potential to meet essential human needs and desires within the ecological and resource

limits of our planet. This paradigm is relevant for all areas including those where chemicals are produced, traded, used, processed, incorporated into products, reused and recycled, disposed of and released into the environment. Sustainable chemistry is a holistic approach for sustainable development considering the entire lifecycle of chemical products and the related system of actors, institutions and culture. This holistic approach distinguishes sustainable chemistry from green chemistry and from operational safe use of chemicals. Sustainable chemistry is building on and goes beyond these two concepts. Therefore, besides health and environment, social conditions, science, research, technical and economic aspects must be considered and balanced within the capacity-limits of our planet. The herewith-presented Concept of Sustainable Chemistry describes the understanding of what sustainable chemistry is about in view of the authors. Based on this assumption, to guard against green washing, to reduce current burdens, and with a view to the SDG, we propose seven Objectives and Guiding Principles of Sustainable Chemistry to be applied in all chemical relevant areas: design and use of benign chemicals; development and use of alternative solutions for problematic applications; reduction of impacts; conservation of natural resources; promotion of reuse and recycling; increase of market opportunities; application of corporate social responsibility. In conclusion we point out action topics promoting the holistic approach that sustainable chemistry entails.

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Smart polymers for drug release and cellular control - triggered release and activation

Mark Bradley

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My talk will be in three parts. Firstly, I will describe polymer microarray technology, which has been developed by the Bradley group. I will introduce the technology, including our unique inkjet mediated fabrication methodologies (which allow over 7000 different substrates to be fabricated on a single

glass slide) and describe how this approach has been used in a large number of stem cell based applications. Secondly, I will discuss how Palladium and Copper catalysts entrapped within a polymeric scaffold can mediate chemistry inside cells, including the formation of both new C-C bonds but also the liberation of “caged” compounds (e.g. drugs). Finally, I will describe some of the group’s polymer chemistry in which Diels-Alder chemistry is used to trigger cargo liberation from nanoparticles within a biological context.

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Emissions and atmospheric chemistry from Havana´ stationary sources

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The determination quantitative of air pollutant emission and dispersion in the atmosphere from main stationary sources in Havana and its effects on atmospheric chemistry, is an urgent and necessary study, taking into the account that mentioned city have the most population of country and a number considerable of emission sources. The knowledge of these emissions and dispersion is a useful tool to know the characteristic the atmospheric chemistry in urbanization.

The results showed atmospheric emissions rate of SO₂ is upper than 29 thousand ton/year while NO₂ emission rate is about 12 300 ton/year. Furthermore, particulate matter (PM₁₀ and PM_{2,5}) reach 3 700 ton/year, which are known for its potential damage for human health and atmospheric chemistry. The most populated municipalities are very close to the fixed sources emit more pollutants into the atmosphere. The influence of urbanization is reflected in the dispersion of emissions pollutants. Finally, this air emission inventory is a previous stage before of that will be allow future implementation of air quality forecasting for Havana city from any air pollution models outputs.

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Soft based hypersonic phononics

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Phononic structures (composite materials in which a periodic distribution of elastic parameters facilitates control of the propagation of phonons, hold the promise to enable transformative material technologies in areas ranging from acoustic and thermal cloaking to thermoelectric devices. This requires strategies to deliberately 'engineer' the phononic band structure of materials in the frequency range of interest. Phononics, the acoustic equivalents of the photonics, are controlled by a larger number of material parameters, as phonon cannot propagate in vacuum. The study of hypersonic phononics (hPnC) imposes substantial demand on fabrication and characterization techniques. Colloid and polymer science offer methods to create novel materials that possess periodic variations of density and elastic properties at length scales commensurate with the wave length of hypersonic phonons and hence visible photons. The key quantity is the dispersion

$\omega(q)$ of high frequency (GHz) acoustic excitations with wave vector q which is measured by the noninvasive high-resolution Brillouin light scattering. The approach involves the exploitation of Bragg-type bandgaps (BGs) that result from the destructive interference of waves in periodic media. However, the sensitivity of BG formation to structural disorder limits the application of self-assembly methods that are susceptible to defect formation. Hybridization gaps (HG), originating from the anti-crossing between local resonant and propagating modes, are robust to structural disorder and occur at wavelengths much larger than the size of the resonant unit. Here, examples based on hierarchical structures will be highlighted: (i) 1D-hPnC to acquire comprehensive understanding, while the incorporation of defects holds a wealth of opportunities to engineer $\omega(q)$. (ii) In colloid based phononics, $\omega(q)$ has revealed both types of band gaps. (iii) particle brush materials with controlled architecture of the grafted chains enable a new strategy to realize HG's (iv) Hierarchically nanostructured matter can involve unprecedented phonon phono propagation mechanisms.

