



**6<sup>th</sup> EuChEMs** | **SEVILLE** Spain  
Chemistry Congress | **11<sup>th</sup>-15<sup>th</sup>** September **2016**

# SCIENTIFIC PRELIMINARY PROGRAM

## Topic Plenaries Advance



Organized by



Platinum Sponsors



Gold Sponsors



Silver Sponsors



Bronze Sponsors



Sponsors



**TOPIC A1- Chemistry Education**



**Paul Yates**

University of Chester, UK

**Defining excellent chemistry teaching**

In November 2015 the United Kingdom government announced their intention to introduce a Teaching Excellence Framework (TEF) to assess the quality of teaching in English universities. The TEF is intended to provide students with more information when selecting an institution to study at, and ultimately will allow the ranking of institutions by teaching quality. Success in the TEF will be linked to the ability to raise tuition fees in line with inflation. The ultimate aim is to allow assessment at the level of individual disciplines.

There has been much debate about what constitutes teaching excellence, but it is likely that the TEF will, at least initially, collect metrics which are regarded as proxies for teaching excellence. These may include graduate salaries, the number of students who complete their course, and existing measures of student satisfaction already collected as part of the National Student Survey. The first stage of the TEF is planned to be implemented in the 2016-2017 academic year.

This presentation will present the current state of the TEF and how it is being implemented, with particular reference to the teaching of chemistry where there are particular teaching demands in the areas of laboratory work and mathematical skills among others. Similarities and differences with other subjects, both within the STEM group and beyond, will be highlighted. There will also be a consideration of the extent to which teaching quality in chemistry can be measured, and the factors that support and reduce the quality of teaching. A crucial factor once the TEF is implemented at discipline level will be who will assess the quality of the teaching, and this will also be discussed.

The implications of attempting to measure teaching quality will be considered. This will include a consideration of the effect of the TEF internationally, and across the nations of the United Kingdom where the TEF is being introduced in England but other nations are expected to introduce similar initiatives. The extent to which students make use of information such as that being collected as part of the TEF will be discussed.

European initiatives which have had a positive effect on the quality of university chemistry teaching, and those who teach it, will be outlined. This will include a consideration of the sustainability of such activities, their long term impact, and the extent to which subsequent activities have become embedded in everyday chemistry teaching.



6<sup>th</sup>  
**EuCheMS**  
Chemistry Congress

SEVILLE Spain  
11<sup>th</sup>-15<sup>th</sup> September 2016  
Organized by  
  
ANQUE  
ASOCIACIÓN NACIONAL DE  
QUÍMICOS DE ESPAÑA  
  
EUROPEAN CHEMICAL  
SCIENCES

### TOPIC A2- Chemistry Society and Public Engagement Education



**Rocco Mazzeo**

University of Bologna, IT

### **Education in chemistry for restoration: a means to help preserving the highest forms of humankind production.**

The last decades the field of conservation and restoration of cultural heritage has been revolutionized by the introduction of new materials, technologies, scientific methods of examination and analytical equipment as well as new information communication technology means. However, even though it is probably too early to draw final conclusions, the question is whether the technical and, above all, the methodological quality of the conservation profession has taken full advantage of all the above mentioned means.

In any case I do believe that this innovation process has led to at least one important achievement. Art objects to be preserved are regarded among the highest forms of humankind production. Therefore, if conservation, beyond its material aspects, more and more represents an occasion of knowledge advancement, it raises quite clearly the overall process to a high cultural level.

The essence of this transformation is primarily linked to the involvement of competencies, body of knowledge and cultures originally far from the field of conservation: primarily the scientific disciplines. Where the field of conservation-restoration is able to promote close interactions among disciplines apparently far from each other, such as chemistry and art history, their distinct body of knowledge can be integrated and perhaps renewed.

To this purpose different type of activities addressed to different audience can be developed. a) specific books addressing all general and applied issues of chemistry, the “alien” scientific discipline primarily involved in conservation, instrumental in collecting and organising the many experiences and advancements that during recent decades have been accumulated often in a disorganised manner; b) inclusion of Chemistry for restoration courses as part of science teaching in university science curricula, may represent an effective tool in attracting new students to the field of science and chemistry in particular; c) engagement of the general public through activities highlighting experiments and games aimed at exploring and presenting the fascinating world of chemistry for cultural heritage.



6<sup>th</sup>  
**EuCheMS**  
Chemistry Congress

SEVILLE Spain  
11<sup>th</sup>-15<sup>th</sup> September 2016  
Organized by  
 ANQUE  
ASOCIACIÓN NACIONAL DE QUÍMICOS DE ESPAÑA  


### TOPIC A3- Benefits Wealth Creation and Society



**Juan Bautista Carda**

Universitat Jaume I, Castellón, ES

### Strategies for International Knowledge Transfer in Ceramic

Universitat Jaume I of Castellón (Spain) is a proactive public university with a firm focus on innovation in the international sphere. Around 10% of our postgraduate students come from abroad, and in the last academic year we welcomed nearly 600 foreign students on exchange programmes. We have academic links with more than 300 universities across the world, former students and ambassadors in 50 countries.

In this context, the socioeconomic area where it is located the University is predominantly ceramic, in which are the main manufacturing ceramic tiles industries in Spain. In that frame, the Solid State Chemistry Group from Inorganic and Organic Chemistry Department of Universitat Jaume I has been leading international collaboration in order to transfer ceramic knowledge both scientific and technological point of view.

Our group is involved in many research lines in collaboration with industry: new ceramic tiles based on recycled materials, glass ceramic glazes with special properties (antibacterial properties, antislip ceramic tiles, phosphorescent ceramic tiles, air cleaning tiles,...) ceramic pigments useful to produce new ceramic applications and photovoltaic technology, which lets the combination of friendly environmental tiles with the use of alternative sources of energy (photovoltaic ceramic tiles).

The Solid State Chemistry group, is member of the European Chemistry and Chemical Engineering Education Network, since where participates in the organizing of short international intensive school about heritage and ceramic. It also organizes international courses of materials in Latin America Universities, such as some places in Colombia, Brazil, Venezuela...

In this presentation, some examples of partnerships with European and Latin America universities and companies will be shown through different exchange programmes, such as "Tempus", "Sócrates", "Erasmus", "ALFA", allowing the contribution of knowledge of foreign universities and research centres. Moreover, we have collaborated with the Spanish International Cooperation Agency to contact to professors and students from around the world.



