



4th European Chemistry Congress

May 11-13, 2017 Barcelona, Spain

Scientific Tracks & Abstracts Day 1

Euro Chemistry 2017

Organic Chemistry | Inorganic Chemistry | Analytical Chemistry | Green Chemistry: Green Chemical Principles | Materials Chemistry

Session Chair

Ju Chou

Florida Gulf Coast University, USA

Session Co-Chair

Judit Tulla-Puche

University of Barcelona, Spain

Session Introduction

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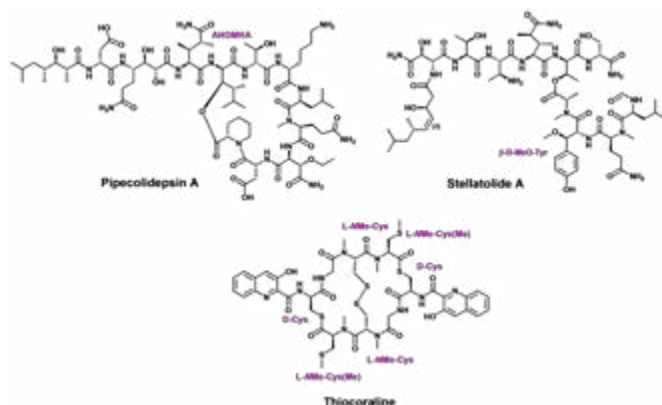
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The synthesis of complex marine depsipeptides

Judit Tulla-Puche¹ and Ramon Y Cajal²^{1,2}University of Barcelona, Spain

Marine organisms are a rich source of bioactive molecules. Among them, cyclodepsipeptides show relevant biological profiles, mostly including cytotoxic and anti HIV activities, and they are, therefore, promising candidates for medicinal chemistry programs. Herein, we report the synthesis of the potent antineoplastic agents pipecolidepsin A and Stellatolide A, “head-to-side-chain” cyclodepsipeptides, where the C-terminus is linked to a γ -hydroxy group via an ester bond, and of thiocoraline, a bicyclic thiodepsipeptide that acts as bisintercalator. The three molecules present extremely challenging structures. Pipecolidepsin A bears the unprecedented and extraordinary bulky AHDMHA residue at the branching point, which makes the construction of the extremely hindered ester bond the major synthetic challenge to overcome. On the other hand, the high propensity of the unnatural γ -MeO-D-Tyr residue in Stellatolide A to suffer decomposition is the main limitation of its assembly. Finally, Thiocoraline’s large amount of cysteines in a rather small structure represents the principal restraint. The successful solid-phase synthetic strategies that resulted in the three synthetic and active cyclodepsipeptides will be discussed.



Biography

Judit Tulla Puche received her Ph.D. in organic chemistry (2004) from the University of Minnesota under the supervision of Prof. George Barany. Her thesis dealt with the solid-phase synthesis of small proteins. After finishing her doctoral studies, she joined the group of Prof. Fernando Albericio at the Institute for Research in Biomedicine (IRB) where she became Research Associate, working on the synthesis of marine antitumor depsipeptides and complex peptides. In 2015, and after obtaining a Ramon y Cajal contract, she moved to the Department of Organic Chemistry at the University of Barcelona to establish her own research group. Her research interests span a broad range of topics at the interfaces of peptide chemistry and chemical biology.

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Green synthesis and characterization of stable gold nanoparticles from various fruits juices and fruit waste for biomedical applications

Ju Chou¹, Bo Yang² and Qingsong Yu³¹Florida Gulf Coast University, USA²Xi'an Shiyu University, China³University of Missouri Columbia, USA

Statement of the Problem: Gold nanoparticles (AuNPs) have diverse biomedical applications. However, when chemically reduced AuNPs were used in biological tests such as toxicity in various cells, the results often varied. One of important factors which lead to inconclusive results is that the chemicals used to make AuNPs might be still present in the AuNPs solutions used. This study focuses on the green synthesis of gold nanoparticles with fruit juices and fruit wasters without adding any toxic chemicals which is crucial for biomedical applications. Gold nanoparticles with different particle sizes were synthesized by the reduction of HAuCl₄ using only fruit juices/extracts. Similar to fruit juices, fruit wastes such as fruit skins were found to contain various antioxidants and were able to make different sizes of gold nanoparticles. The spherical gold nanoparticles could be controlled by adjusting solution pH to obtain small and narrow size distribution. By adjusting the pHs of the solutions and the chemical reaction step, the sizes of AuNPs could be fine-tuned to 4.5±2.0 nm, 5.9±2.5 nm and 6.0±1.5 nm with fruit juices and fruit wastes. For the first time, stable and spherical AuNPs with ultrasmall size of 2.6±1.1nm and uniform distribution were successfully achieved using a fruit extract. UV-visible spectroscopy (UV-vis), transmission electron microscopy (TEM) and high resolution transmission electron microscopy (HRTEM) were used to characterize the morphology and size distribution of AuNPs produced through the green synthesis. The results indicate that AuNPs synthesized in this study are highly stable at room temperature and in general biological medias. More importantly the small and ultrasmall AuNPs were able to be imaged or monitored by dark-field optical microscopy which allows to monitor AuNPs in a live, single cell and this holds great promise in biomedical applications.

Biography

Ju Chou is currently an Associate Professor in the Department of Chemistry and Physics at Florida Gulf Coast University. Dr. Chou received her Ph.D. in chemistry from Chinese Academy of Science, Changchun, China in 1995. After that, Dr. Chou worked as a postdoctoral fellow in RIKEN Research Institute in Japan for a year and then came to the United States as a visiting research scholar working at University of California-Irvine and later at University of California-Santa Barbara. Dr. Chou's research areas include bio-electrochemistry of proteins, bioaccumulation of trace elements in tissues, synthesis and characterization of nanomaterials. Dr. Chou's recent research interests also include green synthesis of gold nanoparticles and environmental analysis of toxic metals in water and human hair. She is also collaborating with biology professors on the application of gold nanoparticles. This research focuses studying toxicity, biocompatibility and transport of gold nanoparticles in membranes and cancer cells.

