

# DAY 1

Scientific Tracks & Abstracts



EuroSciCon Conference on

# Chemistry 2018

February 19-20, 2018

# DAY 1

February 19-20, 2018

## Sessions

Polymer Chemistry | Physical And Theoretical Chemistry | Nano-Chemistry And Technologies | Organic Chemistry | Medicinal & Pharmaceutical Chemistry | Electro-Analytical Chemistry

**Session Chair**  
Jean-Pierre Djukic  
University of Strasbourg, France

**Session Co-Chair**  
Pierre Lutz  
University of Strasbourg, France

### Session Introduction

**Title:** From isotactic polystyrene (iPS) or poly(p-methyl styrene) to semicrystalline iPS / POSS hybrid materials

**Pierre Lutz**, University of Strasbourg, France

**Title:** N-(2-Hydroxyethyl) morpholine HCL salt content by hydrophilic interaction liquid chromatography (HILIC) with charged aerosol detection (CAD)

**David Wang**, Alkermes, USA

**Title:** The percolation scheme for the very basic understanding of the Raman spectra of mixed crystals: apparent universality and possible application

**Olivier Pagès**, University of Lorraine, France

**Title:** Nanostructured and nanocomposite materials for energy conversion

**Sara Cavaliere**, University of Montpellier, France

**Title:** Harnessing multipolar interactions at the nanoscale: a novel opportunity for molecular photonics and bioimaging

**Mireille Blanchard-Desce**, University of Bordeaux, France

**Title:** Synthesis and reactivity of bromocyanobutadiyne: from interstellar chemistry to organic synthesis methodology

**Yann Trolez**, National School of Chemistry of Rennes, France

**Title:** Nanomaterials: in between traditional concepts of understanding matter

**Emil Roduner**, University of Stuttgart, Germany

**Title:** The iPPI-DB initiative

**Olivier Sperandio**, Institut Pasteur, France

**Title:** Electrochemical reactions based on [60] fullerene derivatives

**Guan-Wu Wang**, University of Science and Technology of China, China

**Title:** X-ray standing wave technique applied in the characterization of periodic multilayers

**Meiyi Wu**, Sorbonne University, France

**Title:** Actual issues of monitoring the content of synthetic dyes in food products in the Republic of Belarus using modern analytical methods

**Palianskikh Alena**, Scientific Practical Center of Hygiene, Belarus

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Pierre-J Lutz, J Org Inorg Chem 2018, Volume: 4  
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## FROM ISOTACTIC POLYSTYRENE (IPS) OR POLY(*p*-METHYL STYRENE) TO SEMICRYSTALLINE IPS / POSS HYBRID MATERIALS

**Pierre-J Lutz<sup>1,2</sup>, Maximilian Vielhauer<sup>1,2</sup>, Felix Kirschvink<sup>1</sup>, Luis Valencia<sup>1,2</sup>, Christian Friedrich<sup>1</sup>, Günter Reiter<sup>1</sup> and Rolf Mülhaupt<sup>1</sup>**

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In the present work, the synthesis of iPS is realized by homogeneous catalytic styrene polymerization on a MAO-activated titanium bisphenolate catalyst, in the presence of a non-conjugated diene acting as chain transfer agent (CTA) leading to vinyl-terminated iPS (vinyl-iPS). The polymerization of styrene, with the same catalyst, was also achieved in a cascade of two parallel reactors. Whereas ultra-high-molecular-weight (UHMW) iPS is formed in the absence of the diene, the molar mass  $M_w$  decreases with increasing diene/styrene molar ratio. Hence, the contents of iPS and UHMWiPS are varied without affecting the average molar mass of both blend components. The same catalytic system was tested for the coordination polymerization of *p*-methyl styrene. Vinyl-iPS revealed also a highly efficient CTA for the ring-opening metathesis polymerization (ROMP) of *cis*-cyclooctene, producing polycyclooctene-block-isotactic polystyrene (PCO-b-iPS) as amorphous and semi-crystalline rubber diblock copolymers. Furthermore, crystalline nanostructured inorganic-organic hybrid materials containing isotactic iPS were prepared by means of hydrosilylation coupling of vinyl-iPS with octakis(dimethylsilyloxy)silsesquioxane ( $Q_8M_8H$ ). As a function of the iPS/ $Q_8M_8H$  molar ratio, the formation of linear or star-shaped hybrid architectures is achieved.

### Biography

Pierre-J Lutz is a Professor (Directeur de Recherche Emerite, CNRS) of Polymer Chemistry in Strasbourg. He completed his PhD in Macromolecular Engineering in 1981 from University Strasbourg, France. (supervision P. Rempp). Chargé de Recherche (1981), ICS, (CNRS) postdoc (Prof. H. J. Cantow, Freiburg (Germany)). In 1988, he spent a sabbatical year at the Institute of Macromolecular Chemistry, in Freiburg with Prof. W Burchard as Humboldt Visiting Scientist. In 1996, he was nominated as Directeur de Recherche at the ICS (CNRS-University of Strasbourg). His recent scientific interests are concerned with various polymerization processes structural characterization. From 2012-2015, University of Jena (Germany) (Prof. U. S. Schubert), University of Freiburg (Prof. R. Mülhaupt). Since 2017 Directeur de Recherche Emérite (CNRSHe); has authored more than 170 publications and book chapters and 3 patents. He is a member of the French Polymer Group and the French Chemical Society. He was a member of the American Chemical Society until 2014. His research interests include polymer chemistry- polymers of controlled molecular and structural parameters via ionic polymerization and their characterization; functional homo (or co) polymers including macromonomers, branched polymers, cross-linked polymers, and cyclic polymers (via coordination, living anionic polymerization); complex macromolecular architectures; grafting reactions; self-assembly of block copolymers and; hydrogels designed for biomedical applications. In particular his interests lies in poly(ethylene oxide) (PEO) and related materials designed for biomedical applications; synthesis and characterization of polyethylenes of various molecular architectures and; more recently hybrid polymeric materials.