6<sup>th</sup>  
**EuCheMS**  
Chemistry Congress

SEVILLE Spain  
11<sup>th</sup>-15<sup>th</sup> September 2016  
Organized by  
  
ANQUE  
ASOCIACIÓN NACIONAL DE  
QUÍMICOS DE ESPAÑA  


### TOPIC B1- Sustainable Energy



**James Durrant**

Imperial College London, UK

### Photochemical studies of approaches to artificial photosynthesis

There is increasing interest in the development of artificial photosynthetic systems for solar driven fuel synthesis. My talk will start by reviewing approaches to artificial photosynthesis, and the lessons which can be learnt from biological photosynthesis. I will then go on to address the role of charge carrier dynamics in determining the efficiency of such systems, including both photoelectrodes for water oxidation and reduction and hybrid molecular / inorganic systems for solar driven proton and CO<sub>2</sub> reduction. Experimentally, these studies will be based around transient absorption spectroscopy on timescales from femtoseconds to seconds, which will be correlated with the results of photoelectrochemical analyses of device efficiency. These studies will address the dynamics of charge separation and recombination, as well as the kinetics of water oxidation / reduction at semiconductor / liquid interfaces. Issues which will be addressed will include the underlying photochemistry of oxides, the role of the space charge layers at electrochemical junctions in spatially separating charges, and the role of heterojunctions and catalysts layers in enhancing system efficiency. Particular consideration will be placed on the mechanism of water oxidation / reduction, and the extent to which oxide surfaces function as heterogeneous catalysts for this



**6<sup>th</sup>**  
**EuCheMS**  
Chemistry Congress

**SEVILLE** Spain  
**11<sup>th</sup>-15<sup>th</sup>** September **2016**  
Organized by



ANQUE  
ASOCIACIÓN NACIONAL DE  
QUÍMICOS DE ESPAÑA



EUROPEAN CHEMICAL  
SCIENCE

### TOPIC B2- Environment and Natural Resources Management



**Angel Irabien Gulias**

University of Cantabria.ES

### **From Carbon Dioxide to Sustainable Products: Electrochemical Process Development**

Carbon capture and utilisation (CCU) stands for, in addition to carbon capture storage, the utilisation of CO<sub>2</sub>. The CO<sub>2</sub>, as source of carbon, has the potential to be used in the manufacture of fuels, carbonates, polymers and chemicals. Being on development-to-demonstration phases, CCU represents a new economy for CO<sub>2</sub>, as used as raw material.

Capture, transport, CO<sub>2</sub> transformation and CO<sub>2</sub> product consumption represents the value chain of the CCU technology. Electrochemical reduction is one of the innovative technologies under development for the chemical transformation of CO<sub>2</sub> into useful products.

Electrochemical reduction of CO<sub>2</sub> requires the use of an electric current (in this case, created from a renewable energy source) to produce the required electrons. Products that can be formed include formic acid, carbon monoxide, methanol, methane and other hydrocarbons. In a modern day context it is another way in which renewable electrical energy may be converted into a more manageable form..This area of CCU is particularly appealing to countries with high alternative energy capacities such as hydro-electric power and has been highlighted by Der Norsk Veritas as a viable strategy for Norway in a recent policy briefing paper. Advances in electrocatalysis are needed to provide stable, inexpensive, selective catalysts so that the full potential of electrochemical reduction can be explored.

Formic acid is one of the carbon dioxide derived product based on the electrocatalytic reduction of carbon dioxide, which shows promising results based on the use of nanoparticles and new electrodes design. Methanol has been also explored (3) and ionic liquids show promising results to increase the faradaic efficiency.



**6<sup>th</sup>**  
**EuCheMS**  
Chemistry Congress

**SEVILLE** Spain  
**11<sup>th</sup>-15<sup>th</sup>** September **2016**  
Organized by

**TOPIC B3- Sustainable Chemistry**



**Jean-Luc DUBOIS**

ARKEMA Colombes, FR

**Alternative routes to acrylic acid**

Acrylic acid is an important chemical compound for the chemical industry. It has numerous and diverse applications such as in superabsorbants for diapers, in coating resins (as acrylates) and in water treatment (as copolymers with acrylamide), in rheology additives, and other resins.

It is currently produced mostly from propylene through a 2 stages oxidation. The industry has been looking for alternative routes either to improve its sustainability and to diversify the sourcing of raw materials or to improve the economics. Therefore various solutions have been investigated, including propane direct oxidation (1 step); but also glycerol oxydehydration (2 steps); fermentation of sugars to Lactic acid or 3-Hydroxypropionic acid followed by a dehydration step; ethylene (eventually produced from ethanol) carbonylation followed by a ring opening of the propiolactone; addition reaction between acetic acid and formaldehyde (and variations around this concept); and more recently oxidative coupling of methanol and ethanol.

Advantages and disadvantages of each route will be discussed, including the constraints and challenges. Since the first criteria for sustainability is to develop processes that are economically attractive, the main constraints in the cost of production and catalyst and process development will be presented.



6<sup>th</sup>  
**EuCheMS**  
Chemistry Congress

SEVILLE Spain  
11<sup>th</sup>-15<sup>th</sup> September 2016  
Organized by  
  
ANQUE  
ASOCIACIÓN NACIONAL DE  
QUÍMICOS DE ESPAÑA  


### TOPIC B4- Food Chemistry



**Elke Anklam,**

Research Centre European Commission, BE

### Food Safety and Quality Control in 2030 - are we prepared?

The provision of safe, nutritious, high quality and affordable food is the central objective of the legislative framework of most jurisdictions and consumers in developed economies currently enjoy a high level of food safety. Still, large public health and economic gains can be reaped by improving diets and lifestyles, seeing the increasing rates in overweight, obesity, poor diets and physical inactivity. These risk factors are known to raise the likelihood of diet-related non-communicable diseases such as cardiovascular diseases, diabetes, and cancer. The resulting enormous costs-of-illness burden the health and social security systems and slow-down economic development and growth.

Besides food safety control it is likewise important to ensure the quality and authenticity of food and moreover to prevent food fraud. This is however not new, as adulteration of food has a history, dating back to ancient times. As the underlying aim of food adulteration is to maximise revenues, it is obvious that high priced products risk being tainted. Food fraud cases damage the reputation of the industry and hamper trade.

Therefore, current challenges to the global food system as we know it today might be exacerbated in the future as new and even more complex ones will emerge. New technologies, climate and demographic changes, consumer behaviour or trade disruptions have the potential to put the current policy and legislative frameworks related to food and nutrition under significant stress.