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Electrodeposition of nickel on glassy carbon electrode: The rotating disk study

Batric Pesic

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Electrodeposition of nickel was studied by using rotating disk technique. The electrode substrate was glassy carbon disk cut from a glassy carbon wafer produced by Toshiba. The disk was mounted on a rotation speed controlled rotator made by IBM Instruments. The electrochemical deposition was studied from nickel ammonium sulfate solutions of different concentrations and pH, as the reaction parameters. The electrochemical techniques used were cyclic voltammetry, linear sweep voltammetry, and chronoamperometry. The key feature of this study is that amount of electrodeposited disk was determined by two methods i.e. charge passed and amount of nickel deposited at particular time intervals, such as 15, 30 and 60 seconds. Charge was determined by using a coulometer wired in line with the working electrode. Nickel deposited was determined by dissolution in nitric acid and analysis by atomic absorption. Both types of data were used in Levich equation for determination of kinetic parameters, such as reaction order, activation energy, etc. For example, it was found that electrodeposition of nickel is of first order, and that the activation energy was only 2.7 kcal/mol indicating, a mass transfer controlled reaction. The current efficiency was a function of concentration, increasing with the increase of nickel concentration. Morphology of electrodeposit was very smooth as confirmed by atomic force microscopy.

Biography

Batric Pesic is a distinguished Professor at the University of Idaho. He has received BS degree in Metallurgical Engineering from the University of Belgrade; MS (1976) and PhD (1982) from the University of Utah, USA. Upon graduation, he moved to Canada and worked for HBMS, Flin Flon, Manitoba. In 1983, he joined the University of Idaho, USA. His research interests have been, initially in extractive metallurgy, followed by environmental subjects. Currently, he is doing his research on electrochemistry of molten salts. He has extensive consulting experience with major chemical and metallurgical corporations in North America, Europe and Africa.

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Hydrogen generation from hydrous hydrazine using Ir-based nanocatalysts

Davide Motta

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Modern society relies on oil and hydrocarbon to satisfy its energy requirements. However, the usage of oil is depleting the world resources and increases the emission of greenhouse gases, leading to grave consequences for the whole planet. In this optics the research for new cleaner and renewable energy sources is necessary more than needed, between this hydrogen has created a lot of interest as both fuel and energy carriers. Hydrogen has an energy density three times higher than petroleum i.e., 120 kJ g^{-1} , can be released with high efficiency using fuel cell systems combined with electrical engines. Moreover, fuel cells are clean energy systems that produce only water as by-product, in this way the level of pollutant and greenhouse gases can be reduced in the atmosphere. Main drawback for hydrogen application is the need to find an efficient and safe method of transportation. From this point of view, chemical liquid storage systems like hydrazine and formic acid are really promising platform for large scale application of fuel cell system. We used iridium-based catalysts to catalyze the decomposition of hydrous hydrazine into molecular hydrogen and nitrogen. The catalyst has been prepared using different preparation methods like deposition-precipitation and sol-immobilization and bimetallic systems using other metals such as Fe and Ni. The activity of the catalysts have been measured showing promising results for the generation of H_2 , while the catalysts have been characterized by different techniques like TEM, XPS, SEM and CO-chemisorption.

Biography

Davide Motta is a PhD student at Cardiff University, as part of CDT in Catalysis between the University of Bath, Bristol and Cardiff University. He has done his Master's degree in Industrial Chemistry from the University of Milan in 2014 and a Master of Research in Catalysis from the Cardiff University in 2015.

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Phosphor solutions for the reduction of the time dependant intensity variation of AC LEDs

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AC driven LEDs show very high wall plug efficiency combined with a good colour rendering and long-term stability. For general lighting, LEDs have surpassed the traditional incandescent and fluorescent lamps years ago. (1) However, LEDs still have a tremendous drawback, which is known as flicker. Perceived flicker is caused by the time dependant variation of the luminous intensity of a light source. The consequences for humans under such illumination situations expand from headaches to neurological problems, even including epileptic seizure (2). Since many research activities in this field are conducted to solve or to reduce problems accompanied by flicker, we came up with a possible solution to it. Since the zero point of an AC current cannot be turned out completely, the solution must be based on the used conversion layer (mostly a phosphor particle or ceramic layer) or a combination of a driver systems and the used converter in order to smoothen the Flicker to 100%. In this work a couple of standard LED phosphors have been tested, such as $Y_3Al_5O_{12}:Ce^{3+}$, $BaMgAl_{10}O_{17}:Eu^{2+}Mn^{2+}$, $CaAlSiN_3:Eu^{2+}$, $Ca_3Sc_2Si_3O_{12}:Ce^{3+}Mn^{2+}$ and $Sr_2P_2O_7:Eu^{2+}Mn^{2+}$ with respect to flicker reduction. It will be demonstrated why $Y_3Al_5O_{12}:Ce^{3+}$ won't lead to a solution for this problem and possible solutions will be discussed. The capability of other phosphors to reduce flicker will be shown. From these findings requirements for the development of novel phosphors to reduce the flicker problem will be drawn. A prediction will be given concerning the future potential of this technique and achievements so far will be presented.

Biography

Simon Korte has gained his bachelor degree in chemical engineering and his master degree, specialising on material science, at the University of Applied Science MUnster. Subsequently he started his PhD studies at the University of Applied Science MUnster and does his research on "luminescent materials for flicker reduction of AC-LEDs" in the working group of Prof. Thomas Justel.

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On the VUV luminescence and degradation of UV-C emitting phosphors

Mike Broxtermann¹ and Thomas Justel²^{1,2}Munster University of Applied Sciences, Germany

Xenon comprising excimer discharge lamps represent themselves as an efficient source of vacuum ultraviolet radiation, which may find an application, e.g. for disinfection purposes by the use of suitable photoluminescent conversion materials.^{1,2} Among these conversion phosphors there are some doped yttrium ortho-phosphates, as well as respective lutetium or lanthanum containing derivatives, exhibiting promising properties.^{3,4} A common design for phosphor converted Xe excimer lamps consists of a discharge vessel made from quartz glass, which is coated with a thin layer of phosphor particles (around 10 - 50 μm) on the inner side. Experimental results demonstrate that all of the above mentioned PO_4 -based phosphor materials exhibit a distinct degradation resulting in a mayor loss of lamp UV radiation output over just a few days of operation time. Recovery of aged phosphor material enabled the investigation of that performance loss which could be traced back to a strong new absorption in the UV range. This is accompanied by well fitting excitation bands spreading over the UV spectral range as well as a corresponding broad band emission peaking in the deep red. Immersing analysis of the undoped phosphate compounds YPO_4 , LuPO_4 and LaPO_4 evidenced, that these aging effects find their origin within the phosphate host material itself being directly exposed to the plasma discharge, most probably to the existence of phosphorous III in $[\text{Ne}]3s^2$ electron configuration. Further work is thus conducted on the understanding as well as on the obviation of phosphor aging throughout the application of protective particle coatings.

