

# 7<sup>th</sup> World Congress on Chemistry

November 13-15, 2017 Athens, Greece

Plenary  
Day 1





## Wolfgang Tremel

Johannes Gutenberg University Mainz, Germany

### Inorganic nanoparticles as enzyme mimics


A long-standing goal of biomimetic chemistry is the design and synthesis of functional enzyme mimics. The past three decades have seen a wide variety of materials including metal complexes, polymers and other biomolecules that mimic the structure and function of naturally occurring enzymes. Among these, inorganic nanoparticles bear a huge potential, because they are more stable than their natural counterparts, while having large surface areas and sizes comparable to those of natural enzymes. Therefore, a considerable number of “artificial enzymes” derived from inorganic nanomaterials has been reported. We highlight recent progress in the field of enzymatically active inorganic nanomaterials. They are discussed based on nanoparticle properties in solution, particle uptake in cells and clearance and based on catalytic activities of nanoparticles compared to those of the natural enzyme. The aim of this overview is to determine - or even predict - which chemical type of

nanoparticles is of special interest for further research in enzyme mimetics. Of all nanoparticles discussed, vanadium oxide, molybdenum oxide, cerium oxide, magnetite nanoparticles and molybdenum oxide films showed catalytic activities and stabilities comparable or superior to those of natural enzymes. Some medical and biotechnological applications of enzyme mimics and some prospects for further research are outlined.

### Biography

Wolfgang Tremel studied chemistry and medicine at the universities in Bielefeld and Münster. He received his PhD in chemistry from the University of Münster in 1984. After postdoctoral stays at the Hahn-Meitner Institute in Berlin, the DESY/HASYLAB in Hamburg, Cornell University and Iowa State University he moved to Münster to complete his Habilitation. 1991 he joined the chemistry department in Mainz as an associate professor and was promoted full professor for inorganic chemistry in 1996. He has served several years as department chairman and as chairman of the materials science center. He has been an editorial board member of the Journal of Solid State Chemistry and Chemistry of Materials and an associate editor of the Journal of Solid State Chemistry. He is currently an associated editor of Dalton Transactions. He has  $\pi$ 400 publications that have been cited  $\pi$ 10000 times. His current publication h-index is 53.

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 Notes:

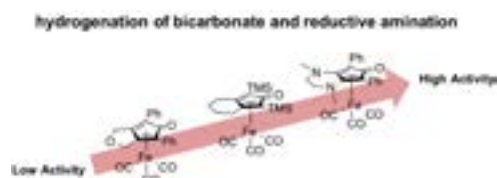


## Jean-Luc Renaud

University of Caen Normandy, France

### Bifunctional iron catalysts: synthesis and applications

Economic constraints and environmental concerns in chemistry have led to increased demand for the replacement of noble metals used in chemical processes by Earth-abundant ones. Iron-catalyzed reduction has received intensive attention and some iron complexes have shown activities and selectivity that are competitive with those of noble metals. However, exchanging noble metals for cheap, abundant, and biocompatible iron complexes to perform reduction is not the sole criterion to render such complexes attractive for industrial applications; the catalytic activities and the price of the ligand must also be taken into account. Based on a "transition metal frustrated Lewis pair" approach, cyclopentadienone iron tricarbonyl complexes have been designed. Their application in reduction and alkylation, as well as a detailed mechanistic study will be presented (Figure 1).



### Recent Publications

1. Bauer I and Knölker H (2015) Iron Catalysis in Organic Synthesis. *Chemical Reviews* 115:3170-

3387.

2. Renaud J L and Gaillard S (2016) Recent Advances in Iron- and Cobalt-Complex-Catalyzed Tandem/Consecutive Processes Involving Hydrogenation. *Synthesis* 48(21):3659-3683.
3. Moulin S, Dentel H, Pagnoux-Ozherelyeva A, Gaillard S, Poater A, Cavallo L, Lohier JF and Renaud J L (2013) Bifunctional (cyclopentadienone)iron-tricarbonyl complexes: synthesis, computational studies and application in reductive amination. *Chemistry - A European Journal* 19(52):17881-90
4. Thai T T, Mérel D S, Poater A, Gaillard S and Renaud J L (2015) Highly active phosphine-free bifunctional iron complex for hydrogenation of bicarbonate and reductive amination. *Chemistry - A European Journal* 21(19):7066-7070.
5. Mérel D S, Lohier JF, Gaillard S and Renaud J L (2013) Bifunctional Iron Complexes: Efficient Catalysts for C=O and C=N Reduction in Water. *ChemCatChem* 5:2939-2945.

### Biography

Jean-Luc Renaud obtained his Ph.D. degree in 1998 under the supervision of Aubert and Malacria (Paris VI University). He was a Lavoisier Postdoctoral fellow in 1999 with Lautens (University of Toronto) then moved to the University of Louvain-La-Neuve in the team of Prof. Riant. In 2000, he was appointed as Maître de Conférences at the University of Rennes and accepted a Professor position at the University of Caen in 2008. The research interests focus on organometallic catalysis (Fe, Co, Cu, Ru, Ir) and their application in fine chemical synthesis (hydrogenation, cycloaddition and coupling reactions).

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# 7<sup>th</sup> World Congress on Chemistry

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## Scientific Tracks & Abstracts Day 1

Chemistry World 2017



# Major Sessions:

Monday, November 13, 2017 | Day 1

Nano chemistry | Medicinal Chemistry | Organic Chemistry | Industrial Chemistry | Pharmaceutical Chemistry  
Atmospheric Chemistry | Physical Chemistry | Polymer Chemistry

## Session Chair

**Jean-Luc RENAUD**

Jean-Luc RENAUD, University of Caen Normandy, France

## Session Introduction

**Title: Synthesis of Novel Types of Nucleosides and Nucleotide Mimetics as Potential Anticancer Agents**

Nuno Manuel Xavier, Universidade de Lisboa, Portugal

**Title: Recent Experimental and Theoretical Developments of Ion Specific "Hofmeister" Phenomena**

Andrea Salis, University of Cagliari, Italy

**Title: Light, a powerful tool for the synthesis of metal nanoparticles and nanocomposites**

Lavinia BALAN, CNRS Institute of Materials Science of Mulhouse, France

**Title: Micro And Nano Molecularly Imprinted Polymers (Mips) For Analytical, Environmental And Forensic Applications**

Eduardo Pereira, University in Concepcion, Chile

**Title: Transition Metal Vinylidene Mediated Catalysis for Use in Organic Synthesis**

Chulbom Lee, Seoul National University, South Korea

**Title: A small molecule inhibitor of HSP70 has cytotoxicity against various cancers**

Injae Shin, Yonsei University, Korea

**Title: Porous support for phase change materials with integrated enhancement of thermal Conductivity and capacity**

Ge Wang, University of Science and Technology Beijing, China

**Title: Comparison of Different Sample Preparation Techniques for the Analysis of Small Molecules in Biological Fluids**