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The transition path time distribution - protein folding, quantum mechanics, tunneling times and uncertainty

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Recent experimental measurements of the transition path time distributions of proteins present theory with challenges. They lead to barrier heights which are much lower than the free energies of activation of the observed transitions. Secondly, can one use the transition path time distribution to obtain insight into some of the intriguing questions of quantum mechanics, such as how long does it take to tunnel? In this talk, I introduce the paradigm of a transition path barrier height for the protein folding problem, and show that it should be smaller than the activation energy, resolving the low barrier

height puzzle. The transition path distribution for a parabolic barrier is derived for arbitrary memory friction. In the second phase of this talk, the quantum mechanical transition path time probability distribution will be discussed. Standard approaches to tunneling times are replaced by considering time correlation functions. The formalism is used to study the quantum dynamics of thermal position correlation functions. Highlights are the proof of a vanishing mean tunneling time at the parabolic barrier crossover temperature and that increasing the length of the path traversed decreases the mean transition time. The mean transition path time is used to define a coarse-grained momentum for passage from one side of the barrier to the other. The product of the uncertainty in this momentum with the uncertainty in the location of the particle is shown under certain conditions to be smaller than the $\hbar/2$ formal uncertainty limit.

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Risks of a false decision on conformity of a multicomponent material and quality of chemical analytical results

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Comparing chemical analytical (test) results with the material specification, regulatory or acceptance limits of the component content, one should decide whether the tested sample (batch/lot) conforms or not. It is known that measurement uncertainty, which characterizes the quality of a result, leads to risks of false decisions. Evaluation of

such risks for a multicomponent material or object involves calculation of probabilities of false decisions for the different components of the material or object (particular consumer's and/or producer's risks). At the same time, even when conformity assessment for each component of a sample is successful, the total probability of a false decision (total consumer's risk or producer's risk) on the conformity of the sample as a whole may still be significant. The total risk due to measurement uncertainty can be evaluated as a combination of the particular risks of conformity assessment of the sample components, whenever there is independence among their test results. Possible correlation can be viewed as a further quality parameter of the results, influencing the total risk of false decisions. It should be also taken into account at the risk evaluation.

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Heating with inorganic nanoparticles: applications in life science

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The capability of being able to release heat upon remote electromagnetic (EM) exposure has opened new opportunities for a variety of goals in life sciences. Local heating with colloidal nanoparticles (NPs) has been used for killing tumoral cells, drug-release applications, ultralow detection of tumoral markers, imaging *in vivo* and *in vitro*, or even sterilization. In the frame of oncological hyperthermia, both magnetic and plasmonic NPs have been investigated as nanoheaters and can be remotely activated by radiation that do not or minimally

interact with physiological tissues and fluids. Actually, the major challenge concerning colloidal chemistry within this framework resides in being able to produce NPs that absorb in EM regions where tissue absorption remains minimum, i.e., biological windows. Engineered nanomaterials with tailored heating performance, as well as suitable organic coatings, are continuously developed toward more efficient interactions with EM radiation and the performance of more complex tasks in biological environments. Moreover, these materials can be used simultaneously as contrast agents by using imaging techniques that rely on their magnetic (e.g., MRI) or plasmonic behavior (e.g., OI), thereby enabling theranostic NPs. In this talk, several examples of nanoheaters for applications in life science will be discussed.