1 U. Kogelschatz, Dielectric-barrier Discharges: Their History, Discharge Physics, and Industrial Applications, *Plasma Chem. Plasma Process.* 2003, 23, p. 1

2 Patent US 6398970 B1

3 T. Justel, P. Huppert, W. Mayr, D.U. Wiechert, Temperature-dependent spectra of $\text{YPO}_4:\text{Me}$ (Me = Ce, Pr, Nd, Bi), *J. Lumin.* 2004, 106, p. 225

4 Patent US20140099798 A1

Biography

Mike Broxtermann has completed his bachelor and master studies at the Ruhr-University Bochum, Germany. Afterwards he has started his PhD studies on the analysis and improvement of UV emitting phosphor converted Xe-excimer lamps at the MUnster University of Applied Sciences. The respective research project "Hg free UV Radiation Sources for Energy Efficient Water Treatment" is supported by the German federal ministry of education and research (BMBF). Mike Broxtermann himself is an awardee of the German foundation economics (sdw).

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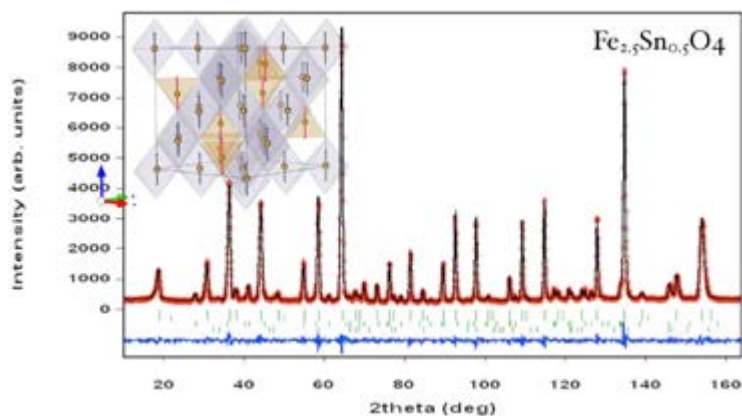
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Oxide materials chemistry using single crystal and powder X-ray and neutron diffraction

Tilo Sohnel

University of Auckland, New Zealand

Mixed transition-metal oxides (MTMO) including stannate phases have promising material properties and are known for the ability to tailor particular features for different uses. They are currently being explored as possible alternative substrates in many emerging high-tech applications such as electrode materials in lithium-ion batteries and as conducting oxides in gas detector sensors [1-3]. The presentation will an overview about the preparation, crystallographic and characterization based on X-ray and neutron diffraction techniques of two groups of mixed transition metal-main group metal oxide materials and spinel compound. Layered oxide structures have been widely studied for their potential use in applications ranging from ferroelectricity to giant magnetoresistance in the field of semiconductor materials. The Fe based layered oxide $\text{Fe}_{4-x}\text{Mn}_x\text{Si}_2\text{Sn}_7\text{O}_{16}$ provides a novel situation in oxide compounds. It can be described as a composite of intermetallic (FeSn_6) clusters and $(\text{Fe}/\text{MnO}_6)/(\text{SnO}_6)$ oxide layers within the one structure. SiO_4 tetrahedra separate these layers which leads to electronic and magnetic isolation of the repeated layers by about 7 Å resulting in a nearly perfectly 2D oxide system comparable to a one layer thick oxide “thin film”. In this study, starting with $\text{Fe}_4\text{Si}_2\text{Sn}_7\text{O}_{16}$, we focus on analysing the electronic structure and its relationship to unique magnetic properties [4-5]. The presentation also summarizes the crystal and magnetic structures of novel iron and tin containing quaternary spinel structures $(\text{M}_{2-x}\text{Fex})\text{SnO}_4$ ($M = \text{Mn}, \text{Zn}$ and $0 \leq x \leq 2$). Neutron and synchrotron X-ray powder diffraction in combination with spectroscopic investigations (Mössbauer, IR and UV-Vis), magnetic measurements and SEM/EDX have been performed on the $(\text{M}_{2-x}\text{Fex})\text{SnO}_4$ systems to find out the exact mechanism of Fe substitution, how much Fe and in what oxidation state is substituted and the effects upon the crystal and magnetic structure.



Biography

Tilo Söhnel did his PhD at the Technical University of Dresden, Germany, in the field of inorganic solid-state chemistry. After different post-doctoral positions in Germany and Auckland, he started as lecturer at the University of Auckland and is currently Associate Professor. His research interest lies in the field of experimental and theoretical chemistry of solid state compounds and inorganic materials such as mixed main group metal / transition metal cluster compounds and complex transition metal oxides. This includes the preparation and characterization of novel tin and antimony cluster compounds with promising materials properties and the calculation of band structures of solid-state compounds to investigate the crystal structure and the electronic structure. For the identification of these compounds the group intensively uses X-ray and neutron single crystal and powder diffraction techniques.

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High temperature ceramic ionic conductors for hydrogen separation

Cecilia Mortalo
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The production of pure hydrogen usually requires its extraction from a gas mixture. One of the critical stages related to the use of hydrogen as an energy carrier is the development of efficient and competitive techniques that separate hydrogen from other by-products such as steam, hydrocarbons, carbon dioxide and other gases. Membranes for hydrogen purification represent an appealing alternative to the current commercially available pressure swing adsorption technology. In this context, mixed ionic and electronic conducting (MIEC) materials are considered attractive as dense ceramic membranes due to their extremely high selectivity at high temperature ($\geq 600^\circ\text{C}$): hydrogen is incorporated into their lattice as charge protonic defects, thus providing a non-galvanic separation, i.e. without external power. Furthermore, the properties of these oxides (i.e. working temperatures, durability) endow membranes that could be directly integrated into industrial processes or used in the catalytic membrane reactors. Recently, $\text{BaCe}_{0.65}\text{Zr}_{0.20}\text{Y}_{0.15}\text{O}_{3-\delta}$ and doped-ceria composites were explored by our group as potential membrane for hydrogen separation, reaching hydrogen flux values among the highest ever reported for bulk MIEC membranes ($0.27 \text{ mL}\cdot\text{min}^{-1}\cdot\text{cm}^{-2}$ at 755°C). This talk provides a comprehensive overview of the recent trends in such MIEC materials for H_2 separation. The long term stability of the investigated systems under harsh environments containing H_2O vapour, CO, CO_2 , and sulphides is also shown.