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## N-(2-HYDROXYETHYL) MORPHOLINE HCL SALT CONTENT BY HYDROPHILIC INTERACTION LIQUID CHROMATOGRAPHY (HILIC) WITH CHARGED AEROSOL DETECTION (CAD)

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The utility of charged aerosol detection (CAD) for quantitation has received considerable attention in the pharmaceutical industry. The operating principle of drying and applying a charge to particles in the eluent stream which are directly measured at an electrometer provides a repeatable response when analyzing compounds which lack a UV chromophore. Due to the molecular chemistry of the morpholine alcohol HCL salt, it was found that neither traditional HPLC-UV nor GC-FID analysis was capable of detecting residual amounts present in the drug substance. Further development studies examining different combinations of mobile phases, organic additives, columns (C8, C18, and HILIC) with a CAD detector were performed. It was determined that HCL salt format of a morpholine compound could be successfully analyzed by an HPLC –CAD method with a HILIC column. The method proved capable of controlling residual morpholine alcohol residual in a drug substance.

### Biography

D Wang has completed his PhD from Florida International University. He is a Senior Scientist at Alkermes, a global biopharmaceutical company. He has published more than 12 papers and presentations in reputed journals and scientific conferences.

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## THE PERCOLATION SCHEME FOR THE VERY BASIC UNDERSTANDING OF THE RAMAN SPECTRA OF MIXED CRYSTALS: APPARENT UNIVERSALITY AND POSSIBLE APPLICATION

**Olivier Pagès**

Université de Lorraine, France

**G**enerally, while dealing with mixed crystals, the crucial issue is to determine whether the atom substitution is ideally random or due to local clustering/anti-clustering. In the latter case, the next issue is to estimate the deviation from random substitution via some relevant order parameter. Raman scattering is interesting with respect to the raised issues because it probes the force constant of a chemical bond, which is a local property. As such, it is presumably sensitive to the local environment of a bond. Moreover, Raman scattering is conveniently operated at the laboratory scale, being non-destructive, fast, and relates to the crystal in volume. However, if we refer to the admitted models for the description of the abundant Raman spectra of the mixed crystals with cubic structure, worked out at the emergence of such systems in the sixties, namely the modified-random-element-isodisplacement (MREI) model and the cluster model, they both fail to account for the natural complexity of the Raman spectra of most random mixed crystals, not to mention about the non-random ones. Basically the MREI model falls short of explaining the natural complexity in question, while the cluster model overestimates it by far. Over the past decade we have introduced a novel model to discuss the Raman spectra of the mixed crystals with cubic structure, the so-called percolation model that seems to apply universally. Moreover, as this model distinguishes between the vibrations of like bonds depending on whether they vibrate in like or foreign environment, it offers a possibility to formalize any trend towards local clustering/anti-clustering (like environment favored/disfavored) via the Raman intensities. In this communication we provide a comprehensive overview of the percolation scheme covering various vibrations addressed in a Raman experiment (the purely-mechanical TO modes as well as the polar LO and phonon-polariton ones), supported by *ab initio* calculations.

### Biography

Olivier Pagès has completed his PhD in Solid State Physics on "Study by Raman scattering of the electronic band bending at the interface between semiconductor compounds" from Université Paul Sabatier (Toulouse III, France). He then conducted Postdoctoral studies at the Birkbeck College (London University, UK) for 1.5 years on "Dielectric approaches of percolation phenomena occurring in highly complex binary polymeric mixtures of the insulating-conducting type". He is presently the Director of the Laboratoire de Chimie et Physique – Approche Multi-Echelle des Milieux Complexes (LCP-A2MC) de l'Université de Lorraine (Nancy-Metz, France). His field of research is concerned with the introduction of a percolation-based approach for the very basic understanding of the vibrational properties of the mixed crystals that can be viewed as the most simple out of complicated systems. He has published more than 65 papers in reputed journals on the subject.

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## NANOSTRUCTURED AND NANOCOMPOSITE MATERIALS FOR ENERGY CONVERSION

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To overcome the degradation of component materials over time, that are still hindering the widespread adoption of Proton Exchange Membrane Fuel Cells (PEMFC), novel materials and original methods of elaboration are needed. Our approach is based on the use of nanofibres and their multiscale assembly to produce innovative energy materials with specific architectures and interfaces, and improved properties. Such materials are prepared with the versatile, cost-effective and up-scalable electrospinning technique. The nanometre size and the 1D morphology of the fibres and the porous structure of the obtained web are expected to bring associated advanced properties, in particular with regard to directional and mechanical properties and mass transport, with beneficial effects on the performance and lifetime of the resulting membrane-electrode assemblies. Due to its inherent adaptability and applicability, electrospinning can be applied to all stages of the preparation of PEMFC core materials, from electrolyte membranes to electrodes. On the one hand, we are developing composite ionomer membranes based on electrospun webs of inorganic materials and polymers, as well as their chemical functionalization, which demonstrated to reinforce the membranes while keeping high proton conductivity; on the other hand, we are preparing nanofibrous electrocatalyst supports including carbon, metal, metal carbide, oxide nanofibres and nanotubes with extended durability and high electrical conductivity. In parallel, we are developing Pt deposition techniques leading to extended metal surfaces onto the electrospun materials, including Ni and Cu galvanostatic displacement, self-terminated Pt electrodeposition and electrochemical atomic layer deposition. These novel morphologies will enable higher platinum exploitation and increased stability. The assembly of these materials will allow the development of a new generation of PEMFC materials in which the components are fabricated entirely by electrospinning and with the possibility of scale-up at industrial level.

### Biography

Sara Cavaliere is Lecturer at the University of Montpellier, Institut Charles Gerhardt for Molecular Chemistry and Materials since 2009. She received her PhD in Chemistry and Materials Science in 2006 in Versailles, France, after graduating from University of Milan, Italy. She worked as Postdoctoral Fellow at the University of Freiburg, Germany, and Lyon, France. Her research interests focus on design, synthesis and characterisation of nanostructured and nanofibrous materials for proton exchange membrane fuel cells and water electrolyzers. In 2017 she was awarded the CNRS Bronze Medal and joined the Institut Universitaire de France as a Junior Member.