Sena Caglar Andac, Istanbul University, Turkey

**Title: Synthesis of heteroatomic thiazole-based copolymers for organic semiconductors**

Byanne Malluhi, Texas A&M University, Qatar

## Synthesis of novel types of nucleosides and nucleotide mimetics as potential anticancer agents

Nuno Manuel Xavier

University of Lisbon, Portugal

Synthetic nucleosides, nucleotides and their analogs or mimetics constitute relevant groups of molecules in medicinal chemistry, due to their propensity to exhibit biological activities. A number of compounds of these types are in clinical use against cancer and viral infections, acting through incorporation into nucleic acids and/or by inhibition of enzymes involved in their biosynthesis. However, some drawbacks limit their use, such as low oral bioavailability and the acquisition of resistance by cancer cells or virus towards their action. The development of novel bioactive nucleoside/nucleotide-like structures that may overcome these issues and act by innovative mechanisms of action remains of interest. Within this context, in this communication the synthesis of novel azido nucleosides, their phosphoramidates and of structurally diverse N-glycosyl derivatives containing D-glucuronamide moieties will be presented. Azido furanosyl and pyranosyl nucleosides were synthesized by N-glycosylation of purine or pyrimidine derivatives with azido 1-O-acetyl glycosyl donors and were subsequently converted into nucleoside phosphoramidates as potential mimetics of nucleoside monophosphates. 1-O-Acetyl glucuronamides were prepared and employed as precursors for the access to N-glycosylsulfonamides and N-glycosylphosphoramidates, in which the sulfonamide and the phosphoramidate moieties were planned as phosphate bioisosteres. N-Substituents of different polar character were introduced at C-6. Among the motifs installed was the benzyltriazole system, leading to novel types of potential nucleotide mimetics. Glucuronamide-based nucleosides as well as related N-glycosyl triazole analogs were also accessed. The evaluation of the compounds' antiproliferative effects on cancer cells revealed some active molecules at micromolar concentration range. Studies aiming at giving insight into the mode of action of the most potent compounds were performed. The synthetic methods and the results of the biological assays will be disclosed herein.

## Recent Publications

1. L P Jordheim, D Durantel, F Zoulim and C Dumontet (2013) Advances in the development of nucleoside and nucleotide analogues for cancer and viral diseases. *Nature Reviews. Drug Discovery* 12(6):447-464.
2. N M Xavier (2017) Recent advances on nucleotide analogs and mimetics: synthesis and biological properties in Elsevier Reference Module in Chemistry, Molecular Sciences and Chemical Engineering, DOI: 10.1016/B978-0-12-409547-2.12655-1.
3. M Serpi, V Ferrari and F Pertusati (2016) Nucleoside derived antibiotics to fight microbial drug resistance: new utilities for an established class of drugs? *Journal of Medicinal Chemistry* 59(23):10343–10382.
4. N M Xavier, R Gonçalves-Pereira, R Jorda, E Řezníčková, V Kryštof and M C Oliveira (2017) Synthesis and antiproliferative evaluation of novel azido nucleosides and their phosphoramidate derivatives. *Pure Appl. Chem.* 89(9):1267–1281.
5. N M Xavier, A Porcheron, D Batista, R Jorda, E Řezníčková, V Kryštof and M C Oliveira (2017) Exploitation of new structurally diverse d-glucuronamide-containing N-glycosyl compounds: synthesis and anticancer potential. *Organic and Biomolecular Chemistry* 15(21):4667-4680.

## Biography

Nuno M. Xavier (b. Nov. 1982, Vila Real, Portugal) graduated in Chemistry from the University of Lisbon in 2005. He received a dual Ph.D. degree in Organic Chemistry from the University of Lisbon and from the National Institute of Applied Sciences of Lyon (INSA Lyon) in 2011, where he worked in the development of new carbohydrate-based antimicrobial agents. He was afterwards a Postdoctoral Researcher at the University of Natural Resources and Life Sciences of Vienna (BOKU), where he focused on the synthesis of new heptose derivatives of antibacterial potential. After another post-doctoral period at the Faculty of Sciences, University of Lisbon, he became in 2014, Researcher (FCT Investigator) at this Institution. His scientific interests are within Organic and Medicinal Chemistry and are devoted to the development, using efficient synthetic methodologies, of new bioactive carbohydrate-containing molecules of potential therapeutic application. He has been particularly dedicated to the design and synthesis of structurally new nucleosides and nucleotide analogues as potential anticancer agents. His research activities have been reported in ca. 30 publications and are frequently presented and discussed in international scientific symposia.

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## Recent Experimental and Theoretical Developments of Ion Specific "Hofmeister" Phenomena

**Andrea Salis**

University of Cagliari, Italy

Ion specific phenomena are perhaps the longest unsolved puzzle of chemistry. About 130 years ago Franz Hofmeister observed that egg white proteins solubility was salt specific. He ordered the salts in an efficiency sequence universally known as the "Hofmeister series". During the 20<sup>th</sup> century a myriad of experiments showed that salt or, better, ion specificity is ubiquitous in chemistry (solution chemistry, colloidal science, electrochemistry) and biology. Unfortunately, our available theories of electrolytes (Debye-Hückel, 1923) and colloid stability (DLVO, 1941-1948) fail to explain and predict ion specificity. That is, LiI, NaCl, and CsF should behave in the same way because they are all 1:1 electrolytes. But they do not. In 1997 Collins proposed a phenomenological set of

rules known as the law of matching water affinities (LMWA). LMWA explains and predicts at a qualitative level the order of ion-ion and ion-surface site interactions. The same year Ninham proposed the inclusion of additional quantum mechanical dispersion forces acting on ions which are missing from conventional theories. Ion dispersion forces and LMWA approaches appeared to conflict. In this presentation some recent experimental results, based on turbidimetric and dynamic light scattering measurements of model protein systems, are shown. These results can be rationalized only by considering that both approaches are at work.

### Biography

Andrea Salis has completed his PhD at the age of 29 years from University of Cagliari, Italy. He is associated professor of Physical Chemistry and leads a research team focusing on Biointerfaces and Biocatalysis at the University of Cagliari. He has published 55 papers in peer review international journals and serving as an Associate Editor of the journal "Biocatalysis" (De Gruyter publisher).