Biography

Cecilia Mortalo is graduated in Chemistry and has completed his PhD at University of Modena and Reggio Emilia (Italy) in 2005. Since 2005 she has been a researcher at the Institute of Condensed Matter Chemistry and Technologies for Energy of the Italian National Research Council. Her research activity is focused on the preparation and study of advanced ceramic ionic conductors for high temperature energy applications, in particular solid oxide fuel cells and hydrogen separation membranes. She has published more than 20 papers and 60 proceedings of national and international conferences.

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Session Chair
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Session Introduction

- Title: Moving microdroplets in 3D using photochemopropulsion**
David L Officer, University of Wollongong, Australia
- Title: Understanding underlying chemistry for renewable energy materials and environmental remedies using first principles-based computational modelings**
Byunghan Han, Yonsei University, South Korea
- Title: Organic semiconductor materials for high efficiency dye-sensitized solar cells**
Hwan Kyu Kim, Korea University, Korea
- Title: Construction of functional structure by precise molecular-design**
Hui Li, Beijing Institute of Technology, China
- Title: Band-gap engineering for graphene by using low energy alkali metal ions**
Jinwook Chung, Pohang University of Science and Technology, Korea
- Title: Development and validation of a voltammetric method for the determination of antimony in aqueous medium**
Hugo Romero B, Technical University of Machala, Ecuador
- Title: P-BGCE - photoreduction of benzophenone in green chemistry using an alternate solvent ethyl alcohol**
Geeta Verma, Chandra Shekhar Azad Govt Post Graduate Nodal College, India
- Title: Synthesis of 5-membered heterocyclic systems by the pummerer reaction**
Diego Gamba-Sanchez, University of Los Andes, Colombia
- Title: Fused multifunctionalized dibenzoselenophenes from tetraynes**
Yimin Hu, Anhui Normal University, China
- Title: Miniaturized wire ion trap for portable mass spectrometry**
Daniel Austin, Brigham Young University, USA

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Moving microdroplets in 3D using photochemopropulsion

David L Officer, Yang Xiao, Sara Zarghami, Klaudia Wagner and Pawel Wagner
University of Wollongong, Australia

The ability to selectively transport chemical species in a controlled fashion, typically against chemical and electrochemical gradients, has been the cornerstone of the development of complex natural systems. In 2013, the Nobel Prize in Physiology or Medicine was awarded to Rothman, Schekman and SUDhof "for their discoveries of machinery regulating vesicle traffic, a major transport system in our cells". Vesicles are closed cellular structures formed from lipid bilayers that are used to actively transport macromolecules from inside cells to the outside fluid by a process known as exocytosis or between cells by a variety of mechanisms. In exocytosis, the macromolecules are contained in the vesicle that isolates them from the rest of the cell and which eventually fuses with the cell membrane to release the macromolecular cargo to the outside of the cell. Emulating such structures and processes in the fluid environment is considered one of the grand challenges confronting nanoscience today and has the potential to add revolutionary capabilities to fluidic platforms that could be used to transport medicine in the human body, act as chemical messengers for signal transduction in sensing or other systems, move cargo around microfluidic devices, or even be utilized for transport in artificial cellular systems. We have developed lipophilic droplets whose movement and direction can be controlled on or in an aqueous medium solely by photo-driven "chemopropulsion" (photochemopropulsion). In this presentation, we will demonstrate how the droplets can be "pushed" or "pulled" by light in 3D, are able to carry "cargo", and undertake sequential chemical reactions through the interaction of two or more droplets.

Biography

David Officer is Professor of Organic Chemistry in the Intelligent Polymer Research Institute and the Australian Research Council Centre of Excellence for Electromaterials Science at the University of Wollongong, Wollongong, Australia. He joined the lecturing staff at Massey University, New Zealand in 1986 and during the following 20 years, he became founding Director of the Nanomaterials Research Centre and Professor in Chemistry in the Institute of Fundamental Sciences. In 2007, he moved to the University of Wollongong. He has published more than 200 papers in the areas of graphene and porphyrin chemistry, conducting polymers, nanomaterials and solar cells.

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Understanding underlying chemistry for renewable energy materials and environmental remedies using first principles-based computational modelings

Byunghan Han

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First principles-based computational modelings propose key descriptors and design concepts for discovering highly active materials in renewable energy system application. Density functional theory calculations combined with statistical mechanical formalism identify optimum catalysts for oxygen (hydrogen) reduction (oxidation) and evolution reactions beyond conventional Pt used in fuel cell and Li-ion batteries. In this talk, the author will present the reaction mechanism of environmentally toxic gases with water and suggest how to remove them by designing efficient filters. Organic iodine and POCl₃ are introduced as the examples.

Biography

Byunghan Han obtained his PhD degree in MIT at the Department of Material Science and Engineering. He was a Research Associate in MIT and Stanford University for four years. From 2015, he has been working at Yonsei University as an Associate Professor. His research interests are developing emerging energy materials for renewable energy devices. He was introduced as 10 most leading young scientists in the Korean newspaper. He was awarded a medal from International Advanced Association of Materials in 2016. He is an Associate Editor of *Scientific Reports*.