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## HARNESSING MULTIPOLAR INTERACTIONS AT THE NANOSCALE: A NOVEL OPPORTUNITY FOR MOLECULAR PHOTONICS AND BIOIMAGING

**Mireille H Blanchard Desce<sup>1</sup>**

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In the last decades inorganic nanoparticles have attracted growing attention in the field of nanophotonics, especially for bioimaging purposes. Among them, luminescent metal-, semiconductor- or oxide-based hard nanoparticles have been the most widely used. Yet, they raise concern with respect to toxicity and/or degradability issues. In that context, purely organic fluorescent nanoparticles hold foremost promises. With that goal in mind, we have developed original bottom-up strategies towards biocompatible ultrabright molecular-based nanoparticles specifically engineered as nanotools for bioimaging. Our strategy is based on the design/synthesis of dedicated multipolar dyes as interacting building blocks of nanoparticles which are readily prepared using expeditious and green protocols involving self-aggregation/nanoprecipitation of the dyes in water. Manipulation of molecular confinement of such engineered dyes provides an effective and innovative way to tune and enhance the luminescence and nonlinear optical responses of the nanoparticles by controlling and taking advantage of interchromophoric electrostatic interactions. This route led to biocompatible, ultra-bright pure nanoparticles that combine unprecedented brightness, remarkable colloidal stability and absence of toxicity, providing superior substitutes to quantum dots. Their luminescence can be tuned in the whole visible down to the NIR region. These nanoparticles can be used as ultra-sensitive contrast agents for *in vivo* two-photon angiography in small animals. Moreover, hyper-bright NIR-emitting nanoparticles (named HiFONs) of controlled size which show unprecedented photostability and excellent biocompatibility can be successfully imaged and tracked at the single particle level in water and used as nanotools in multicolor single particle tracking at video rate experiments to explore cellular compartments. Finally, nanointerfacial field promoted fluorescence amplification has been demonstrated for the first time in core-shell binary nanoparticles made from dedicated complementary dyes. This intriguing phenomenon opens a new avenue in the field of molecular nanophotonics.

### Biography

Mireille H Blanchard-Desce after studies at Ecole Normale Supérieure in Paris, has completed her PhD from University Pierre and Marie Curie under the supervision of Jean-Marie Lehn at the College de France and Postdoctoral studies at the Institute of Physical Chemical Biology in Paris. She is currently the Head of the molecular photonics and imaging team at the Institute of Molecular Science in Bordeaux University. She has an excellent track record in her research field as evidenced by over 260 publications in reputed journals with H index: 56, 6 book chapters, 7 patents, over 100 invited lectures at conferences and awards.

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## SYNTHESIS AND REACTIVITY OF BROMOCYANOBUTADIYNE: FROM INTERSTELLAR CHEMISTRY TO ORGANIC SYNTHESIS METHODOLOGY

Yann Trolez

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Some cyanopolyynes (the formula of which is  $R-(C\equiv C)_n-CN$  with  $R = H$  or  $Me$ ) have been detected in the interstellar medium (ISM) and on titan for some of them. Our laboratory has been studying from several years these compounds by synthesizing them and studying their chemical or photochemical reactivity. However, despite the low number of atoms these compounds possess, their synthesis in laboratory still remains a scientific challenge. Thus, we have recently described a synthetic pathway for cyanopolyynes having two conjugated  $C\equiv C$  triple bonds ( $n=2$ ), but their superior counterparts ( $n=3$ ) stay elusive so far. To solve this problem, we synthesized the bromocyanobutadiyne (5-bromopenta-2,4-diyne;  $Br-C\equiv C-C\equiv C-CN$ ) and reacted it with different terminal alkynes under Cadiot-Chodkiewicz conditions. Surprisingly, the corresponding cyanopolyynes were not obtained but more complex compounds, resulting from cascade reactions, were isolated. In particular, a diene was obtained stereoselectively when using monoacetylenic reactants. When using triisopropylsilylbutadiyne, a functionalized benzofulvene was obtained. The characterization of these unexpected products is based on X-ray crystallography, among other usual techniques. The mechanisms of formation of these products, which were studied both experimentally and theoretically, will be discussed.



Figure1: Reactivity of bromocyanobutadiyne with triisopropylsilylacetylene and triisopropylsilylbutadiyne.

## Recent Publication

V Vuitton, R V Yelle and V G Anicich (2006) The nitrogen chemistry of titan's upper atmosphere revealed. *Astrophys. J.* 647(2):L175-L178.

Y Trolez and J C Guillemin (2005) Synthesis and characterization of 2,4-pentadienenitrile - A key compound in space science. *Angew. Chem. Int. Ed.* 44:7224-7226.

N Kerisit, L Toupet, Y Trolez and J C Guillemin (2013) Methylcyanobutadiyne: synthesis, X-ray structure and photochemistry; towards an explanation of its formation in the Interstellar Medium. *Chem. Eur. J.* 19:17683-17686.

N Kerisit, C Rouxel, S Colombel Rouen, L Toupet, J C Guillemin and Y Trolez (2016) Synthesis, chemistry, and photochemistry of methylcyanobutadiyne in the context of space science. *J. Org. Chem.* 81:3560-3567.

N Kerisit, L Toupet, P Larini, L Perrin, J C Guillemin and Y Trolez (2015) Straightforward synthesis of 5-bromopenta-2,4-diyne nitrile and its reactivity towards terminal alkynes: a direct access to diene and benzofulvene scaffolds. *Chem. Eur. J.* 21:6042-6047

## Biography

Yann Trolez has completed his PhD in 2010 from the University of Strasbourg under the guidance of Jean-Paul Collin and Jean-Pierre Sauvage where he worked on rotaxane-based molecular machines. He then moved to ETH Zürich in François Diederich group as a Postdoctoral Fellow where he worked on alleno-acetylenic compounds bearing interesting optoelectronic properties. In 2011, he was appointed as Assistant Professor at the Ecole Nationale Supérieure de Chimie de Rennes where he now works on organic interstellar chemistry and on new cyanated compounds having interesting optical properties. He has published about 30 papers in peer-review international journals.

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## NANOMATERIALS: IN BETWEEN TRADITIONAL CONCEPTS OF UNDERSTANDING MATTER

**Emil Roduner**

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**W**e classify macroscopic amounts of matter according to various concepts, as metals, semiconductors, insulators, atoms, molecules, complexes, polymers, and so on. Each of these terms triggers a specific image that has a consistent meaning throughout the scientific community. But which of these describe adequately an isolated nanocluster like Pt<sub>13</sub>? We use Newtonian mechanics to describe the frictionless, periodic motion of a system consisting of a few particles, and we can give trajectories and the momentum of every particle at each instant of time. In contrast, systems consisting of large numbers of particles are treated thermodynamically as ensembles in which the information of individual particles is lost and available only as a statistical average. Spontaneous processes occur under heat dissipation, are not normally periodic and approach an equilibrium characterized by a minimum in free energy. Is Newtonian mechanics or thermodynamics more appropriate for treating nanoclusters? Many of the concepts that we use to describe macroscopic amounts of matter break down for nanomaterials. Metals turn into semiconductors and insulators; phase transition temperatures shift dramatically, and the transitions broaden and disappear completely so that the Gibbs phase rule loses its meaning. Heat and temperature that are normally understood to represent kinetic energy are no longer well defined. According to traditional definition we may find that a small system cools down instead of heating up when we deposit more energy on it, pretending a negative heat capacity. Small systems are getting increasingly relevant in chemistry and physics, e.g. in catalysis, molecular electronics or energy devices. It is here where one starts to find amazing and perhaps disturbing phenomena, and these are becoming a hot field of research. Even in an expected thermodynamic system one may find quantum phenomena. The question comes up how we manage the transition between unexpectedly incompatible descriptions.