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## Light, a powerful tool for the synthesis of metal nanoparticles and nanocomposites

**Lavinia Balan**

Institute of Materials Science of Mulhouse - CNRS, France

The size dependent properties of noble metal nanoparticles (MNPs) have created a great promise because of their use in a variety of optical, electronic and biomedical applications. Nowadays, a great diversity of techniques and methods were developed for their synthesis: chemical, thermal, photochemical or biological. Among them, the photochemical approach has proven an excellent tool to synthesize nanoparticles and also nanocomposites materials as well in the investigation of the mechanistic aspects of their formation. Moreover, this “green” and “highly flexible” approach allows a sharp spacial and temporal control of the chemical reactions. Thus, photochemistry is used to produce MNPs through the photo reduction of a metal precursor by transient species arising from the photocleavage of a radical generator in aqueous solution or directly on a glass surface in order to produce plasmonic surfaces. Improving the efficiency of the process and controlling the NPs morphology require a careful optimization of the photonic and chemical parameters. This innovative photochemical approach

was also used to design advanced nanomaterials such as metal/polymer nanocomposites. Hybrid nanocomposites were obtained by combining the in situ photoreduction with the photopolymerization of multifunctional acrylate monomers. In such systems, specific interactions between the macromolecular network and nascent particles was found to control the access of metal atoms to the different crystalline planes of the growing particles, which is necessary to obtain anisotropic nanoobjects. The ultimate step of this photochemical approach is concerned with the spatial assembling of MNPs in the polymer matrix. Thus, controlling both the synthesis and multi-scale organization (nano, micro and macro) of such cross-linked organic-inorganic nanomaterials opens promising prospects in the field of advanced materials.

### Biography

Lavinia Balan obtained her PhD degree from the University Henry Poincaré in Nancy, France, in 2005. Her PhD was devoted to the elaboration of an original material for the anode of Li-ion batteries. Since 2006, she is a CNRS Senior Researcher. Her lines of research are concerned with photo chemical synthesis and design of metal nanoparticles and metal/polymer nanocomposites for advanced applications. She holds five patents, published more than 90 papers in reputed journals and is a member of 10 editorial boards of journals in the field of nanomaterials and nanotechnology.

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## Micro and nano molecularly imprinted polymers (MIPS) for analytical, environmental and forensic applications

**Eduardo Pereira**

University of Concepción, Chile

New classes of organic pollutants including poly-aromatic hydrocarbons (PAHs), antibiotics, endocrine disrupting compounds (ECDs), pharmaceuticals, personal care products (PPCPs), and toxins coming from cyanobacteria, such as microcystin-LR, in very low concentration, part-per-trillion (ppt) range, have been identified. On the other hand, Forensic Chemistry is an area of the chemistry devoted to the analysis of several substances, most of the organic molecules, that might be important or might have been used in the commission of a crime. Forensic chemistry employs most of the analytical chemistry knowledge and tools to analyze evidence, such as fiber, paints, explosives, fire debris, glass, soil, documents, and firearms. Moreover, the enzyme-linked immunosorbent assay (ELISA) is used for quantitative determination of the analytes. The

disadvantages of this technology are the low stability of reagents, the need for refrigerated transport and storage, batch-to-batch (or clone-to-clone) variability, and the high cost of producing antibodies are often cited as problems. In this work we have developed materials and nanomaterials based on molecularly imprinted polymers containing the optimal combination of monomers, crosslinker, initiator and solvent, having high capability and selectivity of molecular recognition with ability to be used in solid phase extraction, analytical detection and quantitative diagnosis assay for target organic molecules coming from environmental and forensic samples.

### Biography

Eduardo Pereira has completed his PhD from University of Concepción, Chile. He is Full Professor and Dean of the Faculty of Chemical Science at University of Concepción. In addition, he is the current President of the Chilean Chemical Society (SCHQ) and Latin-American Federation of Chemical Associations (FLAQ). He is the leader of a research team focusing on to develop materials and nanomaterials with molecular recognition capability and the applications in analytical, environmental and forensic chemistry. He has published more than 70 papers in reputed journals, several book chapters and more than 150 communications in conferences, symposia and meetings.

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## Transition metal vinylidene mediated catalysis for use in organic synthesis

**Chulbom Lee**

Seoul National University, South Korea

Transition metal vinylidene is organometallic complexes derived from alkynes that are isomeric to more well-known pi- and sigma-alkyne complexes. Our laboratory has been engaged in the development of C-C bond-forming methods that make use of alkynes via mechanisms involving a transition metal vinylidene species as a catalytic intermediate. A wide range of new reactions has been developed, which include enyne cycloisomerizations, and various tandem processes effecting hydrative, alkylative, and carboxylative cyclizations. Recently, in a departure from these C-C bond forming cyclization processes, our explorations have been focused on the oxygen-transfer to

the metal-bound unsaturated carbene. This approach has led to the discovery of the alkyne oxygenative additions that occur through the intermediacy of a metallocetene arising from oxidation of the metal vinylidene. Discussed in this presentation will be the design, implementation and mechanistic studies of the oxygenative transition metal vinylidene-mediated catalytic reactions.

### Biography

Chulbom Lee has completed his PhD from Stanford University and Postdoctoral studies from Memorial Sloan-Kettering Cancer Center. He is currently working as a Professor of Chemistry at Seoul National University, while serving as Chair of the International Affairs Committee of the Korean Chemical Society. He has published more than 50 papers in the areas of natural product total synthesis and transition metal mediated catalysis, and has been serving as an Editorial Board Member of Chemical Reviews and Organic Chemistry Frontiers.

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## small molecule inhibitor of Hsp70 has cytotoxicity against various cancers

**Injae Shin**

Yonsei University, Korea

Hsp70 acts as an anti-apoptotic factor and protects cells from various apoptotic stresses. Hsp70 is highly expressed in many cancer cells and its overexpression correlates with tumor development and resistance to chemotherapy. By using cell-based, high-throughput screening of an imidazole library and target identification with affinity chromatography, a small molecule named apoptozole (Az) that inhibits Hsp70 activity was discovered. This substance inhibits Hsp70 activity by binding to its ATPase domain but does not affect other heat shock proteins such as Hsp40, Hsp60, and Hsp90. We also conducted structure-activity relationship study. Treatment of cells with Az induces an array of apoptotic phenotypes in various cancer cell lines. The inhibitor blocks the interaction of Hsp70 with Apaf-1 but does

not affect the interaction of Hsp70 with ASK1, JNK, Bax, and AIF, thereby inducing caspase-dependent apoptosis. In addition, the inhibitor remarkably reduces tumors in nude mouse models xenografted with cancer cells without affecting the viability. Interestingly, treatment of cancer cells and tumor-xenografted mice with a combination of a Hsp70 inhibitor and doxorubicin enhances apoptosis in comparison with a single treatment with either doxorubicin or the inhibitor. I will discuss the current progress made in Az-induced cancer cell death.