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Organic semiconductor materials for high efficiency dye-sensitized solar cells

Hwan Kyu Kim, Yu Kyung Eom, Sung Ho Kang and In Taek Choi
Korea University, Korea

Dye-sensitized solar cells (DSSCs) have attracted much interest as a promising renewable energy supply device based on the merits of low-cost, flexibility and easy fabrication. Very recently, a variety of organic dyes using inexpensive metals has been prepared for DSSCs. A state of the art DSC based on porphyrin-based solar cells with cobalt-based electrolyte has exceeded the conversion efficiency of 13.1%. For the high PCE of D- π -A sensitizer-based DSSCs, the structural modifications of a π -bridge, including tuning the energy levels and the improvement of intramolecular charge transfer (ICT) from D to A of the sensitizer, are particularly essential. We demonstrate that new thieno[3,2-b][1]benzothiophene (TBT)-based D- π -A sensitizers and D- π -A structured Zn(II)-porphyrin sensitizers based on the structural modification of SM315 as a world champion dye for efficient retardation of charge recombination and fast dye regeneration were synthesized. The device with new porphyrin sensitizers exhibited the higher photovoltaic conversion efficiency (PCE) than those of the devices with SM315 as a world champion porphyrin dye. To further improve the maximum efficiency of the DSSCs, by replacing the TBT π -bridge with the alkylated thieno[3,2-b]indole (TI) moiety, the TI-based DSSC exhibits a highest PCE (12.45%) than does TBT-based DSSC (9.67%). Furthermore, the first parallel-connected (PC) tandem DSSCs in the top cell with a TI-based sensitizer and bottom cell with a porphyrin-based sensitizer were demonstrated and an extremely high efficiency of 14.64% was achieved. In this presentation, new strategy on materials paradigm for low-cost, long-term stable, highly efficient dye-sensitized solar cells will be described.

Biography

Hwan Kyu Kim received PhD from Carnegie Mellon University. After postdoctoral associate in Materials Science and Engineering at Cornell University, he joined ETRI as a project leader of polymeric photonic device group. After his career at Hannam University where he became Professor of Polymer Science and Engineering, he was invited as a distinguished professor to Korea University in 2007. He had executed the president-ship of both Korean Society of Photoscience and Korean Organic Photovoltaics Society. His current research focuses on developing advanced organic and polymeric semiconductors for dye-sensitized solar cells, perovskite solar cells as well as solar energy conversion.

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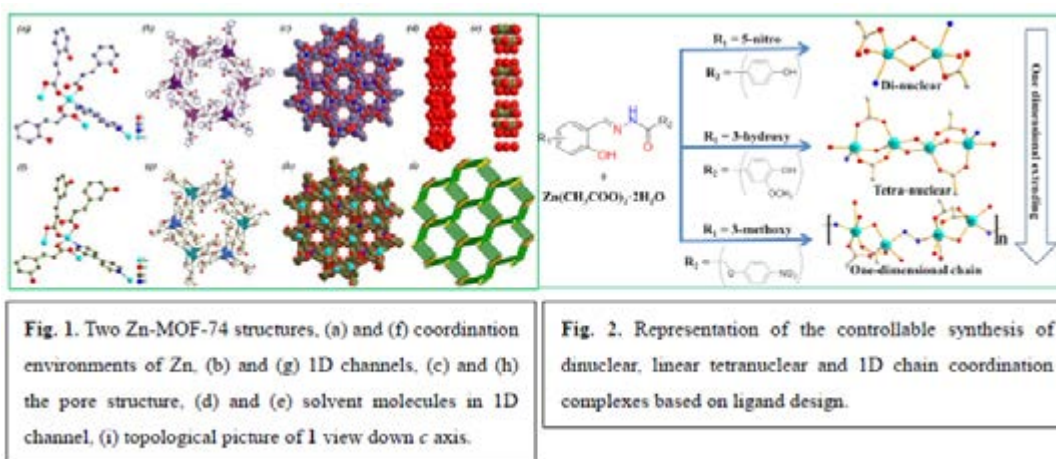
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Construction of functional structure by precise molecular-design

Hui Li

Beijing Institute of Technology, China

The precise construction of functional structures is a challenge for chemists. We are interested and have worked in this topic for a long time. For example, two MOF-74 analogs with OH groups on 1D channel surfaces have been synthesized through multi-component self-assembly at room temperature, which exhibit unique luminescent selectivity (Fig.1). 1 Another interesting work is the controllable synthesis of dinuclear, linear tetranuclear and 1D chain coordination complexes based on ligand design (Fig.2). 2



Biography

Hui Li obtained her Ph.D. degree in State Key Laboratory of Coordination Chemistry, Nanjing University. She has worked in University of Nottingham, U.K. as a Royal Society K. C. Wong Research Fellow. After then, she worked in National Taiwan University. In 2003, she joined Department of Chem., Beijing Institute of Technology. She has worked in Fraser Stoddart's Lab. for CD-POM complexes. Her research field covers Coordination Chem., Supramolecular Chem. and Crystallography.

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Band-gap engineering for graphene by using low energy alkali metal ions

Jinwook Chung

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Despite its superb electronic properties over other materials, graphene still remains as a tantalizing candidate to be actively utilized in electronic applications mainly because of its linear gapless band spectrum. Since the massless Dirac fermions in graphene showing ballistic charge transport even at room temperature are ideal charge carriers for fast circuit devices, extensive research efforts have been made to open a tunable bandgap in graphene with several different schemes. In this talk, we introduce a new scheme of forming and fine-tuning a bandgap for a range suitable for most applications by using slow alkali metal ions. We also demonstrate the on-off switching capability by controlling the size and mid-gap energy (or Dirac point) of the bandgap independently by adding other neutral atoms. Our density-functional theory calculations for the band suggest that the sublattice asymmetry enhanced by the doped ions drives the behavior of the ion-induced bandgap in graphene.

Biography

Jinwook Chung has completed his PhD at the age of 32 years from Brown University and postdoctoral studies from Massachusetts Institute of Technology in USA. He is the director of Surface and Nanomaterial Physics Lab, Pohang Institute of Science and Technology in Korea. He has published more than 96 SCI papers in reputed journals and has been serving as an editorial board member of several journals including Applied Physics A (1997~2003), Science Letters (2014~), and Madridge Journal of Nanotechnology & Nanoscience (2016).