### Biography

Emil Roduner studied Chemistry at the University of Zürich and at the Rensselaer Polytechnic Institute in Troy, NY. In 1988, he was awarded the Werner Prize by the Swiss Chemical Society for developing muon spin resonance to a universal method for studying structure and reaction behaviour of free radicals. During 1995-2012 he held a Chair of Physical Chemistry at the University of Stuttgart. After retirement he accepted a part-time Professorship at the University of Pretoria in South Africa. He wrote an advanced textbook, *Nanosopic Materials: Size-Dependent Phenomena and Growth Principles* (RSC, 2014). His research interests include studies on structure, size-effects and magnetism of platinum nano-clusters and dynamics of molecules in the pores of zeolites, mechanisms of elementary steps in catalysis, kinetic isotope effects, degradation and proton conductivity of fuel cell polymer membranes. In South Africa, he is working on the electrochemical conversion of CO<sub>2</sub> to liquid fuels using solar energy.

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## THE IPPI-DB INITIATIVE

### Olivier Sperandio<sup>1,2</sup>

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<sup>2</sup>Inserm, French Institute for Health and Medical Research, France

**T**he iPPI-DB initiative consists of collecting pharmacological data and gaining knowledge about protein-protein interaction (PPI) modulators. First, it provides the scientific community with a set of web-based tools, both chemical probe-centric and target-centric, to query our iPPI-DB database of PPI modulators. Second, it uses this data collection into adapted chemoinformatics technologies as a mean to identify the physico-chemical properties and the privileged chemical substructures that can facilitate the modulation of PPI targets. This presentation will describe the full re-foundation of our database and of the last developed tools to query it as well as our last results about the design of PPI-tailored libraries and of privileged chemical structures for PPI. During the speech, I will also describe our new web application for maintaining iPPI-DB which has been designed for remote contribution in order to build a community of contributors and co-authors.

### Biography

Olivier Sperandio has more than 15 years of experience in Bioinformatics and Drug Design. He obtained his Master's degree from the University of Alabama at Birmingham in Biochemistry and Bioinformatics during a 3-year stage in the US in the lab of Dr. Stephen C. Harvey. Then, he obtained an industrial PhD at the company MEDIT SA in partnership with the University Paris Descartes (Lab of Pr. Christiane Garbay) in virtual screening, in silico drug design and the design of computational chemistry tools. He was then recruited Junior Researcher at the Inserm as a Drug Designer within the Inserm CDithem. In 2010, he was recruited as a Senior Research Associate (CR1) at the Inserm within the lab of Dr. Bruno Villoutreix with the project of characterizing the chemical space of Protein-Protein Interaction inhibitors. He is now Group Leader in Chemoinformatics in the structural bioinformatics unit of Pr. Michael Nilges at Institut Pasteur in Paris.

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## ELECTROCHEMICAL REACTIONS BASED ON [60] FULLERENE DERIVATIVES

## Guan-Wu Wang

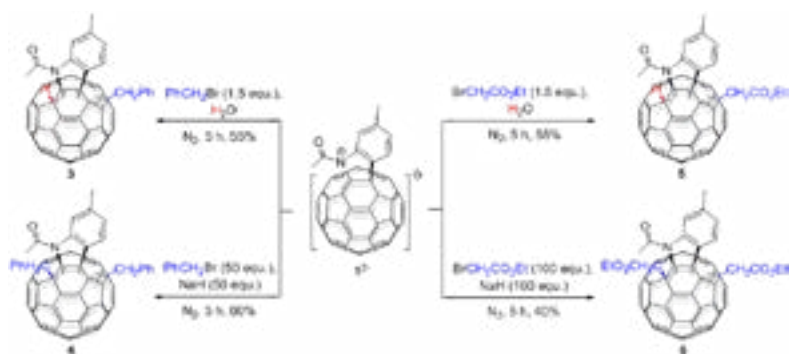
University of Science and Technology of China, China

Electrochemical organic reactions have attracted increasing attentions of organic chemists. Fullerenes and their derivatives are electron-deficient molecules, and therefore they are electrophiles. If they are reduced by controlled potential electrolysis (CPE) and thus would undergo an umpolung process, the formed negatively charged fullerenes and fullerene derivatives are nucleophiles. I will present our recent progress in the electrochemical reactions of fullerene derivatives. Several types of natural fullerene derivatives, which were synthesized by the methodologies developed by us, can be reduced to dianionic species by CPE. The formed dianionic species can then react with different electrophiles such as benzyl bromide, ethyl bromoacetate, diethyl bromomalonate, acyl chlorides, and chloroformates to provide new functionalized fullerenes with new addition patterns.

## Biography

Guan-Wu Wang is currently a full time Professor at the University of Science and Technology of China. He obtained his BS, MS and PhD from Lanzhou University in 1987, 1990, 1993, respectively. He then did his Postdoctoral work at Fudan University, Kyoto University, University of Kentucky, University of Chicago and Yale University. In May of 2000 he joined the University of Science and Technology of China as an awardee of the "Hundred Talents Program" of the Chinese Academy of Sciences (1999). He was awarded a National Science Fund for Distinguished Young Scholars (2001). He currently serves an Editorial Board Member of *Chinese Science Bulletin*, *Chinese Journal of Organic Chemistry*, *Mini-Reviews in Organic Chemistry*, *Current Organocatalysis*, *Acta Chimica Sinica*, and *Current Organic Chemistry*. He has published over 200 scientific papers. His research interests include fullerene chemistry, mechanochemistry and C-H activation reactions.