### Biography

Injae Shin received his BS degree in 1985 and MS degree in Chemistry from Seoul National University, Korea in 1987. His PhD research was performed at University of Minnesota from 1991-1995 and his Postdoctoral studies at University of California at Berkeley from 1995-1998. He is a Director of Center for Biofunctional Molecules and an Underwood Distinguished Professor at Yonsei University. His research interests include the synthesis of biologically and chemically interesting compounds, the development of bioactive molecules that can be used for biological and biomedical studies, and functional studies of glycans using chemical tools including glycan microarrays.

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 Notes:

## Porous support for phase change materials with integrated enhancement of thermal conductivity and capacity

Ge Wang

University of Science and Technology Beijing, China

Phase change materials (PCMs) have been widely developed in thermophysical storage technologies. However, issues with leakage in the liquid phase and low thermal conductivity of pure PCMs block their real-world applications. Typically, porous support can stabilize the PCMs through surface tension action and capillary forces. However, support with high porosity usually leads to amorphous structures and low thermal conductivity, which is inadequate for meeting most power conversion targets. Therefore, designing novel support with both an integrated high loading capacity and large thermal conductive properties still remains a challenge. Recently, our group developed a one-design many-functions strategy to create metal-organic frameworks (MOFs) derived porous carbons and 3D porous carbon support for PCMs. For example, a highly porous carbon (HPC) from MOFs have been fabricated by using a control carbonization method. The large mesopores of the support guarantee a high

loading percentage of PEG molecules, and the micropores induced the surface tension and capillary force to ensure the high thermal stability of the shape stabilized PCMs. The phase change enthalpy of shape stabilized PCMs is close to pure PEG and the thermal conductivity of PEG can be further improved through porous carbon. 3D conductive network carbon has been synthesized by employing a direct-calcined CQDs-derived porous carbon from the aldol reaction. 3D porous carbon offered large loading space for PCMs, meanwhile, the graphitized sp<sup>2</sup>-hybrid carbon nanosheets provide thermally conductive network and improve thermal conductivity. These SS-PCMs exhibit excellent thermal conductivity and power capacity.

### Biography

Ge Wang has completed her PhD in Chemistry from Michigan Technological University in 2002. Currently she is a Professor and PhD supervisor in the School of Material Science and Engineering at the University of Science and Technology Beijing. In 2012, she became a special Chair Professor endowed by the Chang Jiang Scholars Program of the Ministry of Education. Her research interests focus on creating complex materials structures with nanoscale precision using chemical approaches, and studying their functionalities including catalytic, energy storage and energy saving properties, etc.

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## Comparison of Different Sample Preparation Techniques for the Analysis of Small Molecules in Biological Fluids

**Sena Caglar Andac**  
Istanbul University, Turkey

Biological matrices consisting of high molecular weight matrices i.e. endogenous substances, metabolites, proteins, blood cells and coexisting drugs are often difficult to handle for chromatographic analysis. To purify and enrich the target analytes and drugs in these complex matrices an effective sample pretreatment step is essential. Biological sample pretreatment has always been a forgotten part of the biopharmaceutical analysis. Among the sample pretreatment techniques, traditional off-line sample processing like liquid-liquid extraction, protein precipitation, and solid phase extraction are gradually becoming a limiting bottleneck in the chromatographic analysis. On-line and fully automated techniques have been in demand recently.

For this purpose, new systems and coupled devices put on the market by several companies. In this presentation, importance of sample pretreatment in chromatography, manual and automated sample preparation techniques, comparison of these techniques and chromatographic method development steps will be discussed. Some applications of drug determination in complex bio-fluids will be presented under the consideration of current publications. Current trends and the future prospects of sample preparation will be overviewed.

### 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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## Synthesis of heteroatomic thiazole-based copolymers for organic semiconductors

Byanne Malluhi, Maciej Barlog, Hassan S Bazzi and Mohammed Al-Hashimi  
Texas A&M University, Qatar

The development of efficient and low-cost polymeric semiconductors is a longstanding scientific goal. Major research effort has been delegated to the design of polymeric materials with excellent electron transport properties and ambient stability for their potential applications in transistors, solar cells, consumer electronics, etc. In recent years, there has been particular interest in developing solution-processable n-type semiconductor compounds. Of these compounds, copolymerized thiazole-based heteroatomic polymers have recently shown impressive potential as active materials in organic electronics. These thiazole-based heteroatomic compounds are characterized by their closely packed  $\pi$  arrangement and rigid backbone structure. Herein, we will study the design and

synthesis of different pyrrole thiazole-based ladder polymeric structures. We will report the chemical, optical, and mechanical properties of different alkyl branching of the thiazole-based core and different copolymerization structures. The polymers exhibited excellent solubility, broad absorption spectrum, and sufficient electrochemical and thermal stability. Furthermore, we investigate the copolymerization of fluorinated and non-fluorinated thiadiazole-based polymers. The fluorinated thiadiazole polymers are expected to show higher electron mobility and exhibit better photovoltaic performance. With such successful outcomes, the future of high-performance and ambient stable polymeric semiconductors remains promising and near.

### Biography

Byanne Malluhi is an undergraduate Chemical Engineering student at Texas A&M University at Qatar.

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# 7<sup>th</sup> World Congress on Chemistry

November 13-15, 2017 Athens, Greece

Plenary  
Day 2

Chemistry World 2017





## Wei Min Huang

Nanyang Technological University, Singapore

### Elastic shape memory polymeric materials and their potential applications in comfort fitting for flexible wearable items


The shape memory effect (SME) refers to the capability of a piece of pre-deformed material to return its original shape, but only at the presence of the right stimulus. Typical stimuli include temperature variation (via either heating or cooling), chemicals, and light etc. The materials have such a feature are called shape memory materials (SMMs). We have seen a number of shape memory polymers at present. However, most of them are not elastic enough for flexible wearable items, such as shoes, at room temperature. We have recently developed a series of highly elastic (tailorable) shape memory polymeric materials to get rid of this problem, and furthermore, the items, such as shoes, made of this type of material can be programmed for comfort fitting

at body temperature for each individual. Hence, we are now able to realize customized fabrication at a low cost in a DIY manner. In this talk, we will introduce the major features of such materials, and show their potential applications in comfort fitting of wearable items.