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Development and validation of a voltammetric method for the determination of antimony in aqueous medium

Hugo Romero B, Thalia Vera, Kathy Gadvay, Kerly Dávila, Fredis Pesantez and Cristhian Vega
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The objective of this research was to develop and validate a voltammetric method for the determination of antimony in aqueous medium. First, solutions of 5, 10, 15 and 20 mg L⁻¹ of Sb were prepared, using 0.5M phosphoric acid as supporting electrolyte. Additionally, nitrogen was bubbled at 99% purity to remove oxygen from solutions. To measure the concentration of antimony the anodic stripping voltammetry technique was applied, by using a potentiostat multi-channel PARSTAT mark with Versa Princeton Applied Research Studio software. To carry out the registration of voltammograms, a three-electrode system was used, which consisted of glassy carbon as working electrode, Ag / AgCl as reference electrode and a platinum electrode as a counter electrode. In a first stage of the process, a chronoamperometry to $E = -1.2$ V was applied for a time pre-concentration of 50 s, to achieve this electrodeposition of metallic antimony (Sb⁰) on the surface of the glassy carbon electrode. Next, a linear sweep voltammetry with potentials between -1.2 V and $E_i = E_f = 0.5$ V was applied at a rate of $v = 20$ mV s⁻¹. To validate the method for quantification of antimony determined linearity, precision, accuracy, detection limit and quantitation limit. The linearity of the method was demonstrated from the proportionality coefficient of 0.9961. The coefficient of variation (CV) had a value of 14.2%, indicating that the accuracy of the method is acceptable. Meanwhile the accuracy is within the criteria for consideration of the method, because a 114% recovery was determined. Additionally it was found that the detection limit and quantitation limit values correspond to 1.45 mg 4.42 mg L⁻¹ and L⁻¹ respectively.

Biography

Hugo Romero Bonilla has completed the Master's Program in chemistry at the Pontificia Catholic University of Valparaiso, Chile. Currently (2016) he completed the PhD program in environmental science in San Marcos University, Perú. He works as a researcher and professor at the Faculty of Chemistry at the Technical University of Machala, Ecuador where he has served as Director of Chemical Research Center and Director of the Center for Technology Development. Your research lines are Biotechnology and Applied Electrochemistry. He has published some scientific articles papers in reputed journals such as New Biotechnology, Progress in Organic Coatings, Talanta, Advances in Chemistry and Analytical Chemistry Research.

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Notes:

4th European Chemistry Congress

May 11-13, 2017 Barcelona, Spain

P-BGCE - photoreduction of benzophenone in green chemistry using an alternate solvent ethyl alcohol

Geeta Verma

Chandra Shekhar Azad Govt Post Graduate Nodal College, India

Green Chemistry is an approach to the synthesis, processing and use of chemicals that reduces risks to humans and the environment. A synthesis of benzopinacol from benzophenone is carried out using ethanol as a solvent. This is a free radical reaction and reduction of benzophenone occurred by sunlight via UV radiation. Benzopinacol is a catalyst of the formation of unsaturated polyesters. It is also used as an organic synthesis intermediate and as an initiator of polymerization by free radicals. Characterization of Benzopinacol was done by using spectroscopic technique like IR, NMR etc. Results positively show that solvent ethyl alcohol can be used as an alternative for photoreduction of benzophenone in case of non availability of isopropyl alcohol.

Biography

Geeta Verma had completed her Ph.D at the age of 26 years from Central drug Research Institute Lucknow and Awadh University, Faizabad. She has published 16 research papers including interdisciplinary topics in reputed International Journals. Awarded patent during CDRI research work 2003, Best Professor of the year 2015 from M.P. Employees Jankalyan Sangh. UGC Sponsored Research Project work done by her published and selected as Best paper award by International Academy of Science and Technology 2015 and Excellence in Service on Independence day 2016. She has won the Indus Foundation awards for Teaching Excellence 2016. Her suggestions for family problems were selected as winners in Daily Newspaper.

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Notes:

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Synthesis of 5-membered heterocyclic systems by the pummerer reaction

Diego Gamba-Sanchez, Juan Rueda-Espinosa and Andres Gomez-Angel
University of Los Andes, Colombia

The Pummerer reaction has been studied for many years as a powerful method to form C-Nu bonds, its applications in total synthesis of natural products has been recently reviewed showing its great potential. We recently published a new method to obtain oxazolines by Pummerer chemistry, and the goal of the current study is to extend the scope of this methodology to the synthesis of other heterocyclic systems. The results include approaches to pyrroles, oxazoles, thiazoles and the application of the methodology to the total synthesis of siphonazole and muscoride A.

Biography

Diego Gamba-Sanchez obtained his PhD in 2010 from the Ecole Polytechnique at Palaiseau. After one year as a postdoctoral associate in the laboratory of Prof. Thorsten Bach, he moved back to Colombia and started his independent career at the Universidad de los Andes in Bogotá. His research focused on new methodologies using Pummerer chemistry and the development of synthetic routes to natural products.

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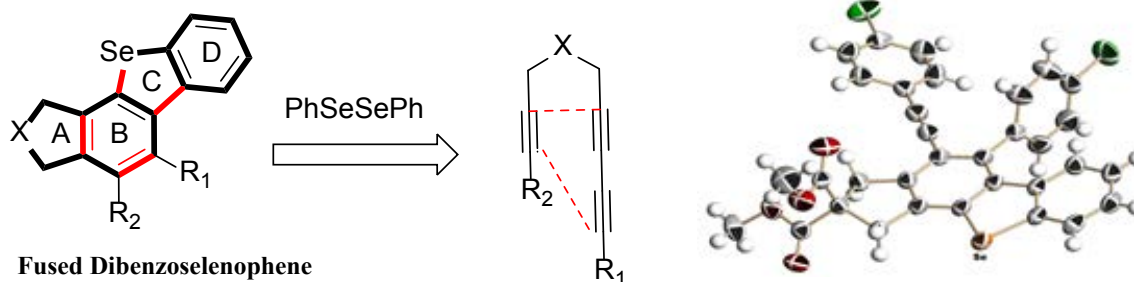
May 11-13, 2017 Barcelona, Spain

Fused multifunctionalized dibenzoselenophenes from tetrynes

Yimin Hu

Anhui Normal University, China

Selenium, an essential trace element and antioxidant, is used in the prevention of various cancers. Daily supplements of Selenium reportedly reduce the risk of several types of cancer in patients with a history of skin cancer. Dibenzoselenophene and dibenzoselenophenes are important intermediates in the production of perfumes, dyes, plastics, agricultural materials, and drugs. Aryne precursors that can assemble three consecutive functional groups on a benzene ring in a “one-pot” process are compatible with various reagents and functional groups; such precursors are suitable in versatile transformations, thereby greatly expanding the current bounds of aryne chemistry and drug synthesis. Scheme shows novel cyclization method involving freeradical and the subsequent regioselective functionalization of an unactivated C–H bond for the preparation the dibenzoselenophene core. Fused heterocyclic ring systems contain conjugate planes at the A–B–C–D ring junctures. Control of the relative and absolute configurations of these conjugate planes in selenium, and the construction of the tetracyclic framework of the complex heterocyclic system, represent significant synthetic challenges. Compared with ordinary organic selenium derivatives, dibenzoselenophene derivatives prepared in the present experiment have multiple rings, complex and variable structures, and wide application prospect in chemical production and clinical medicines.