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## X-RAY STANDING WAVE TECHNIQUE APPLIED IN THE CHARACTERIZATION OF PERIODIC MULTILAYERS

**Meiyi Wu<sup>1,2</sup>, Karine Le Guen<sup>1,2</sup>, Jean-Michel André<sup>1,2</sup> and-  
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**W**e apply X-ray standing wave technique on multiple spectroscopic methods to characterize the structure of the periodic multilayers which are designed as reflecting mirrors for radiations of certain wavelengths. In this work, we have performed X-ray fluorescence spectroscopy (XRF), hard X-ray photoelectron spectroscopy (HAXPES) and particle induced X-ray emission (PIXE) in order to generate the X-ray standing waves (or Kossel diffraction in the case that the standing waves are due to the interference of the X-ray emission) within the nano scale periodic multilayers or so-called superlattices. The effect of the standing wave can be studied by observing the variation of the spectroscopic intensities as a function of the angle between the surface of the multilayer and the incident radiation/particle beam. Such angular dependence of the spectra provides a depth profile of both elemental and chemical information of the multilayers. The experimental results are compared with theoretical calculations. A fine fit of them indicates a great potential of these characterization methods, of which the PIXE-Kossel method is originally designed by our research group.

### Biography

Meiyi Wu has obtained his bachelor degrees in physics and applications in 2012 from both Wuhan University and Université Claude Bernard Lyon 1. He obtained his master degree in sciences of materials and nano-objects in 2015 from Université Pierre et Marie Curie (Sorbonne Université today). He has been studying as PhD student in Laboratoire de Chimie Physique - Matière et Rayonnement of Sorbonne Université since 2015 and is expecting to obtain his PhD in 2018. During two years, he has published 4 papers in journals and 4 conference papers. He has contributed in multiple international conferences with posters and oral presentations, including an invited talk.

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## ACTUAL ISSUES OF MONITORING THE CONTENT OF SYNTHETIC DYES IN FOOD PRODUCTS IN THE REPUBLIC OF BELARUS USING MODERN ANALYTICAL METHODS

**Palianskikh A<sup>1</sup>, Belyshava L L, Fiodarava T A, Sychik S I and Shevchuk L M**

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**F**ood dyes are widely used in the food industry to give products attractive appearance. Currently there are over 50 such food colourings of natural and synthetic origin. In the Republic of Belarus (RB) and in the countries of the Eurasian Customs Union (CU) 13 synthetic dyes are allowed to be used in the foodstuffs production. In accordance with the existing sanitary and hygienic requirements the content of each of these 13 substances is controlled and should not exceed 50 - 500 mg / kg depending on the nature of the dye and the foodstuff's type. At the same time it is completely forbidden to use synthetic dyes for baby food production. It should be noted that until now there are no uniform approaches for assessing the safety of synthetically produced dyes. As the result in some countries certain synthetic dyes are included in the list of banned substances as dangerous food additives, while in the others the same dyes are still used in food industry. Studies on the discovery of synthetic dyes impact on the human organism are continuing till now and scientists establish more and more new facts concerning the negative impact of some dyes on human health. In this regard, controlling the content of synthetic dyes in food products is an important and urgent task. Today in the Republic of Belarus and in the countries of the Customs Union there is no reliable analytical method which would allow determining all the regulated synthetic dyes in all kinds of food products rapidly and with appropriate repeatability and high accuracy. Thus the aim of this study was to develop a unified method for the simultaneous determination of 17 synthetic dyes in all kinds of food products by high performance liquid chromatography (HPLC).

### Biography

Palianskikh Alena has completed her PhD at the age of 35 from Belarusian State University. She is a senior researcher of the Laboratory of Food Chemistry in Republican Unitary Enterprise "Scientific Practical Center of Hygiene", Minsk, Belarus. The sphere of her interests is analytical chemistry, extraction of organic compounds, chromatographic methods of analysis. The activity of the laboratory is aimed at control the quality and safety of food products produced in the Republic of Belarus and imported to its territory from different countries. She has published more than 10 papers in reputed Belarusian and Russian journals.

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# DAY 2

Scientific Tracks & Abstracts



EuroSciCon Conference on

# Chemistry 2018

February 19-20, 2018



# DAY 2

February 19-20, 2018

## Sessions

Material Science and Chemistry | Environmental Chemistry | Physical and Theoretical Chemistry | Medicinal & Pharmaceutical Chemistry | Organic Chemistry | Polymer Chemistry | Electro-Analytical Chemistry | Spectroscopy |

**Session Chair**  
**Pradeep Varadwaj**  
The University of Tokyo, Japan

**Session Co-Chair**  
**Frédéric Bihel**  
University of Strasbourg, France

### Session Introduction

- Title:** Photovoltaic perovskites  
**Pradeep Varadwaj**, The University of Tokyo, Japan
- Title:** Evaluation of the adsorption efficiency of modified clinoptilolite zeolite in the extraction of hexavalent chromium ions  
**Bruno Ladeira**, Integrated College of Aracruz, Brazil
- Title:** Pulse-induced optoelectronic response of molecular junctions  
**Katawoura Beltako**, Aix-Marseille University, France
- Title:** Carbon dioxide sorption properties of fly ash zeolites differentiated in case of synthesis process  
**Natalia Czuma**, AGH University of Science and Technology, Poland
- Title:** Evaluation of analgesic and sedative activities of *Berberis baluchistanica* extract  
**Imdad Ullah**, University of Balochistan, Pakistan
- Title:** Modification and progressive advancement in the field of electrochemical sensors  
**Karamjeet Kaur**, Punjabi University Patiala, India
- Title:** Mimetic peptides based on promiscuous enzyme as asymmetric catalyst in aldol and michael reactions  
**Saadi Bayat**, Tofigh Daru Research & Engineering Pharmaceutical Company, Iran
- Title:** Density functional theory study of interaction of some halogen acids with polyaniline emeraldine salt gas sensor  
**Ayesha Ashraf**, University of the Punjab, Pakistan
- Title:** Physical properties and antimicrobial activity of chitosan with monoterpene phenols  
**Ozge Kurt**, Anadolu University, Turkey
- Title:** A source of new diagnostic techniques for asthma  
**Katrina Hutchinson**, The National University of Ireland Galway, Ireland

EuroSciCon 

Chemistry 2018

## PHOTOVOLTAIC PEROVSKITES

### Pradeep R Varadwaj<sup>1, 2</sup>, Arpita Varadwaj<sup>1, 2</sup> and Koichi Yamashita<sup>1, 2</sup>

<sup>1</sup>The University of Tokyo, Japan

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**H**alide perovskites are the centre of many recent studies in areas as diverse as chemistry, physics, chemical engineering, materials science and nanotechnologies. They are materials to develop photovoltaic technology for solar energy. To this end, I will briefly discuss the recent research progress in this field and introduce some newly modelled hypothetical  $\text{BMY}_3$  perovskite compounds in 3D that display band structures, octahedral tilting, materials properties, electronic structures and stabilities that are analogous with the most studied methylammonium lead triiodide solar cell semiconductor. Various featured aspects of these materials such as Rashba splitting, as well as the importance of hydrogen-, halogen- and other noncovalent bonding interactions will be discussed to demonstrate how important are they for the design of such highly valued functional materials. A brief discussion will be provided on factors that influence the degradation of these materials.