Foresight is a process that provides the necessary anticipatory intelligence to inform medium- to long-term policy formulation; it enhances forward-looking thinking by gathering a broad range of stakeholders and different knowledge sources to systematically explore the future so as to guide today's decision-making.

This presentation will highlight the critical challenges to the global legislative governance of the food system and will assess the ability of the current food policy frameworks to successfully deal with these challenges. Moreover, it will reflect on the needs for scientific developments in the field of food analysis and for the quality assurance of data.



6<sup>th</sup>  
**EuCheMS**  
Chemistry Congress

SEVILLE Spain  
11<sup>th</sup>-15<sup>th</sup> September 2016  
Organized by  
 ANQUE  
ASOCIACIÓN NACIONAL DE QUÍMICOS DE ESPAÑA  
 EUROPEAN CHEMICAL SCIENCES

### TOPIC C1- Synthesis and reactivity in Metal based Compounds



**Marinella Mazzanti**

École Polytechnique Fédérale de Lausanne. CH

#### Small Molecule Activation by Complexes of Low-valent f Elements

Complexes of low-valent f-elements are excellent candidates for small molecule activation. Different sterical and electronic environments at the U(III) and Ln(II) centers have a critical impact on the nature, structure, stability and reactivity of the reduction products.

Careful tuning of the ligand is also essential to promote multi-electron transfer which is rare in f element chemistry.

Notably, bulky siloxide ligands can be used to isolate stable homo- and heteropolymetallic U(III) complexes which act as multi-electron reducing agents in the reaction with a variety of small molecules such as CS<sub>2</sub>, CO<sub>2</sub> azides, and chalcogenides. Reduction of azides leads to highly reactive nitride-bridged di-uranium complexes that can functionalize small molecules such as CO, CO<sub>2</sub> and CS<sub>2</sub>.

Nitride bridged complexes containing uranium in the oxidation state +III can also be prepared using siloxide supporting ligands and promote unusual reactivity with small molecules.

Moreover, the sterical demand and electron-rich coordination environment of homoleptic siloxide complexes of Eu(II) and Yb(II) leads to the reduction of azobenzene, carbon disulfide and carbon dioxide and the ready release of the reduction products, a prerequisite for the implementation of catalytic cycles.

Finally, siloxide ligands lead to the formation of heterobimetallic complexes enabling the multimetallic cooperativity in uranium mediated reduction of carbon dioxide. The redox chemistry of f element complexes with siloxides and other bulky ligands[6] will be presented together with the structure and properties of original compounds.



6<sup>th</sup>  
**EuCheMS**  
Chemistry Congress

SEVILLE Spain  
11<sup>th</sup>-15<sup>th</sup> September 2016  
Organized by  
ANQUE  
ASOCIACIÓN NACIONAL DE  
QUÍMICOS DE ESPAÑA  
EUROPEAN CHEMICAL  
SCIENCE

**TOPIC C2- Synthesis and reactivity in in Carbon based Compounds**



**Antonio M. Echavarren**

Institute of Chemical Research of Catalonia ICIQ, ES

**Golden Avenues for the Synthesis of Natural Products**

Our group have developed new cascade reactions based on the activation of alkynes cationic gold(I) complexes for the construction of complex cyclic molecules such as orientalol and other sesquiterpenoids. In this lecture, new strategies that have led to the development of efficient routes for synthesis of cannabimovone, ruplellaone A, hushinone, the lundurines, and grandolodine C will be presented.



**6<sup>th</sup>**  
**EuCheMS**  
Chemistry Congress

**SEVILLE** Spain  
**11<sup>th</sup>-15<sup>th</sup>** September **2016**  
Organized by



ANQUE  
ASOCIACIÓN NACIONAL DE  
QUÍMICOS DE ESPAÑA



EUROPEAN CHEMICAL  
SCIENCE

**TOPIC C3- Methods and Mechanisms**



**Alceo Macchioni**

University of Perugia, IT

**Molecular, heterogenized and hydrotalcite-like iridium water oxidation catalysts**

The development of an efficient catalytic system for the oxidation of water, aimed at generating electrons and protons for the photosynthesis of renewable fuels, is one of the most difficult challenges that the scientific community is facing today.

In this contribution, the results of our studies aimed at engineering novel iridium water oxidation catalysts (WOCs) will be illustrated.

Particularly, three classes of WOCs will be considered: molecular organometallic compounds (1), hybrid materials obtained by immobilizing 1 onto TiO<sub>2</sub> (2) and layered double hydroxides doped with iridium (3). Attention will be focused on the effects of changing the nature of L-ancillary ligands in type 1 WOCs (both for catalytic and photocatalytic experiments), the fabrication of robust and recyclable type 2 and 3 WOCs and the possibility of tuning the reactivity of type 3 WOCs by a proper selection of M3-active, M1 and M2 metal centers.



6<sup>th</sup>  
**EuCheMS**  
Chemistry Congress

SEVILLE Spain  
11<sup>th</sup>-15<sup>th</sup> September 2016  
Organized by  
  
ANQUE  
ASOCIACIÓN NACIONAL DE  
QUÍMICOS DE ESPAÑA  


**TOPIC C4- Catalysis in Solution**



**Kyoko Nozaki Nozaki**

University of Tokyo, JP

**Polar Polypropylene: Group 10 Metal Catalyzed Coordination Copolymerization of Propylene with Polar Monomers**

Moderately isospecific homopolymerization of propylene and the copolymerization of propylene and polar monomers were successfully obtained with palladium complexes bearing a phosphine–sulfonate ligand.

The triad isotacticity could be increased to  $mm = 0.59$ , resulting in the formation of crystalline polar polypropylenes, which was supported by the presence of melting points and sharp peaks in the corresponding powder X-ray diffraction patterns.



**6<sup>th</sup>**  
**EuCheMS**  
Chemistry Congress

**SEVILLE** Spain  
**11<sup>th</sup>-15<sup>th</sup>** September **2016**  
Organized by  
  
ANQUE  
ASOCIACIÓN NACIONAL DE  
QUÍMICOS DE ESPAÑA  
  
EUROPEAN CHEMICAL  
SCIENCES

### TOPIC D1- Chemistry in Industry



**Paolo Pollesel**

Eni Spa, IT

### The role of industrial catalytic technologies in the evolving oil refining scenario

The oil production-consumption map is undergoing deep changes due to the discovery of new resources, the development of technologies for the production and processing of non-conventional sources, the evolving regulation, and the economic trend of emerging Countries. These fundamental changes are redefining the worldwide refining industry model with a strong impact on the European refining system. Technology will be a crucial issue to help managing these relevant changes, and catalysis science and technology are particularly important as most of refining technologies are based on catalytic processes.