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Organogels: Original Materials for Therapeutic and Dermo-Cosmetic Applications

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Nowadays, several therapeutic, cosmetic and dermo-cosmetic studies consider gelling agents to produce innovative face and body care formulations. Organogels are an interesting perspective because they possess the ability to confer hardness due to their fibrous structure, and to allow new organoleptic and physicochemical properties of the final product. These formulations are semi-solid systems, in which an organic liquid phase of cosmetic or dermo-cosmetic interest (soybean, almond, emollients, ...) is immobilized by a three dimensional network composed of self-assembled, intertwined gelator fibers. The most commonly employed organogelators in cosmetics are polymers, but these are not the only gelling agents used. Indeed, smaller molecules, Low Molecular-Mass Organic Gelators Organogelators (LMOGs),

may also present similar properties towards organic liquids. LMOGs are frequently used in cosmetology for their desirable physical organization properties within the oil phase or their capacity to jellify the organic liquids in smaller quantities (in the range 0.1– 10 wt%).

In this study, the concept of organogel preparation and characterization from vegetable oils and LMOG (1,3:2,4-Dibenzylidene sorbitol or DBS and 12-hydroxystearic acid or HSA) agreed for therapeutic, cosmetic and dermo-cosmetic applications, has been described and their physicochemical properties (mechanical strength, physical stability, phase transition temperatures, ...) have been investigated. The results show that the determination of LMOG proportion allows modulating the organogel properties. The use of LMOG is beneficial for the formulation consistency and texture, conferring good physical and chemical stability of the final product.

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The kinetics of conversion of carbon monoxide to carbon dioxide on the surface of mixed nano-catalyst in the closed system

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In this article, the kinetics of oxidation process of carbon-monoxide on the nano-catalyst surface was investigated. The investigation was conducted in the different flow conditions

and temperature, at the temperature range of 70-350°C (by the range of $\Delta T=70-350^\circ\text{C}$), depending on the kinetic conversion of carbon monoxide to carbon dioxide in the closed system. It is determined that the speed of conversion process increases (by) 1.30-1.32 times as temperature increases on the surface of catalyst. The conversion of carbon-monoxide to carbon-dioxide runs more rapidly at the low flow rates. Nano-catalyst (are) introduced and tested in a process of neutralizing harmful emissions is presented in this investigation.

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A novel double-layer immobilised biocatalyst for simulated barrel aging production of sweet wine

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The present study was undertaken to assess the simulating barrel aging effects of a novel double-layer immobilised biocatalyst for low temperature wine making. The double-layer biocatalyst consisted of partially delignified and burned oak sawdust (DBOS) with entrapped *Leuconostoc oenos* cells, covered with starch gel containing the alcohol resistant and cryotolerant strain *Saccharomyces cerevisiae* AXAZ-1. The immobilized double-layer biocatalyst was found efficient for high gravity grape must fermentations at low temperature

and high final alcohol concentration. In parallel, this novel biocatalyst was able to convert malic acid to lactic acid and simulating oak barrel ageing through extraction of volatiles of burned oak sawdust producing a sweet wine with higher organoleptic characteristics as shown by GC and SPME GC/MS analysis. Improvement of wine quality compared with wine fermented with free *S. cerevisiae* cells was attributed to malolactic fermentation and lower alcohols production due to the low fermentation temperature. The significance of DBOS is the feasibility of three processes (alcoholic fermentation, malolactic fermentation, oak barrel aging simulation processes) in one batch fermentation reducing the production cost and energy demand in the food industry, giving the opportunity to the consumers to taste an aromatic sweet wine without preservatives.

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Sizing α , β and γ cyclodextrins by capillary electrophoresis and indirect UV detection

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Cyclodextrins have ring structures made of glucose connected by 1,4-glycoside linkage and they differ in the number of glucose on the ring. The interior of cyclodextrin is considerably less hydrophilic than its exterior; therefore, they are useful for carrying hydrophobic molecules. Due to their hydrophilic exterior, they are able to penetrate body tissues, which make them good candidates as drug carriers where

they can release biologically active compounds under specific conditions. However, different sizes of cyclodextrins form different complex with the same molecule, so, it is important to know the size of each cyclodextrin. Indirect UV-capillary electrophoresis and Taylor dispersion analysis are used to size α , β and γ cyclodextrins. Because cyclodextrins have low UV absorbance, indirect UV is used in which the background electrolyte has significantly higher UV absorbance than the target molecules, therefore, resulting in negative peaks. Using TDA, diameters of α - and γ -CD are calculated to be 0.70 nm and 0.86 nm. The small standard deviation indicated the precise and reproducible measurement.

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