#### Biography

Pradeep R Varadwaj completed his PhD in 2008 from Saha Institute of Nuclear Physics (Jadavpur University, Kolkata, INDIA). Okayama National University (JAPAN) has conferred on him a DSc degree in the mid of 2011. He has travelled many countries such as Japan, Canada, Taiwan and South Africa for his Postdoctoral studies. He was a recipient of several of prestigious fellowships, of which the notable ones are JSPS (JAPAN) and Quebec Merit Scholarships (Canada) for foreigners. He is serving as a Senior Research Professor in the Department of Chemical System of the University of Tokyo, Japan since September 2015. His areas of expertise are spectroscopy, noncovalent interactions and materials science. His current research is centred on the theoretical investigations diverse chemical compounds, essential for the fundamental understanding of their chemistry; particularly on the modelling of halide perovskite solar cells. He has published more than 40 papers in reputed journals and has been serving as a reviewer for many journals of international repute.

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## EVALUATION OF THE ADSORPTION EFFICIENCY OF MODIFIED CLINOPTILOLITE ZEOLITE IN THE EXTRACTION OF HEXAVALENT CHROMIUM IONS

**B C Ladeira, J Vassoler, L M D Santana Rocha, T F Bottan  
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The inappropriate disposal of wastewater with hexavalent chromium ions has been causing risks to human health, the environment and industries. The present study aims to minimize the concentration of dichromate ions in contaminated effluents using the adsorption technique to remove ions. Adsorption tests in batch were performed using natural clinoptilolite zeolite in its activated and functionalized form, where it was possible to evaluate the efficiency through the removal of contaminating material. The zeolite modification in order to improve substantially its activity and selectivity was made through the activation with NaCl and the functionalization with BaCl<sub>2</sub>. The modified zeolite was added in a kitassato with a dichromate solution and stirred with the aid of a magnetic stirrer. The analysis of the ions adsorption efficiency was determined with statistical support of the center composite rotational design (CCRD), where the best conditions for three factors was tested. The adsorption efficiency factors and levels studied was the adsorbent particle size (ranging from 0.128 mm to 2.03 mm), the adsorbent material mass (ranging from 1 g to 5 g) and the contact time between zeolite and the solution (ranging from 0.5 h to 2 h). For the chromium ions adsorption, the best condition found was using particles with of 0.128 mm, zeolite mass in 3 g and contact time in 1.25 h at room temperature. The initial chromium concentration of 25 ppm was based on actual values of wastewater effluents in which the zeolite would be used after an initial effluent treatment by precipitation. The application of this adsorbent under the studied conditions for the removal of hexavalent chromium is sufficient to meet the resolution of the National Council for the Environment, CONAMA n° 430, which the valid limit for hexavalent chromium is 0.1 ppm. The chromium sample analysed, reached a 99.6% removal as result, it was possible to reach a final concentration of 0.089 ppm, which is in accord with the limit established by the Brazilian legislation. The concentration of hexavalent chromium ions present in the sample was determined by the 3500-Cr (Colorimetric) analysis method of the Standard Methods for the Examination of Water and Wastewater (1992). The adsorption isotherm which best represented a hexavalent chromium adsorption, under the used conditions, was Langmuir, where in concentrations between 10 and 500 ppm, resulted in R<sup>2</sup> of 0.96 and Q<sub>max</sub> of 13.64 mg/g which is close to Q<sub>exp</sub> of 12.65 mg/g, indicating that the hexavalent chromium adsorption on the solid is a propitious physical process.

### Biography

B C Ladeira has recently completed his graduation in Chemical Engineering from Faculdades Integradas de Aracruz – FAACZ and currently pursuing his Postgraduation in Production Engineering at Universidade Cândido Mendes – UCAM. He has worked as a Research Assistant in the development laboratories of Fibria Celulose SA in Brazil, working with cellulose pulping and bleaching, physical paper assays and nanocellulose pilot plant. Currently, he is a trainee in the field of drug product development at Hovione FarmaCiência SA in Portugal.

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## PULSE-INDUCED OPTOELECTRONIC RESPONSE OF MOLECULAR JUNCTIONS

**K Beltako, N Cavassilas, L Raymond and F Michelini**

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**B**ased on quantum many-body transport formalism, we analyse the quantum dynamics of a donor-acceptor molecule sandwiched between two metallic electrodes throughout the effects of metal-molecule coupling, Coulomb and exciton interactions, and pulse intensity. The photocurrent reveals internal frequencies of the system emerging from a non-equilibrium reorganization of the molecular orbitals which manifests itself in unexpected features of the dynamical electronic structure. Indeed, the time-resolved local density of states we define exhibits two types of signature: a dynamical Rabi shift and Floquet-like states generation. Our combined theoretical-numerical methodology is of strong interest for ultrafast photocurrent spectroscopy, and it also opens avenues toward the possibility of controlling or analysing the internal quantum properties of nanosystems by means of pump-push photocurrent spectroscopy.

### Biography

K Beltako is about to complete his PhD from Aix-Marseille University (AMU) and is Graduated from AMU excellence Master's Program P3TMA. He is working to develop an efficient and faster numerical technique to handle various aspects of time-dependent quantum transport in nanodevices.