This presentation resumes a brief history of the catalytic processes used in refinery operations, with a particular focus on cracking technologies, the core of the modern refineries. It is also discussed on how the development of new catalytic technologies can be a key issue to face the changes and to improve the trend for the downstream oil sector. Two examples of technology innovation will be discussed, in two fields which are extremely relevant for the modern refining system.

One is the efficient exploitation of heavy oils and heavy refinery residues, allowing the transformation of the so-called bottom of the barrel into valuable products, and minimizing the formation of low-value by-products such as fuel oil, tarry residues, and coke. Slurry hydrocracking processes are the most suitable and effective technologies to convert heavy residue into middle distillates, which are the products with the highest market demand.

The other example is in the area of biofuels, where new technologies are becoming crucial in order to cope with the evolving regulations. Environmental regulation is not uniform all over the world. Europe is the area that is historically more ready to update the environmental rules and usually adopts more stringent rules. Europe for example has been the first area to decrease sulphur limit in gasoline and diesel below 10 ppm.

At present European regulations are those that more definitely push the use of biocomponents into the transportation fuels pool. Target share of renewable energy in road fuel is set at 10% for 2020. According to this framework, share of biofuels is strongly increasing and demand will reach 20 Mton/y in Europe by 2020. This substitution of fossil fuels will put even more pressure on the refining industry. The increasing demand together with the higher quality requirements for biofuels can be satisfied only with high-level technologies.



6<sup>th</sup>  
**EuCheMS**  
Chemistry Congress

SEVILLE Spain  
11<sup>th</sup>-15<sup>th</sup> September 2016  
Organized by  
ANQUE  
ASOCIACIÓN NACIONAL DE  
QUÍMICOS DE ESPAÑA  
EUROPEAN CHEMICAL  
SCIENCE

### TOPIC D2- Industrial Processes for the 21st Century



**Stefan Mecking**

University of Konstanz, DE

### Catalytic Functionalization of Seed and Algae Oils

Plant oils are attractive raw materials with a unique long-chain structure. For a utilization as monomers for novel materials[1] or to generate e.g. low molecular weight surfactants or lubricants, often compounds with two reactive groups at the ends of a linear chain are required. This contribution addresses novel catalytic routes to such, symmetric or unsymmetric, a,w-difunctional mid- and long-chain compounds.

To achieve a full incorporation of the entire fatty acid chain length, isomerizing functionalizations[2] are pursued which convert the double bonds deep in the chain of unsaturated fatty acids to a terminal functional group selectively. Further, concepts to multiply the fatty acids chain length are of interest.

This contribution reports novel functionalization approaches and addresses underlying mechanisms and practical aspects like catalyst compatibility with technical grade plant oil substrates under pressure reactor conditions.



**6<sup>th</sup>**  
**EuChE MS**  
**Chemistry Congress**

**SEVILLE** Spain  
**11<sup>th</sup>-15<sup>th</sup>** September **2016**  
Organized by  
  
ANQUE  
ASOCIACIÓN NACIONAL DE  
QUÍMICOS DE ESPAÑA  
  
EUROPEAN CHEMICAL  
SCIENCES

### TOPIC D3- Catalysis at Interfaces



**Ferdi Schüth**

Max-Planck-Institute. DE

### Controlled nanostructures for applications in catalysis

Over the last decades, tremendous progress has been made in the control of catalytic materials on the nanometer size scale. This includes tailoring of pore sizes of catalytic materials by different soft and hard templating techniques, size control of catalytically active metal particles by solution phase synthesis of such particles and subsequent deposition on supports, the placement of catalytic particles in desired locations of structured support materials, and the design of solid environments which resemble ligand motifs of molecular catalysts.

The placement of catalytically active particles in desired locations of structured supports is an interesting technique for the creation for composites with novel properties. Hollow shell supports allow the synthesis of a variety of different catalysts with outstanding performance. Encapsulation of single metal particles in hollow shells made of zirconia, titania or carbon allows the synthesis of catalysts which are stable against sintering, since individual particles are encapsulated and therefore can not migrate towards each other, which prevents sintering. This pathway is highly flexible, if the parameters are fine-tuned, and a wide range of catalysts is accessible. An interesting variant of this process relies on the synthesis of hollow spheres of carbon with mesopores in the carbon shells. If platinum particles are deposited in the mesopores of the shell, the platinum dispersion is thermally extremely stable. Importantly, this material is also a very active and stable fuel cell catalyst, and both rotating disc electrode measurements as well as measurements using a working membrane-electrode-assembly prove the high stability of this system. The approach can be extended to allow the formation of alloyed nanoparticles by confined space alloying.

Modified resorcinol-formaldehyde resins allow incorporation of metal species into the polymer in a highly controlled manner. Subsequent carbonization gives access to carbon-supported metal, alloy, or metal oxide particles. These catalysts were found to be useful for a variety of reactions. RF-gels proved an excellent platform for the synthesis of a wide variety of high performance catalysts.

Finally, the synthesis of solids having ligand motifs of the Periana catalyst for the oxidation of methane to methylbisulfate (which can be hydrolyzed to methanol) has recently become possible. Such solids can be impregnated with suitable platinum species, upon which solid analogues to the Periana system result, with comparable catalytic activity for methane oxidation. In addition, by careful choice of reaction conditions, activities for methane oxidation with a related molecular system could be achieved which are unprecedented in methane activation at TOFs exceeding 25.000 h<sup>-1</sup>



6<sup>th</sup>  
**EuCheMS**  
Chemistry Congress

SEVILLE Spain  
11<sup>th</sup>-15<sup>th</sup> September 2016  
Organized by  
 ANQUE  
ASOCIACIÓN NACIONAL DE  
QUÍMICOS DE ESPAÑA  
 EUROPEAN CHEMICAL  
SCIENCES