### Biography

Wei Min Huang is currently an Associate Professor (tenured) at the School of Mechanical and Aerospace Engineering, Nanyang Technological University, Singapore. With over 20 years of experience on various shape memory materials (alloy, polymer, composite and hybrid), he has published over 180 papers in journals, such as Accounts of Chemical Research, Advanced Drug Delivery Reviews, and Materials Today, and has been invited to review manuscripts from over 200 international journals (including Progress in Polymer Science, Nature Communications, Advanced Materials, and Advanced functional materials, etc), project proposals from American Chemical Society, Hong Kong Research Grants Council, etc, and book proposals from CRC and Elsevier. He has published two books (Thin film shape memory alloys – fundamentals and device applications, Polyurethane shape memory polymers) and is currently on the editorial board of over two dozens of international journals.

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# 7<sup>th</sup> World Congress on Chemistry

November 13-15, 2017 Athens, Greece

## Scientific Tracks & Abstracts Day 2

Chemistry World 2017



# Major Sessions:

Monday, November 14, 2017 | Day 2

Food Chemistry | Analytical Chemistry | Materials Chemistry | Sustainable Chemistry and Chemical Engineering  
Electro Chemistry | Applied Chemistry | Chemical Science

## Session Chair

**Wolfgang Tremel**

Johannes Gutenberg University Mainz, Germany

## Session Chair

**Ge Wang**

University of Science and Technology Beijing, China

## Session Introduction

**Title: Lanthanide complexes - synthesis, characterization and biological evaluation**

Irena Kostova, Medical University, Bulgaria

**Title: Photocyclization of organic compounds as a universal method of creating recording systems for optical memory devices**

M.M. Krayushkin, Russian Academy of Sciences, Moscow

**Title: N-acetyl serotonin protects neuronal cell death induced by oxidative stress via elevation of TrkB/CREB/BDNF and Akt/Nrf<sub>2</sub> pathways**

Mee Ree Kim, Chungnam National University, South Korea

**Title: Visible Light-Mediated Synthesis of Organophosphorus Compounds: Synthetic and Mechanistic Investigations**

Sami Lakhdar, Université de CaenBasse-Normandy, CNRS, France

**Title: Facile Synthesis, Fluorescence and Functional Properties of  $\pi$ -Expanded Fluorenes**

Jagarapu Ramakrishna, Indian Institute of Technology Madras, India

**Title: Synthesis and Properties of Two Classes of Thiazole-Based Organoboron Fluorophores Possessing the AIEE/AIE Effect**

Belskaya Nataliya, Ural Federal University, Russia

**Title: Mechanism of low-temperature ignition of acetaldehyde-oxygen gas mixtures,initiated by peroxy radicals**

Irma Vardanyan, National Academy of Sciences, Armenia

**Title: Hydroxy Apatite Composite Coatings on Mg alloy forMedical Applications**

Mohren Saremi, University of Tehran, Iran.

**Title: Application of the ALA-SCAN method in drug discovery and pharmacodynamics**

Cenk A Andac, Istinye University-Istanbul, Turkey

## Lanthanide complexes – synthesis, characterization and biological evaluation

Irena Kostova

Medical University - Sofia, Bulgaria

There is an increasing requirement for the discovery of new metal-based compounds having better activities than their precursors. Recently a number of lanthanide(III) complexes were reported. These studies highlighted the potential of developing novel lanthanide complexes with improved biological potency. As a part of our continuing work on the synthesis, characterization and applications of lanthanide(III) complexes, it was observed that changes in ligands and reaction conditions had profound effects on selectivity and activity of the products obtained. The present work deals with the synthesis, theoretical, analytical, NMR, FT-IR and FT-Raman spectral investigations, supported by DFT calculations, to understand the structural and bonding features, the intramolecular interactions of biologically active ligands and their lanthanide(III) complexes. Detailed spectral analysis based on both calculated and experimental data confirmed the suggested metal–ligand binding mode. The recorded spectra and the marker bands of characteristic

functional groups were identified, in order to use them as data bank for further application in trace analysis of rare-earth complexes. The overall results confirmed that the DFT approximation is a reliable method for calculations of geometries and vibrational frequencies of the tested ligands and their lanthanide(III) complexes. The cytotoxic effects on different tumor cells and antioxidant activity of the complexes were studied in order to set up a sequence of experimental assays *in vitro* which allow predicting their activity *in vivo*. Our investigations have shown that the complexes reveal promising pharmacological properties more pronounced than for the respective ligands and should be subset to further detailed pharmacological and toxicological evaluation.

### Biography

Irena Kostova has graduated from Mendeleev University - Moscow with the highest grade. She has been appointed as a Research Scientist at Ministry of Environmental. Her PhD and DSc thesis has been awarded by MU-Sofia which is established and maintains relationships with many European Universities. She has published hundreds of publications with more than 3300 citations (IF>150; h-index: 27), scientific book chapters and books for students. Her research interests include the developmental work of coordination chemistry, vibrational spectroscopy, pharmacological investigations etc.

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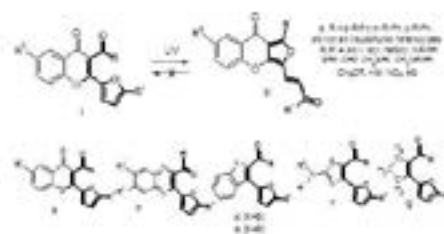
## Photocyclization of organic compounds as a universal method of creating recording systems for optical memory devices

M M Krayushkin

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In recent years, the prospects of an increase in the capacity of data storage media (up to 1 Tera-bytes/cm<sup>3</sup>) are related to the development of multilayer light-sensitive optical discs using light-sensitive organic compounds for data recording and readout. Preparation of the effective compounds, which undergo photochemical transformations providing 3D operative and archival optical memory with ultra-high storage capacity due to non-destructive fluorescence readout, is one of the key problems of molecular electronics. This presentation discusses our results on the development of photochromic and photochromogenic polymer materials and recording media thereof for three-dimensional (3D) bitwise working and archival optical memory. The synthesis of original chromones and their analogues, photochromic diarylethenes, as well as their characterization are reported. The results of spectral-kinetic studies were applied to

the development of polymeric recording layers based on the synthesized compounds and the design of multilayer recording media for optical disks. We demonstrated that UV-irradiated acylchromones and their analogues that show no fluorescence irreversibly rearrange into fluorescent furano[3,4-b] chromenones II. Based on the latter, we have developed multilayered recording media for optical discs of the WORM type.