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## CARBON DIOXIDE SORPTION PROPERTIES OF FLY ASH ZEOLITES DIFFERENTIATED IN CASE OF SYNTHESIS PROCESS

**N Czuma, K Szczurowski, K Zarębska and P Baran**

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**Z**eolite synthesis out of fly ash is a worth noticing, low budget alternative for the production of zeolites compared to natural zeolites or zeolites produced from pure chemicals. Generally, zeolites due to their structure represent interesting properties (ion-exchange, catalytic, sorptive). Based on the sorption properties it is possible to use this material as a sorbent for flue gases impurities such as carbon dioxide. Energy sector in Poland is mainly based on burning of brown and hard coal. Environmental concerns and legal aims oblige to reduce the emission of greenhouse gases emitted to the atmosphere. Due to restrictions on the emission limits, it is crucial to search for differentiated methods for CO<sub>2</sub> capturing adapted for the economy new needs. The use of zeolites such as sorbent in the industrial processes may have a positive ecological result, not only due to the elimination of disadvantages of commonly used CO<sub>2</sub> capture absorption methods, but also due to the usage of waste material as a raw material for the synthesis. Fly ash zeolites may be synthesised by different methods which affect the final product. It influences the type and amount of zeolite present in the synthesized sample and in this way the sorption properties of synthesized materials. In this work, the comparison of CO<sub>2</sub> sorption of 3 fly ash zeolites samples synthesized by differentiated methods were presented. Synthesis methods chosen were: hydrothermal method, fusion method and modified two-step method. Results indicated different sorption capacity due to zeolite type present, synthesis efficiency and for similarities in isotherm shapes connected with the presence of micropores.

### Biography

N Czuma is a PhD student at AGH University of Science and Technology in Kraków, Poland. Her PhD work focuses on fly ash synthesis and its sorption properties in relation to CO<sub>2</sub> and SO<sub>2</sub>. Additionally, her scientific interest focuses on other fly ash uses such as carbonation processes and geopolymer synthesis. She is a member of InnoEnergy PhD School. She had participated in national and international internships including cooperation with EDF Poland S A, Lublin University of Technology, UPC-Universitat Polytechnica de Catalunya and Université Pierre et Marie CURIE.

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## EVALUATION OF ANALGESIC AND SEDATIVE ACTIVITIES OF BERBERIS BALUCHISTANICA EXTRACT

**Imdadullah<sup>1,2</sup>, Muhammad Younis<sup>3</sup> and Shafi Muhammad<sup>4</sup>**

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<sup>4</sup>Department of Pharmacology, Faculty of Pharmacy and Health Sciences, University of Balochistan Quetta Pakistan

**T**he current study was carried out on a crude ethanolic extract of bark and stem of *Berberis baluchistanica* and this plant is endemic to Balochistan. *B. baluchistanica* caused in traditional medicine. Plant was collected from local market and ethanolic extract was carried out. The ethanolic extract was tested for Analgesic and seductive effect. Extract produced significant analgesic effects at the dose of 500 mg/kg in the acetic acid induced writhing test and the formalin test. Sedative effect were determine by traction test and forced swimming test. In traction test time taken by the mice to travel iron rod was significantly increased. In forced swimming test mobility time was significantly decreased. Results were significantly comparable with standard drug diazepam. In conclusion, results suggest that the ethanolic extract of *B. baluchistanica* possess significant analgesic effects also possess sedative effects.

### Biography

Imdadullah is an M.Phil Scholar in Pharmacy Department, University of Balochistan, Quetta Pakistan. After completion of his graduation from the same university he joined the Government Services as Drug Inspector in Health Department, Government of Balochistan Quetta. Since last two years he is serving in the public sector as Secretary Provincial Quality Control Board Balochistan, Quetta.

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## MODIFICATION AND PROGRESSIVE ADVANCEMENT IN THE FIELD OF ELECTROCHEMICAL SENSORS

**Karamjeet Kaur and Jatinder Singh Aulakh**

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The progressive transformation in the field of electrochemical sensors has enhanced the great curiosity in the area of analytical chemistry. The recent advances in the field of electroanalysis i.e., applying electrodes modification by different type of materials such as ligands, conducting polymers, carbon paste, nanomaterials, nanocomposites, nanostructures (CNT, graphene), metallic nanoparticles or magnetic beads, molecular imprinted polymers etc., create the interest in designing electrochemical sensors. Numerous applications has been developed to date consist of voltammetric detection, electrochemical stripping analysis, electrochemiluminescence, as well as electrochemical biosensors and potentiometric sensors show promising progress in selection, binding or transduction characteristics and grasp the requirement goal for environmental control. These modifications have encouraged the field for exciting new potentials and approaches.

### Biography

Karamjeet Kaur is doing her PhD in the field of Analytical Chemistry with research topic "Electrochemical Sensors", from Department of Chemistry, Punjabi University, Patiala, India. She has done projects during her MSc and MPhil. She has 2 publications, 1 book chapter (in press) and communicated 4 articles in reputed journals.

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## MIMETIC PEPTIDES BASED ON PROMISCUOUS ENZYME AS ASYMMETRIC CATALYST IN ALDOL AND MICHAEL REACTIONS

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**B**iocatalysis has emerged as an elegant and green tool for modern organic synthesis due to its high efficiency, good selectivity and environmental acceptability. Although, an enzyme is capable of catalyzing a specific reaction effectively, some unexpected experimental results have indicated that many enzymes are catalytically promiscuous. Mimetic peptides based on enzyme as a kind of important chiral scaffold are broadly identified for their obvious advantages, diverse structures and readily accessibility. Based on promiscuous aldo-keto-reductase enzymes, several mimetic peptides were designed which were synthesized and tested as multifunctional organocatalysts in direct asymmetric aldol and Michael reactions. The asymmetric aldol and Michael reactions, as the most prominent carbon-carbon bond formation reactions, are the central study issues in the field of asymmetric synthesis. In this study, promiscuous aldo-ketoreductase (AKR) is used to catalyze aldol reaction between aromatic aldehydes and ketones. Good yield (up to 75%), moderate enantioselectivity (60%), and high diastereoselectivity (dr) up to 93/7(anti/syn) were obtained. Several mimetic peptides from AKR's active site were designed and synthesized as asymmetric catalysts in the aldol and Michael reactions. The corresponding aldol products were produced with high yields (up to 97%) and excellent diastereoselectivities (up to 99/1) and enantioselectivities (up to 99.9) under mild reaction conditions. These peptides exhibit excellent catalytic activity in terms of yield, diastereoselectivity and enantioselectivity. The secondary structures of peptide catalysts provide an understanding of their mechanism.

### Biography

Saadi Bayat received his BSc in Applied Chemistry at Buali Sina University (Hamedan, Iran, 2000). He did his MSc in Organic Chemistry at Kharazmi University (Tehran, Iran, 2008). Later he enrolled for the PhD programme at Department of Chemistry, Faculty of Science of University of Putra Malaysia (UPM), under the supervision of Prof. Dr. Mohd Basyaruddin Abdul Rahman. The following year, he was offered scholarship from Graduate Research Assistance (GRA), UPM. Moreover, his research program focuses on mimetic peptide as asymmetric catalysis. He was as a Postdoctoral Research Fellow for a year (May 2014-June, 2015) in UPM. He had been selected to receive Endeavor or Scholarship from the Australian government and joined Dr. Bellinda Abott's group in La Trobe University, Melbourne (July 2015-January 2016). He has published almost 20 papers and has been serving as an Editorial Board Member in journals of repute.