### TOPIC E1- Materials Chemistry



**Peter Seeberger**

Max-Planck Institute, DE

### **Automated Glycan Assembly as Basis for Molecular Glycobiology, Vaccine Development and Material Science**

Pure glycans are key to enable biochemical, biophysical and immunological studies aimed at understanding the role of carbohydrates. Described is the development of a fully integrated platform for automated glycan assembly (AGA) based on solid-phase oligosaccharide synthesis<sup>1</sup> and carbohydrate arrays to address biological problems. Particular emphasis in this lecture will be placed on the new automated synthesis platform<sup>2</sup> that has been commercialized. <sup>3,4</sup> Access to defined polysaccharides as long as 50-mers enables now biological as well as materials science investigations. <sup>5</sup> These synthetic polysaccharides can be combined much like “molecular LEGO” to create even larger oligosaccharide assemblies. Quality control of synthetic glycans can now be guaranteed using ion mobility mass spectrometry to very low levels. <sup>6</sup>

Carbohydrate arrays are used as diagnostics and in support of vaccine programs that are based on conjugates with synthetic oligosaccharides to screen blood sera.<sup>7</sup> Case studies of specific vaccines will provide an appreciation for the approach that is now advancing candidates toward clinical testing. <sup>8,9</sup> Fully synthetic vaccine candidates exploit iNKT cells for to induce a robust and protective immune response.<sup>10</sup>



**6<sup>th</sup>**  
**EuCheMS**  
Chemistry Congress

**SEVILLE** Spain  
**11<sup>th</sup>-15<sup>th</sup>** September **2016**  
Organized by



ANQUE  
ASOCIACIÓN NACIONAL DE  
QUÍMICOS DE ESPAÑA



EUROPEAN CHEMICAL  
SCIENCE

### TOPIC E2- Nanomaterials, Devices, Technology and applications



**Luis M. Liz-Marzán**

CIC biomaGUNE, ES

### Synthesis and Chemical Modifications in Metal Nanocrystals

The growth of colloidal metal nanoparticles with controlled size and shape is one of the most promising ways toward the fabrication of nanomaterials and devices. It has been reported that the final nanocrystal shape is defined by the crystalline structure of the initial nuclei, as well as by the presence of ligands and capping agents that help stabilizing certain crystallographic facets. This talk will focus on recent progress on the understanding of the role of surfactants, counter-ions, as well as crystalline structure of seeds during the growth of gold nanocrystals, as well as the morphological changes derived from using such nanorods as seeds for overgrowth through additional gold reduction.

Under different growth conditions, the morphological changes and corresponding optical effects can be drastically different, which may provide important hints related to the growth mechanism of the nanoparticles. Recent understanding on the so-called galvanic replacement reaction will be discussed, in relation with the application of modern electron microscopy and the synthesis of more complex nanocrystals.



**6<sup>th</sup>**  
**EuCheMS**  
Chemistry Congress

**SEVILLE** Spain

**11<sup>th</sup>-15<sup>th</sup>** September **2016**

Organized by



**TOPIC E3- Analytical Techniques, Characterisation and Properties**



**Christoph Janiak**

Universität Düsseldorf, DE

**Metal Nanoparticles in Ionic Liquids - from Synthesis to Catalysis**

We present the use of ionic liquids (ILs) as solvents for the synthesis [1,2] (Fig. 1) and catalytic application [3] of stable metal nanoparticles without the need of additional stabilizers, including their deposition on surfaces [4] (Fig. 2) and quantized charging [5].

Fig 1 Ionic liquids as templates for stable metal nanoparticles without the need of additional stabilizers [1]. Fig. 2 Microwave-induced organometallic precursor decomposition in the presence of thermally reduced graphite oxide (TRGO) in ILs to give metal nanoparticles (M-NPs) deposited on TRGO: (from left to right) Ru-NP@TRGO [4c], Ir-NP@TRGO [4a] and Pt-NP@TRGO-SH [4b]. The IL also exfoliates the TRGO sheets.



**6<sup>th</sup>**  
**EuCheMS**  
Chemistry Congress

**SEVILLE** Spain  
**11<sup>th</sup>-15<sup>th</sup>** September **2016**  
Organized by  
 ANQUE  
ASOCIACIÓN NACIONAL DE  
QUÍMICOS DE ESPAÑA  
 EUROPEAN CHEMICAL  
SCIENCE

### TOPIC E4- Carbon Based Nanochemistry



**Nazario Martín**

Universidad Complutense , ES

### Giant multivalent glycofullerenes as potent inhibitors of Ebola virus infection

In the burgeoning area of nanoscience, the study of carbon nanomaterials for biomedical applications is currently a hot topic which has not been properly addressed so far. These carbon-based nanomaterials upon the appropriate chemical modification has allowed increasing their biocompatibility and to provide new biological properties.

On the other hand, multivalency plays a key role in the protein-glycan recognition events which usually take place in the initial steps of pathogenic infection and also at some stages of the immune response. The search for high-affinity ligands for the study and understanding of the mechanisms involved in multivalent interactions has yielded a wide variety of artificial glycoconjugates. Furthermore, SWCNTs and SWCNHs constitute a less-explored type of unconventional and biocompatible scaffolds for the preparation of new glycoconjugates for a multivalent presentation of carbohydrates.

We have recently shown that fullerene sugar balls, namely hexakis-adducts of [60]fullerene appended with 12, 24 or 36 mannose moieties, act as strong inhibitors for DC-SIGN in an Ebola infection assay model.<sup>1</sup> Furthermore, a drastic increase in the inhibition process to the subnanomolar scale has been observed when the size and mannoses' number are increased in the tridecafullerenes endowed with 120 mannose units decorating the periphery of the molecule.<sup>2</sup>

In this presentation, we report the aforementioned results as well as how SWCNTs and SWCNHs have also been employed as virus mimicking nanocarbons platforms for the multivalent presentation of carbohydrates in an artificial Ebola virus infection model. All carbon nanoforms have been chemically modified by the covalent attachment of glycofullerenes using the CuAAC "click chemistry" approach. This modification dramatically increases the water solubility of these structurally different nanocarbons. Their efficiency to block DC-SIGN mediated viral infection by an artificial Ebola virus has been tested in a cellular experimental assay finding that glycoconjugates based on 3D Dahlia Flower shaped SWCNHs behave as potent inhibitors of viral infection.