### Biography

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 Notes:

## N-acetyl serotonin protects neuronal cell death induced by oxidative stress via elevation of TrkB/CREB/BDNF and Akt/Nrf2 pathways

Mee Ree Kim

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Recently, N-acyl serotonin, present in the intestine, has been reported to exert neuroprotective action against oxidative stress by inducing antioxidant enzymes. However, the mechanism for neuroprotective action of N-acetyl serotonin (NAS) as a precursor of melatonin is not clarified. In this study we focused on the suppressive effect of N-acetyl serotonin on glutamate-induced apoptosis in HT-22 cells, and then examined the molecular mechanism for its anti-apoptotic action. For this purpose, we performed flow cytometry, immunoblotting analyses and antibody-mediated neutralization. When HT-22 cells were preincubated with NAS prior to glutamate treatment, NAS dose-dependently reduced apoptotic bodies and recovered mitochondrial potential in glutamate-treated HT-22 cells. NAS dose-dependently inhibited oxidative stress-induced cell death in HT-22 cells. Moreover, NAS suppressed glutamate-induced apoptosis by suppressing expression of pro-apoptotic factors such as AIF, Bax, calpain, cytochrome c and cleaved caspase-3, whereas it enhanced expression of Bcl-2, an anti-apoptotic factor. In addition, NAS improved phosphorylation of tropomyosin-

related kinase receptor (TrkB) and cAMP response element-binding protein (CREB) as well as expression of brain-derived neurotrophic factor (BDNF), whereas the inclusion of each inhibitor of JNK, p38 or Akt neutralized the neuroprotective effect of NAS, but not that of ERK. Meanwhile, NAS dose-dependently reduced the level of reactive oxygen species, and enhanced the level of glutathione in glutamate-treated HT-22 cells. Moreover, NAS not only increased expression of heme oxygenase-1, NAD(P)H quinone oxidoreductase-1 and glutamate-cysteine ligase catalytic subunit, but also enhanced nuclear translocation of NF-E2-related factor-2. Separately, NAS at 30 mg/kg suppressed scopolamine-induced memory impairment and cell death in CA1 and CA3 regions in mice. In conclusion, NAS shows actions of antioxidant and anti-apoptosis by activating TrkB/CREB/BDNF pathway and expression of antioxidant enzymes in oxidative stress-induced neurotoxicity. Therefore, such effects of NAS may provide the information for the application of NAS against neurodegenerative diseases.

### Biography

Mee Ree Kim has completed her PhD from Seoul National University and is a Visiting Professor at Wisconsin-Madison University, Department of Toxicology. She is the former President of Korean Food Related Academic Association. She has published more than 120 papers in reputed journals and has been serving as an Editorial Board Member of reputed such as Journal of Medicinal Food.

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## Visible light-mediated synthesis of organophosphorus compounds: synthetic and mechanistic investigations

Sami Lakhdar

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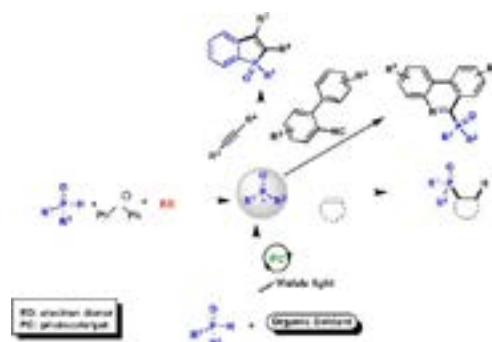
Reactions involving phosphorus centered radicals play a pivotal role in the construction of organophosphorus ligands, biologically active molecules and p- conjugated molecules. Common synthetic approaches for the generation of such radicals imply the use of harsh reaction conditions. In this communication, we show that access to a large variety of organophosphorus compounds can be achieved under mild reaction conditions through: i) visible light photoredox catalysis or ii) visible light irradiation of Electron-Donor-Acceptor complexes (EDA). The scope and limitations of these methods will be discussed with a special focus on their mechanistic aspects.

### Recent Publications

1. D E C Corbridge (2013) Phosphorus: Chemistry, Biochemistry and Technology, 6th ed, CRC Press: Boca Raton, FL.
2. L D A Quin (2000) Guide to Organophosphorus Chemistry; Wiley Interscience: New York.
3. V Quint, F Morlet-Savary, J F Lohier, J Lalevée, A C Gaumont and S Lakhdar (2016) Metal-free, visible light-photocatalyzed synthesis of benzo[b] phosphole oxides: synthetic and mechanistic

investigations. Journal of American Chemical Society 138(23):7436–7441.

4. L Noël-Duchesneau, E Lagadic, F Morlet-Savary, J F Lohier, I Chataigner, M Breugst, J Lalevée, A C Gaumont and S Lakhdar (2016) Metal-free synthesis of 6-phosphorylated phenanthridines: synthetic and mechanistic insights. Organic Letters 18(22):5900–5903.
5. G Fausti, F Morlet-Savary, J Lalevée, A C Gaumont and S Lakhdar (2017) Chemistry- A European Journal 23:1–6.



### Biography

Sami lakhdar is working as a professor at University of Caen Basse-Normandie, France. He has his research experience in the field of organic and inorganic chemistry

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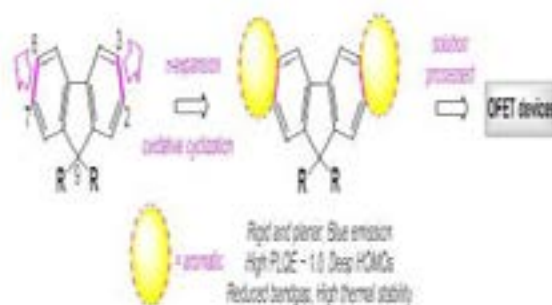
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## Facile synthesis, fluorescence and functional properties of $\pi$ -expanded fluorenes

Jagarapu Ramakrishna and Parthasarathy Venkatakrishnan  
Indian Institute of Technology Madras, India

$\pi$ -Expanded 2D fluorenes were synthesized via double annulation at 2,3 and 6,7-faces of fluorene employing DDQ-mediated oxidative cyclization method with very high regioselectivity. All the newly synthesized larger fluorenes were thoroughly characterized by <sup>1</sup>H and <sup>13</sup>C NMR, IR spectroscopy, and high-resolution mass spectrometry. The rigid and planar fluorenes thus obtained led to near-UV absorbance, bright blue emission with very high close-to-unity fluorescence quantum yields, and deep HOMO energy levels with excellent thermal stabilities. In addition, single crystal X-ray analyses of the newly synthesized fluorenes revealed potential  $\pi$ - $\pi$  stacking that was found to depend on the substituents at either 9-position or at the aromatic ring. As these electron-rich fluorenes are very well soluble in common organic solvents, we have fabricated OFET devices for them

via the solution-process method and have characterized their charge transport performances. Some of these interesting results will be showcased in this presentation.