Biography

Yimin Hu has completed his PhD from Nanjing University and postdoctoral studies from Bowling Green State University. He has published more than 35 papers in reputed journals and has received the Thieme Chemistry Journal award for 2010 by the editorial boards of the journals Synlett, Synthesis, and Synfacts. His research area focused on palladium catalyzed cascade and HDDA cycloaddition reaction by means of C–H activation and Heck coupling process to construct a complementary approach to the remarkably powerful Domino reaction.

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Miniaturized wire ion trap for portable mass spectrometry

Daniel Austin

Brigham Young University, USA

Biography

Daniel E. Austin is an Associate Professor in Department of Chemistry and Biochemistry at Brigham Young University, USA.

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Notes:



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Scientific Tracks & Abstracts Day 2

Euro Chemistry 2017

Physical Chemistry | Environmental Chemistry | Theoretical Chemistry

Session Chair
Goncagul Serdaroglu
Cumhuriyet University, Turkey

Session Co-Chair
Dorothee ARNS
Petrochemicals Europe, Belgium

Session Introduction

- Title:** **Highly porous bio-based nanofibrous aerogels for removing cationic dyes from aqueous solutions**
Sara Mousavi, ZHAW Life Sciences and Facility Management, Switzerland
- Title:** **Hydrazine-borane derivatives as promising chemical hydrogen storage system. A boron-nitrogen bond study by UV-photoelectron spectroscopy and quantum calculations**
Javier Torres Escalona, IPREM, France
- Title:** **The features of diamond nucleation on nanolevel prediction of diamondization of multilayered graphene**
Pavel B Sorokin, National University of Science and Technology MISiS, Russian Federation
- Title:** **CNFs-supported Pd series catalysts comparison for hydrogen evolution from additive free formic acid decomposition**
Felipe Sanchez, Cardiff University, UK
- Title:** **How macroeconomic factors shape the European petrochemicals industry**
Dorothee ARNS, Petrochemicals Europe, Belgium
- Title:** **Transfer dehydrogenation of 1-phenylethanol over supported palladium nanoparticles under mild conditions**
Reem AlBilali, University of Dammam, Saudi Arabia
- Title:** **Substituent effect on reactivity of β CCM: A computational study**
Goncagul Serdaroglu, Cumhuriyet University, Turkey
- Title:** **DFT studies on copolymers of 3,4-Ethylenedioxythiophene/3-methylthiophene and pyrene**
Nevin Kaniskan, Anadolu University, Turkey
- Title:** **DNA N6-methyladenine modification from unicellular eukaryotes to mammals**
Hailin Wang, Chinese Academy of Sciences, China
- Title:** **Influence of different parameter in air gap membrane distillation for seawater desalination**
Rochd Sanaa, Ben Msik Universite Hassan2 Casablanca, Morocco
- Title:** **First principles study on the reaction mechanisms of hydrolysis reaction of PCl_3 and $POCl_3$**
Hyunwook Jung, Yonsei University, Korea
- Title:** **Physical and chemical characterisation of captagon tablets seized in Dubai in 2016**
Samar Gewily, Dubai Police Forensic Laboratory, UAE

4th European Chemistry Congress

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Highly porous bio-based nanofibrous aerogels for removing cationic dyes from aqueous solutions

Sara Mousavi^{1,2}, Fabian Deuber¹, Farhad Shahraki², Majid Aliabadi³ and Christian Adhart¹¹ZHAW Life Sciences and Facility Management, Switzerland²Department of chemical engineering, university of Sistan & Baluchestan, Iran³Department of chemical engineering, Azad university of Birjand, Iran

The use of synthetic dyes in different industries such as paper, textile, paint, printing, and plastics is inevitable. Environmental concerns due to their UV and temperature stability together with their inhibiting effects on photosynthetic activities ask for improved dye removing processes. Dye adsorption is a promising method in dye removing process, as it is cost efficient, easy and flexible without any new toxic by-products. Difficulties such as separating the adsorbent after the removal process together with their low efficiency were overcome by the development of new adsorbents based on electrospun nanofiber membranes. However, besides all the outstanding properties of electrospun nanofiber membranes such as their huge specific surface area tailored surface functionality and fiber uniformity, they are still facing challenges such as low mechanical stability and unfavorable mass transport properties. To overcome these problems, a robust 3D sponge like aerogel with high porosity, mechanical stability, and flexibility as well as low density was developed using pullulan: nanofibers are electrospun from the natural and edible polysaccharide pullulan followed by cutting in dioxane, proceeding with a freeze casting process and finally thermally crosslinked [1]. The pullulan based super elastic and environmentally friendly aerogel is used as a highly efficient adsorbent to remove cationic dyes from aqueous solutions. Dye adsorption is pH dependent and recycling of the aerogel adsorbent is demonstrated.