6<sup>th</sup>  
**EuCheMS**  
Chemistry Congress

SEVILLE Spain  
11<sup>th</sup>-15<sup>th</sup> September 2016  
Organized by  
ANQUE  
ASOCIACIÓN NACIONAL DE  
QUÍMICOS DE ESPAÑA  
EUROPEAN CHEMICAL  
SCIENCE

### TOPIC F1- States of Matter



**John Maier**

University of Basel, CH

### Electronic spectrum of C<sub>60</sub><sup>+</sup> in the gas-phase at 6K

After the discovery of C<sub>60</sub> (1), the question of its relevance to the diffuse interstellar bands was raised. In 1987 H.W.Kroto wrote: "The present observations indicate that C<sub>60</sub> might survive in the general interstellar medium (probably as the ion C<sub>60</sub><sup>+</sup>)" (2). In 1994 two diffuse interstellar bands (DIBs) at 9632 and 9577 Å were detected and proposed to be the absorption features of C<sub>60</sub><sup>+</sup> (3). This was based on the proximity of these wavelengths to the two prominent absorption bands of C<sub>60</sub><sup>+</sup> measured by us in a neon matrix in 1993 (4).

Confirmation of the assignment required the gas phase spectrum of C<sub>60</sub><sup>+</sup> and has taken 20 years. The approach which succeeded confines C<sub>60</sub><sup>+</sup> ions in a radiofrequency trap, cools them by collisions with high density helium allowing formation of the weakly bound C<sub>60</sub><sup>+</sup>– He complexes below 10 K. The photofragmentation spectrum of this mass-selected complex is then recorded using a cw laser. In order to infer the position of the absorption features of the bare C<sub>60</sub><sup>+</sup> ion, measurements on C<sub>60</sub><sup>+</sup>– He<sub>2</sub> were also made. The spectra show that the presence of a helium atom shifts the absorptions by less than 0.2 Å, much less than the accuracy of the astronomical measurements. The two absorption features in the laboratory have band maxima at 9632.7(1) and 9577.5(1) Å, exactly the DIB wavelengths, and the widths and relative intensities agree. This leads to the first definite identification of now five bands among the five hundred or so DIBs known and proves the presence of gaseous C<sub>60</sub><sup>+</sup> in the interstellar medium (5), (6).

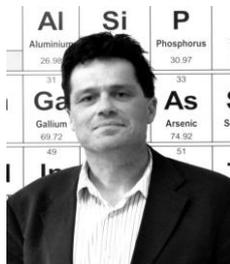
The electronic spectrum of cold C<sub>70</sub><sup>+</sup> has also been obtained by this approach. The implications for the relevance of fullerene cations in general in the interstellar medium can be discussed.



6<sup>th</sup>  
**EuCheMS**  
Chemistry Congress

SEVILLE Spain  
11<sup>th</sup>-15<sup>th</sup> September 2016  
Organized by  
ANQUE  
ASOCIACIÓN NACIONAL DE  
QUÍMICOS DE ESPAÑA  
EUROPEAN CHEMICAL  
SCIENCE

### TOPIC F2- Properties of Materials



#### Matthew Rosseinsky

University of Liverpool , UK

#### Design of Advanced Materials?

The development of advanced materials will increasingly rely on our ability to assemble complex compositions in an ordered and predictable manner to generate enhanced properties. It is attractive to harness the ever-increasing power of computation in the search for new materials, but the scale and nature of the problem make brute force de novo approaches challenging, while “big data” searches for analogues of existing structures in databases cannot identify potentially transformative new structures. Building chemical knowledge into computational tools used together with experiment offers a different approach. I will present an example of crystal chemically-informed computational identification of a new solid oxide fuel cell cathode (1).

This integrated approach has recently allowed us to combine permanent magnetism and electrical polarisation in a single phase material above room temperature (2), a major challenge in materials synthesis because of the competing electronic structure requirements of these two ground states. As a counterpoint, we have recently used a non-computational multiple length scale symmetry control strategy to switch both of these long-range orders in a magnetoelectric multiferroic at room temperature (3). This emphasises the enduring importance of developing the crystal chemical understanding that drives “classical” approaches to materials design.



6<sup>th</sup>  
**EuCheMS**  
Chemistry Congress

SEVILLE Spain  
11<sup>th</sup>-15<sup>th</sup> September 2016  
Organized by  
ANQUE  
ASOCIACIÓN NACIONAL DE  
QUÍMICOS DE ESPAÑA  
EUROPEAN CHEMICAL  
SCIENCES

### TOPIC F3- Polymers



**Harm-Anton Klok**

Polymers Laboratory LP. CH

### Mechanochemistry of surface-grafted polymers

Mechanical forces can trigger chemical reactions of polymers. Mechanical activation of polymers is typically accomplished using e.g. turbulent and elongational flow fields as well as ultrasound. This presentation will introduce surface-initiated polymerization reactions as an alternative mechanochemical tool to subject polymers to elongational forces.

Surface-initiated polymerization techniques can be used to generate assemblies of chain-end tethered polymers that are spaced at distances that are so short that neighboring chains are forced into a stretched conformation (“polymer brushes”). This approach is characterized by a number of unique features that make it very attractive for polymer mechanochemistry. These include (i) the absence of a need for an external force field to induce chain elongation and (ii) the possibility to systematically investigate the influence of chain stretching on chemical reactivity by varying the film thickness and grafting density. It will be shown how swelling-induced chain stretching can result in mechanochemically augmented hydrolytic bond cleavage and degrafting of surface-tethered polymer chains. These degrafting reactions can be modulated by adjusting the layer thickness as well as grafting density of the polymer brush films as well as the nature of the surface-tethered polymerization initiator.

Understanding these fundamental phenomena may pave the way towards novel responsive surfaces.



**6<sup>th</sup>**  
**EuCheMS**  
Chemistry Congress

**SEVILLE** Spain  
**11<sup>th</sup>-15<sup>th</sup>** September **2016**  
Organized by  
 ANQUE  
ASOCIACIÓN NACIONAL DE QUÍMICOS DE ESPAÑA  
 EUROPEAN CHEMICAL SCIENCES

### **TOPIC F4- Innovative Computational Environments for Molecular Science**



**Gabor Terstyanszky**

University of Westminster, UK

### **European Research Infrastructure for the Chemistry Community**

Currently there are isolated “islands” of research facilities and e-infrastructure resources that are not available for the whole Chemistry community in Europe. Integrating existing research facilities with computing and data resources into an European Research Infrastructure, called Sumo-Chem RI, will enable joint research involving Computational and Experimental Chemistry and even other research communities.

It will have an open architecture to allow its extension with further research facilities and resources to be used by scientists.