### Biography

Jagarapu Ramakrishna is currently pursuing his PhD in Functional Organic Materials under the guidance of P Venkatakrishnan at IIT Madras, India. He is currently in final year of his PhD degree and expecting to defend his thesis early in 2018. His research interests are in the area of Synthetic Organic Chemistry, Organic Photonic, Electronic and Energy Materials.

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## Synthesis and properties of two classes of thiazole-based organoboron fluorophores possessing the AIEE/AIE effect

Belskaya Nataliya<sup>1</sup>, Kseniya I Lugovik<sup>1</sup>, Alexander K Eltyshv<sup>1</sup>, Polina O Suntsova<sup>1</sup>, Pavel Slepukhin<sup>2</sup> and Enrico Benassi<sup>3</sup>

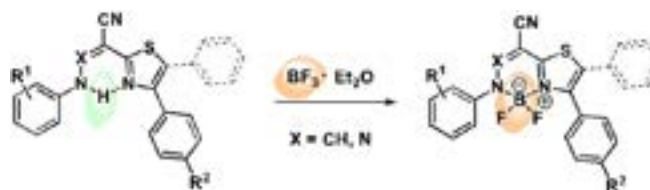
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Luminescent organoboron molecular systems have been receiving an increasing amount of interest over the past few decades. The presence of boron in the structure of organic compounds leads to substantial modifications in the molecule's electronic structure due to the electron deficiency of boron. Some boron complexes featuring diketones, iminoketones azo dyes,  $\beta$ -enaminones,  $\beta$ -ketoiminates, and hydrazones have shown high fluorescence in the solid state and either aggregation-induced emission (AIE) or aggregation-induced emission enhancement (AIEE). However, although BF<sub>2</sub> complexes are actively being synthesized and investigated, only a few examples of AIE/AIEE-active luminophores have been reported in the literature due to the deficiency of appropriate frameworks. Moreover, the number of known AIE/AIEE-active boron complexes that efficiently emit in the solid state is still limited. We recently reported the synthesis and photo physical characteristics of the aryl enamine and aryl aza-enamine thiazoles, which show weak fluorescence in solution

that was proven to be caused by intramolecular hydrogen bonding and that is very sensitive to the microenvironment. The structure of these thiazole derivatives includes a convenient combination of functionalities and may be used as a bidentate N, N-ligand to synthesize BF<sub>2</sub> complexes. We report now about synthesis of two new series of promising thiazole-containing BF<sub>2</sub> complexes and their spectroscopic and photo physical characterization. These investigations were performed in solution, powder and aggregation states. Solvato(fluoro)chromism was also explored. Some structure-property relationships were rationalized by DFT calculations.



### Biography

Belskaya Nataliya has completed her Doctor Sciences thesis at Ural Federal University, Russia in 2011. She was appointed as Associate Professor at Ural Federal University in 2006, becoming a full Professor at the same university in 2012. Till 2017, 75 publications have appeared in international and Russian journals about her work that have been cited over 200 times. Her research is focused on the chemistry of heterocyclic compounds, pericyclic reaction and design, synthesis and investigation of fluorescent compounds in the solutions, suspension and solid state.

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## Mechanism of low-temperature ignition of acetaldehyde-oxygen gas mixtures, initiated by peroxy radicals

I A Vardanyan, A M Arustamyan, A B Harutyunyan, A S Martirosyan and S V Tsarukyan

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During the low temperature ignition of acetaldehyde-oxygen mixtures, initiated by peroxide compound, adsorbed on the reactor surface, at its heating, a decrease of the ignition temperature, depending on the surface nature, has been detected. In the case of  $H_3BO_3$ , it drops to the room temperature, but in the case of NaCl it was remarkably higher. The reason of such heterogeneous nature of the ignition of aldehyde-oxygen mixtures was not clear. Taking into account the possibility of the interaction of adsorbed peroxy radicals with acetaldehyde and methane the comparison and the analysis data of has been made. The general attention has been focused on the comparison of data, received in the

case of  $H_3BO_3$  and NaCl. The correlation between the rate of heterogeneous interaction of peroxy radicals and the ignition temperature of above mentioned mixtures has been established. Taking into account the experimental fact, that the rate of peroxy radicals ( $CH_3O_2$ ) reaction with organic compound (methane, aldehyde) on the  $H_3BO_3$  surface is more than on the NaCl surface and that this is in accordance with lower ignition temperature in the case of  $H_3BO_3$  surface than in the case of NaCl surface, it was concluded, that the essence of the heterogeneous nature of the initiation of the ignition process of  $CH_3CHO + O_2$  mixtures consists in set of the fire by a radical process going on the surface. Bearing in mind the possibility of heterogeneous interaction of  $C_2H_5O_2$  radicals with  $C_2H_5CHO$ , it is possible to consist that this explanation is available and for the ignition of  $C_2H_5CHO-O_2$  mixtures.

### Biography

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## Hydroxy Apatite Composite Coatings on Mg alloy for Medical Applications

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Mg and its alloys are important engineering materials with widespread applications especially in aerospace and automobile industries for their light weight and good strength /weight ratio. Moreover, in recent years they have been the focus of research for medical applications due to their biocompatibility, biodegradability and nontoxicity. Mg and Mg alloys are good candidates for use in orthopedic applications as temporary implants because in addition to the above mentioned properties they have also module of elasticity near to the human bone. However such application faces limitations due to high corrosion rate and H<sub>2</sub> gas formation. The corrosion of Mg alloy is desirable in temporary implants but it should be controlled to retain its properties during healing process of fractured bone. But H<sub>2</sub> formation is a considerable obstacle because it also interferes in healing process. The corrosion of Mg and Mg alloys can be controlled by applying different methods among them surface coating is the most efficient and easy to perform. Hydroxyapatite is the most suitable biocompatible ceramic material with composition near to human bone which is used as coating in medical applications. Application of biocompatible HA coating on