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Ayesha Ashraf, J Org Inorg Chem 2018, Volume: 4  
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## DENSITY FUNCTIONAL THEORY STUDY OF INTERACTION OF SOME HALOGEN ACIDS WITH POLYANILINE EMERALDINE SALT GAS SENSOR

**Ayesha Ashraf**

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Based on density functional theory (DFT) calculations, the ability of a conducting polymer; polyaniline emeraldine salt (PAN-ES) as the sensor for HCl and HBr gas molecules have been investigated. The polymer structures are modelled theoretically through oligomer approach. The selectivity and sensitivity of PAN-ES (with 2-8 even number of oligomers) among two of the halogen acids are simulated at UB3LYP/6-31G (d) level. Various features like the energy of interaction, natural bond orbital and Mulliken charge analyses are also in line with the analysis from optimized geometric parameters to calculate the detecting ability of PAN-ES towards halogen acids in terms of charge transfer. Interaction energies between donor and acceptor molecules are calculated and corrected for basis set superposition error (BSSE). Comparatively larger forces of attraction among sensor and analyte were observed in *n*PAN ES-HBr complex as compared to *n*PAN ES-HCl. To find out the differences in IP, EA, charge separations between donors and acceptors and electron distribution in the acceptor units, spectral properties were analyzed. It is observed that electronic properties of *n*PAN ES are sensitive to the interaction of *n*PAN ES with HBr and HCl by calculating the energy gaps between HOMO and LUMO. The theoretical approach helps to conclude that polyaniline conducting polymers shows more selectivity towards HBr as compared to that for HCl and this outcome agrees with reported results based on experimental observations.

### Biography

Ayesha Ashraf has completed her M.Phil from Institute of Chemistry, Pakistan and PhD Studies from University of the Punjab, Pakistan. She has been received 3rd position in M.phil 2011-2013 Fall, Institute of Chemistry, University of the Punjab, Lahore, Pakistan. And DPCC Research scholarship awarded for 201. She has recently published 01 paper in reputed journals in short time.

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## PHYSICAL PROPERTIES AND ANTIMICROBIAL ACTIVITY OF CHITOSAN WITH MONOTERPENE PHENOLS

**Kurt O, Celebi H, Karaca N and Demirci F**

Anadolu University, Turkey

In the recent years, development of environmental awareness and eco-friendly plastic utilization has gained importance instead of petroleum-based synthetic plastics. Chitosan is a natural polymer obtained from deacetylation of chitin in various quality grades. It is nontoxic, biodegradable, biofunctional and biocompatible with antimicrobial characteristics. The film-forming property of chitosan has found many applications in tissue engineering, drug delivery and packaging. Monoterpenes are one of the major components of essential oils, which are fragrant blends derived from plants. Many of the monoterpenes are found in the nutrients of humans as well. In this present study, the monoterpene phenols, carvacrol and thymol were used for preparation of chitosan composite films to expand its use. Composite films have been prepared by stirring aqueous solution of chitosan and carvacrol/thymol in different ratios in the presence of diluted acetic acid and ethanol. *In vitro* antimicrobial activity evaluation as well as water-vapor permeability, solubility in water, pH measurement and moisture content of the films formed was conducted for characterization.

### Biography

Kurt O has completed her undergraduate education from the Gazi University followed by Postgraduate Studies at the Anadolu University in Chemical Engineering. She has been working on several scientific research projects for 2 years.

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## A SOURCE OF NEW DIAGNOSTIC TECHNIQUES FOR ASTHMA

**Katrina Hutchinson<sup>1,3</sup>, John Faul<sup>2</sup>, Michael Louw<sup>1</sup> and Yury Rochev<sup>3</sup>**

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**E**pidemiological studies have linked asthma with vitamin D deficiency (VDD). Asthma, like VDD, is highly prevalent in Ireland. Vitamin D receptor (VDR) gene polymorphisms have been associated with asthma and allergy susceptibility. The objective of this project is to set up new biochemical methods in a clinical laboratory for diagnosing and treating asthma, and to deepen our knowledge of the illness's pathophysiology. We successfully completed verification of the total 25-hydroxyvitamin D (25OHD or  $C_{27}H_{44}O_2$ ) assays on Abbott Architect. New tests for eosinophil cationic protein (ECP), IL10, IL17a, VDR, cathelicidin antimicrobial peptide (CAMP) and for 4 single nucleotide polymorphisms (SNPs) were employed for diagnostic and research testing. We found associations between vitamin D levels ( $C_{27}H_{44}O_2$ ) and airway obstruction in adults' asthma and body mass index in healthy Irish adults. A negative association was recorded between 25OHD and IgE levels in paediatric patients. In general we observed no significant benefit of vitamin D supplementation in asthmatics. However improvement in asthma control was noticeable in some patients with specific genotypes. We showed an association of TaqI and Apal polymorphisms of the VDR gene with a susceptibility to asthma in Irish patients. Also, we demonstrated that paediatric patients with TC for TaqI, and CC and CT genotypes for Apal have a significantly low level of IL-10 and increased white blood cells (neutrophils in particular), and that they were associated with poor asthma control. Vitamin D's role in respiratory disorders has not yet been fully investigated. Research is still at an early stage, but our preliminary results seem encouraging. Further and more extensive studies, using a larger sample, will be necessary to confirm our findings, to examine links between vitamin D and VDR gene polymorphisms in specific asthma phenotypes, and to investigate the possibility of using VDR SNPs as biomarkers for susceptibility to asthma.

### Biography

Katrina Hutchinson has a MD from Moscow State Medical University and she is currently completing her PhD in the School of Chemistry in the National University of Ireland, Galway. She has published several articles based on her research. Since 2000 she has been the Head of the Clinical Chemistry, Immunology, Serology and Molecular Biology departments at Eurofins-Biomnis, Ireland. She was short-listed by Enterprise Ireland for the Irish Scientist of the Year in 2013, and she has been an active participant in national and international conferences relating to Clinical Chemistry, Endocrinology and Immunology.

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