Computational Chemists will be able to design and implement applications as a service to simulate molecular properties using the computing and data resources of the RI. The Experimental Chemists will design and run laboratory experiments aimed at checking the results of the performed simulations using the research facilities of the research infrastructure. This infrastructure will allow designing more advanced experiments and creating more accurate simulations using European, regional and national research facilities and e-infrastructure resources through an intuitive and seamless virtual access considering different levels of their expertise and skills.

The major innovation of Sumo-Chem will be the scientific data management covering the whole lifecycle of data using metadata, ontologies and provenance based on advanced data and computing services. Sumo-Chem RI will also enable and support multi-disciplinary research in cooperation with ESFRI and other major research initiatives to address climate, energy and life science societal challenges. The Chemistry community identified eight use cases as first users of the infrastructure to represent the heterogeneity of this community.

The presentation will outline the concept of the Sumo-Chem RI, how it will provide access to e-infrastructure resources and research facilities, how it will manage data and how the selected use cases will use this RI.



**6<sup>th</sup>**  
**EuCheMS**  
Chemistry Congress

**SEVILLE** Spain  
**11<sup>th</sup>-15<sup>th</sup>** September **2016**  
Organized by



ANQUE  
ASOCIACIÓN NACIONAL DE  
QUÍMICOS DE ESPAÑA



EUROPEAN CHEMICAL  
SCIENCE

### TOPIC G1- Analytical and Physical Methods



**Alfredo Sanz-Medel**

University of Oviedo, ES

### Advances on plasma ion sources and mass analysers for deeper insights into chemical speciation and proteomics

The classical boundaries and tools of Atomic Spectrometry are blurring nowadays. Atomic spectroscopists one day studying photon/atoms interactions, are today investigating also the molecules constituting their samples (i.e. chemical speciation). On the other hand, more and more bioscientists are learning to make use of analytical strategies of atomic spectrometry and chemical speciation (e.g. in proteomics). The outstanding analytical potential of mass spectrometry (MS) is becoming the chemical ladder to scalate from isotopes, atoms, elements and molecules up to nanoparticles and nanostructures of matter. An atmospheric plasma ion source (e.g. ICP) with a mass analyser and an appropriate separation could form the basis for analysing directly metalloproteins. In any case that elemental speciation using ICP-MS, should be completed with the corresponding molecular (MALDI- or ESI-MS) information for “integrated” chemical speciation.

These combinations are opening new avenues and insights in bioscience. Traditionally, the biologically relevant non-metals S and P have been elusive to sensitive ICP-MS determinations. However, the new ICP(QQQ)MS instruments enable S and P analysis at very low limits of detection (orders of magnitude better than ICP-MS used before).

This sensitive S and P determinations turns out to be of critical importance to allow direct absolute quantification of proteins or of protein phosphorylations (by S and P simultaneous determinations) for targeted proteomics. Also, highly amplified ICP-MS detections can be achieved by tagging the protein of interest with metal nanoparticles (NPs). The high number of ICP-MS detectable atoms, per NP tag, enables a much higher sensitivity of the corresponding proteins by metal NPs tagged immunoassays.

What is more, such amplifications can be enhanced by orders of magnitude if we select a special NP (e.g. ZnS(Mn) QDs) which, by a spontaneous catalytic reduction, deposits on its surface relatively huge amounts of native gold from a Au(III) proper solution. Subsequent elemental detection of this Au by ICP-MS allows an ultra-sensitive indirect determination of the NP-tagged protein. We will illustrate the developed immunoplatform and its extraordinary performance for real-life determinations of extremely low levels in human serum of “early alarm biomarkers” of cancer (e.g. prostate specific antigen, PSA). A less known low-pressure plasma-MS instrumental development is the Pulsed Glow Discharge-Mass Spectrometer (PP-GDMS(TOF)) developed in part in our laboratory.

Characteristics and analytical applications, simultaneous speciation, elemental depth profiling of nm-layered materials and elemental/molecular screening of polymeric materials will be described. At this moment the first worldwide commercial PP-GDMS(TOF) is available in our Research Group in Oviedo and its actual analytical potential for nm-depth profiling and speciation in the solid will also be discussed.



6<sup>th</sup>  
**EuCheMS**  
Chemistry Congress

SEVILLE Spain  
11<sup>th</sup>-15<sup>th</sup> September 2016  
Organized by  
ANQUE  
ASOCIACIÓN NACIONAL DE  
QUÍMICOS DE ESPAÑA  
EUROPEAN CHEMICAL  
SCIENCE

### TOPIC G2- Determination of Structure and Physical Properties



**Armin Gölzhäuser**

University of Bielefeld, DE

### Imaging, Modification, and Analysis of Nanostructures with Helium Ions

The Helium Ion Microscope (HIM) is a scanning microscope that utilizes a focused beam of helium ions to image and modify materials with high spatial resolution and chemical sensitivity. A HIM can be envisioned as a scanning electron microscope (SEM) with a helium ion beam. The helium ion beam can be focused into a smaller diameter than an electron beam, and the HIM is thus capable to resolve features down to 0.25 nm. Helium ions are also more surface sensitive than electrons and they interact more strongly with matter. HIM images thus show much stronger chemical and topographical contrasts than SEM images. The HIM is further capable to image not only conductive, but also insulating samples without special treatment. This allows the investigation of unstained biomaterials and cell surfaces. When applying higher ion currents, the HIM can be also used for the modification and the milling of materials.

The presentation will contain various examples of HIM imaging. A particular focus is laid on the imaging of 2D materials. 1 nm thick carbon nanomembranes (CNMs) [1] can be engineered with a controlled thickness, elasticity, conductivity and porosity [2,3,4]. HIM images provide valuable information to understand the structure of CNMs and their formation process [5]. The capability of the HIM for nanolithography will be shown by examples of milling CNMs and graphene, where nanopores with diameters down to 1.3 nm were fabricated. HIM imaging of different carbon materials as well as of biological cells [6] will also be discussed.



**6<sup>th</sup>**  
**EuCheMS**  
Chemistry Congress

**SEVILLE** Spain  
**11<sup>th</sup>-15<sup>th</sup>** September **2016**  
Organized by



ANQUE  
ASOCIACIÓN NACIONAL DE  
QUÍMICOS DE ESPAÑA



EUROPEAN CHEMICAL  
SCIENCE

**TOPIC G3- Chemical Dynamics**



**Juergen Troe Troe**

University of Goettingen, DE

**Insight into Reaction Mechanisms through Quantitative Kinetics**

Thermally, chemically, or photochemically activated molecular species often possess a variety of pathways for reaction. Insight into details of these mechanisms can be obtained by kinetic experiments combined with quantum-chemical and rate theories.