Mg alloys can reduce corrosion rate and consequently reduce H<sub>2</sub> formation. However, its brittle nature is a major problem for use at load bearing sites of body implants. Moreover the application of HA in orthopedic implants suffers from its low toughness and poor wear resistance. This leads to the focus on developing composite coatings with incorporation of various biopolymers and reinforcing material to improve its mechanical behavior. In our research works we have made different composites of HA with Chitosan as a biopolymer, CNT and Graphene. The composites were prepared and applied on Mg alloy ( AZ31) by electrochemical cathodic deposition using CNT or Chitosan as dispersion in the electrolyte solution. In the next attempt graphene and HA particles were dispersed in the electrolyte and the composite of HA-Graphene deposited in an electrophoretic process. he morphological studies showed uniform dispersion of particles in the coating and further electrochemical tests using Tafel polarization and EIS methods confirmed remarkable improvement corrosion resistance of the composite coatings. Nano indentation method was used to check the mechanical behavior of the coating and the results showed considerable improvement in mechanical properties.

### Biography

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## Application of the ALA-SCAN method in drug discovery and pharmacodynamics

**Cenk A Andac**

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In drug discovery and pharmacodynamics, alanine scanning (ALA-SCAN) is a method used to determine the contribution of an amino acid residue (other than alanine or glycine) to the stability or function of a given protein or peptide. In addition, point-mutations to alanine (or glycine) allows researchers to determine essential/non-essential interactions between the peptide/non-peptide ligands and their receptors, which provide crucial information in drug discovery. In vivo applications of the ALA-SCAN technique involves site-directed mutagenesis or random mutations constituted by PCR library, which may be costly. On the other hand, a more cost-effective method of ALA-SCAN has

been computationally utilized in theoretical chemistry. Here, specific examples for the in-silico version of the ALA-SCAN technique applied in our computer-assisted drug development laboratory will be given.

### Biography

Cenk A Andac works as an Assistant Professor in the School of Pharmacy at Istinye University-Istanbul, Turkey. He has completed his Master's degree and PhD work as the Faculty of Pharmacy at the University of Wisconsin-Madison, WI, USA (UW-Pharmacy, USA). He had been involved in teaching Drug Actions & Delivery, and Pharmaceutical Biochemistry & Biotechnology courses at UW-Pharmacy, USA for four and half years. He has also taught Medical Pharmacology courses as an assistant professor for three years in Medical school in Turkey. His current researches are development of novel anticancer agents inhibiting G-coupled receptors in cancer stem cells; development of novel aminoglycoside antibiotics; determination of 3D structures of biological and synthetic compounds by NMR techniques; computer-assisted drug development by AMBER, CHARMM and Quantum mechanics; Pharmacokinetics and Pharmacodynamics properties of drug-receptor interactions. He currently holds a patent for a potentially active anti-cancer agent against breast cancer.

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# 7<sup>th</sup> World Congress on Chemistry

November 13-15, 2017 Athens, Greece

## Video Presentation Day 2



## A study of fluorine substitution on solution processable benzo [1, 2, 5] thiadiazole based copolymers for optoelectronic applications

Amira Abouhadid

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Polymer solar cells (PSCs) have attracted great attention in recent years due to their advantages of low cost, light-weight, easy fabrication and capability to be fabricated into large area flexible devices. Herein, we designed and synthesized a series of four novel thermally stable low-band-gap (LBG) conjugated polymers (P1-P4) based on benzo [1,2,5] thiadiazole (BT) as a building block. BT is well known electron-withdrawing unit which has been sandwiched with two electron donating octylthiophene units; a monomer in this designed polymer series. We copolymerized with various fluorinated and non-fluorinated BT in order to compare optoelectronic properties. The thermal stability of the polymers is studied by differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA). Optical properties of the polymers are measured by UV-Visible spectrophotometer. Theoretical calculations (DFT studies) and electrochemical cyclic voltammetry (CV) measurement suggested that the fluorine atom could decrease the molecular

energy levels highest occupied molecular orbital and lowest unoccupied molecular orbital (HOMO and LUMO) of the resulting polymers distinctly. Presence of fluorine atom in the conjugated backbone tunable optoelectronic properties could be expected. Moreover, we discuss the effect of the fluorine atom on the absorption spectra, crystalline properties, hole mobilities, and blend morphologies of the conjugated polymers.

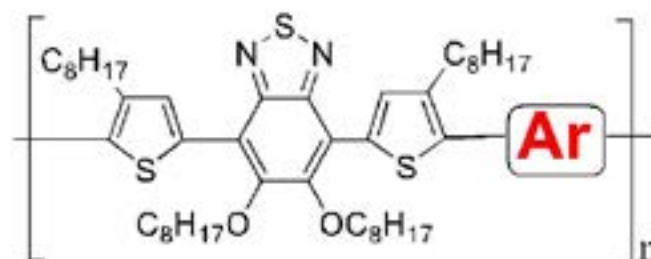


Figure 1. benzo [1,2,5] thiadiazole based conjugated polymers

### Biography

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## Relativistic origin of classical thermodynamics as an alternative to the concept of probability

**A Yu Zakharov**

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The problem of the non-contradictory microscopic foundation of both thermodynamics and kinetics remains unsolved. Thus, statistical mechanics is an ill-posed theory. In addition to internal contradictions, there are several difficult fundamental problems in this theory such as (i) the equivalence criteria for the statistical ensembles are not known, (ii) there are no exact methods or a priori accuracy estimates of approximate methods for calculating partition functions, (iii) the problem of closure of equations for partial distribution functions leads to use uncontrolled additional probabilistic hypotheses such as weakening correlations principle. The purpose of this study is to develop a method for probability-free describing the evolution of many-particle systems with

account relativistic effects. In our papers, a new description of the evolution of a system of particles with retarded interactions is proposed. The qualitative properties of the solutions of this relativistic equation with respect to the microscopic density are investigated. It is proved that the solutions possess the property of irreversibility in time. Therefore, there is no need to use any kind of probabilistic concepts in the microscopic foundation of classical thermodynamics. The further purpose of our research is to construct a microscopic kinetic theory of many-particle systems, including the processes of thermodynamic equilibration at different scales, the calculation of thermodynamic and kinetic properties.

### Biography

A Yu Zakharov has completed his PhD from Donetsk Physico-Technical Institute, Academy of Sciences of Ukrainian SSR and Postdoctoral studies from Donetsk Polytechnical Institute, USSR. He is Professor in Yaroslav-the-Wise Novgorod State University. He has published more than 70 papers in reputed journals and six monographs.

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