This talk illustrates the state of the art by describing thermal decomposition studies of unsaturated fluorocarbons, bond activation experiments with transition metal(oxide) cations, and non-Born-Oppenheimer collisional energy transfer and open-electronic shell radical reaction processes.



6<sup>th</sup>  
**EuCheMS**  
Chemistry Congress

SEVILLE Spain  
11<sup>th</sup>-15<sup>th</sup> September 2016  
Organized by  
 ANQUE  
ASOCIACIÓN NACIONAL DE QUÍMICOS DE ESPAÑA  
 EUROPEAN CHEMICAL SCIENCES

### **TOPIC H1- Drug Discovery and Chemical Biology**



**William Zuercher**

University of North Carolina at Chapel Hill, USA

### **Illuminating the historically understudied kinome with open access chemical probes**

Despite the approval of more than 30 small molecule kinase inhibitors for the treatment of human disease since the turn of the century, the kinome remains to be more fully elucidated. Indeed, over 80% of human kinases are poorly studied and have insufficiently understood roles in human (patho)biology.

Access to high-quality chemical and biological enabling reagents is a critical step to enabling researchers to shift their attention towards such historically understudied proteins. In this presentation, we will present examples of our efforts to generate and make openly available chemical probe sets for kinases which have received scant attention to date.

We will also describe our strategy to experimentally prioritize members of the historically understudied kinome.



**6<sup>th</sup>**  
**EuCheMS**  
Chemistry Congress

**SEVILLE** Spain  
**11<sup>th</sup>-15<sup>th</sup>** September **2016**  
Organized by

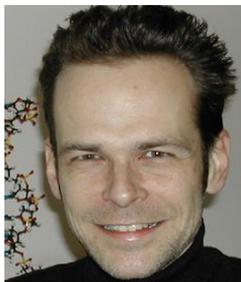


ANQUE  
ASOCIACIÓN NACIONAL DE  
QUÍMICOS DE ESPAÑA



EUROPEAN CHEMICAL  
SCIENCE

### TOPIC H2- Bio-macromolecules



**Ronald Micura**

University of Innsbruck, AT

### Chemically modified RNA to explore riboswitch and ribozyme function

Riboswitches are gene regulation elements in mRNA that function without the assistance of proteins, responding instead to the specific recognition of small-molecule ligands.[1] Likewise, ribozymes that accelerate specific cleavage of their own phosphate backbones play important biological roles, including self-scission during rolling-circle replication of RNA genomes, co-transcriptional processing of retrotransposons, and metabolite-dependent gene expression regulation in bacteria.[2]

This talk will cover our recent investigations on mRNA riboswitches and ribozymes, using chemical and biophysical methods, including NMR and fluorescence spectroscopy, and single-molecule fluorescence resonance energy transfer (smFRET) imaging. Chemical modification of these RNA systems is a prerequisite not only to apply spectroscopic methods but also to probe their function by atomic mutagenesis approaches. For that, access to the appropriate modification pattern implies intensive efforts in chemical synthesis.[3]

Unprecedented insight has been achieved into the dynamics of selected riboswitches[4,5] and of novel ribozyme classes that shed new light on the mechanism of RNA-mediated transcriptional and translational regulation, and on ribozyme catalysis.[6,7]



**6<sup>th</sup>**  
**EuCheMS**  
Chemistry Congress

**SEVILLE** Spain  
**11<sup>th</sup>-15<sup>th</sup>** September **2016**  
Organized by  
  
ANQUE  
ASOCIACIÓN NACIONAL DE  
QUÍMICOS DE ESPAÑA  
  
EUROPEAN CHEMICAL  
SCIENCES

### **TOPIC H3- Methods and Applications**



#### **Silvio Aime**

University of Torino , Italy

#### **Design and testing of Probes for Functional and Molecular Imaging. Exploring routes to enhance sensitivity and specificity of MRI agents**

The possibility of exploiting the superb anatomical resolution of MRI continues to make this modality highly desirable for Molecular Imaging applications in spite of the low sensitivity of the currently available contrast agents. Whereas chemists have tackled this issue by designing novel structures endowed with enhanced sensitivity, important achievements have also been reached by using nanocarriers (e.g. apoferritin, LDL or liposomes, etc.) able to deliver a large number of paramagnetic agents to the targeting sites. This approach is bringing relevant insights also to the emerging field of imaging-guided drug delivery (“theranostics”)1. Besides paramagnetic relaxation systems (e.g. Gd(III) or Mn(II) complexes), two new classes of frequency-encoding probes, namely the CEST agents (CEST= Chemical Exchange Saturation Transfer) and the class of hyperpolarized molecules, have been considered as powerful tools for MR-Molecular Imaging applications.

The use of frequency-encoding agents has opened the interesting perspective of detecting more than one agent in the same anatomical region2. Moreover, hyperpolarized molecules have the potential for being a real breakthrough as diagnostic agents reporting on cellular metabolism and transport across cellular membranes3. The design of properly functionalized precursors has allowed to achieve the formation of hyperpolarized molecules (e.g. pyruvate) by the route based on the use of para-Hydrogen4.

All together, the development in the design and testing of new probes has significantly improved the potential of MRI in respect to competing imaging modalities.



6<sup>th</sup>  
**EuCheMS**  
Chemistry Congress

SEVILLE Spain  
11<sup>th</sup>-15<sup>th</sup> September 2016  
Organized by  
ANQUE  
ASOCIACIÓN NACIONAL DE  
QUÍMICOS DE ESPAÑA  
EUROPEAN CHEMICAL  
SCIENCE

### TOPIC H4- In-silico Methods in Life Sciences



**Rebecca Wade-**

University of Heidelberg.DE

### In silico prediction of biomolecular recognition

I will describe the application of molecular modelling and Brownian [1] and molecular dynamics simulation methods to studying how proteins recognise their diverse binding partners. We consider specific and non-specific interactions between proteins and between proteins [2,3] and inorganic surfaces [4,5]. Implications for protein and small molecule design will be discussed.



6<sup>th</sup>  
**EuCheMS**  
Chemistry Congress

SEVILLE Spain  
11<sup>th</sup>-15<sup>th</sup> September 2016  
Organized by  
 ANQUE  
ASOCIACIÓN NACIONAL DE QUÍMICOS DE ESPAÑA  