Biography

Sara Mousavi is from Zhaw, Switzerland

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Notes:

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May 11-13, 2017 Barcelona, Spain

Hydrazine-borane derivatives as promising chemical hydrogen storage system. A boron-nitrogen bond study by UV-photoelectron spectroscopy and quantum calculations

Javier Torres Escalona¹, Anna Chrostowska¹, Clovis Darrigan¹, Alain Dargelos¹, Alain Gracia¹ and Jean-Claude Guillemin²
IPREM, France

The major challenge of the XXI century is probably related to our ability to provide an efficient and cost-effective energy transition, but also to propose alternative solutions and processes environmentally friendly. The discovery of new sources and new methods of operation will determine our energies for the future. Thus, all forms of research dedicated to this problem are to consider, especially as conventional reserves deplete. In this context, hydrogen is one of the principal candidates as clean fuel and hydrazine-borane derivatives are promising as chemical hydrogen storage systems. On the other hand, ultraviolet photoelectron spectroscopy (UV-PES) is a well-established technique to provide ionization energies of molecules in gas phase. These experimental data supported by quantum calculations for the consistency of the assignments of PE bands allow to reach fundamental information about electronic structure and bonding that is obtained by no other technique. Representative examples to illustrate the advantages and wide applicability of this approach will be exclusively chosen from our research in the field hydrazine-borane derivatives and in particular on the nature of boron-nitrogen bond versus substitution on each atom.

Biography

Javier Torres Escalona has completed his Master in Chemistry at age of 25 years from Castilla-La Mancha University. He is currently a 3rd year PhD candidate at the Pau University doing his doctoral research at the Research Institute on Analytical Sciences and Physical Chemistry for Environment and Materials (IPREM).

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The features of diamond nucleation on nanolevel prediction of diamondization of multilayered graphene

Pavel B Sorokin

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Since the isolation in 2004 graphene continues to attract significant attention from the scientific community. Despite of the fact that graphene is under detailed investigation more than 10 years it still serve as a source for unusual effects. Here I will show that multilayer graphene surface can be used a base for formation of diamond nanofilms [1] facilitated by chemical adsorption of adatoms on the multilayer graphene surface, and explain how the pressure of phase transition is reduced and formally turns negative. For the first time we obtain, by *ab initio* computations of the Gibbs free energy, a phase diagram (P, T, h) of quasi-two-dimensional carbon—diamond film versus multilayered graphene. It describes accurately the role of film thickness h and shows feasibility of creating novel quasi-2D materials. In such “chemically induced” phase transition both chemistry and compression concurrently serve as the driving factors for diamond film formation. I will continued to discuss this effect through the ultrastiff films with hexagonal diamond (lonsdaleite) type structure and further show that under the particular external conditions and using particular adsorbate atoms films with the specific structure can be formed [3]. The process of diamond phase nucleation was further investigated on the atomic level. The critical size of graphene hydrogenated region which can initiate graphene diamondization was estimated. The nonlinear dependence of size of graphene hydrogenated region upon the number of layers predicted the maximal thickness of the film which can be formed by chemically induced phase transition [3]. This research was supported by Ministry of Education and Science of the Russian Federation in the framework of Increase Competitiveness Program of NUST «MISiS» (№ K2-2015-033).

1. A.G. Kvashnin et al. Nano Letters 14 (2014) 676
2. L.Yu. Antipina et al. J. Phys. Chem. C 119 (2015) 2828
3. S.V. Erohin et al. submitted (2017)

Biography

Pavel Sorokin has completed his PhD at the age of 25 years from Lebedev Physical Institute of RAS, Moscow and postdoctoral study from Rice University. He is the leading researcher of Inorganic Nanomaterials Laboratory in National University of Science and Technology "MISiS". He has published more than 80 papers in reputed journals.

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CNFs-supported Pd series catalysts comparison for hydrogen evolution from additive free formic acid decomposition

Felipe Sánchez¹, Alberto Villa² and Nikolaos Dimitratos¹¹Cardiff University, UK²University of Milan, Italy

Searching for a safe and efficient H₂ generation/storage material has become a serious challenge toward a fuel-cell-based H₂ economy as a long-term solution. Herein we report the development of Pd nanoparticles catalysts supported on 5 different carbon nanofibers (CNFs): three different grades and nitrogen and oxygen functionalisations; each one via sol-immobilisation and impregnation techniques. Thorough characterisation has been carried out by XRD, XPS, TEM, SEM-EDX. The catalysts have been evaluated for the formic acid dehydrogenation, which has potential to be a safe and convenient H₂ carrier under mild conditions. Those catalysts prepared by sol-immobilisation technique exhibit more activity when compared with catalysts prepared by impregnation due to the higher metal loading and higher Pd⁰/Pd ratio, smaller particle size (Fig. 1) and lower binding energies, leading to an improved activity due to the weaker interaction between the Pd nanoparticles and the formic acid. The heat treatment on CNFs has an important effect on catalyst activity, increasing with the annealing temperature (Fig. 2). Oxygen functionalities present a higher initial activity that could be addressed to a favoured deprotonation step due to the presence of O- on the surface, leading to an easier dehydrogenation of formic acid. However, deactivation was observed after 30 minutes due to CO evolution. The most active catalyst reached a remarkable TOF of 979 h⁻¹ and high selectivity (>99%) at 30°C. Being this a great value for formic acid dehydrogenation at mild conditions however, further investigation is necessary in order to decrease the CO formation and improve reusability.

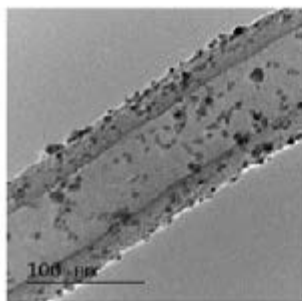


Figure 1. Bright field TEM micrograph of PdSI/CNF-HHT

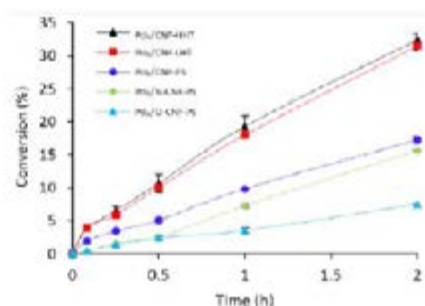


Figure 2. Formic acid dehydrogenation reaction on Pd on different supports.

Biography

Felipe Sánchez is from department of chemical engineering in Málaga. Currently, he joined in Cardiff University for PhD and pursuing 3rd year.

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4th European Chemistry Congress

May 11-13, 2017 Barcelona, Spain

How macroeconomic factors shape the European petrochemicals industry

Dorothee ARNS

Petrochemicals Europe, Belgium

The intervention will focus on the following elements: How the European Petrochemicals industry contributes in a sustainable way to the economic and societal well-being of Europe. How chemical markets evolve. Why a lower oil price doesn't change the situation for the European Petrochemicals industry. The competitiveness challenge for the European Petrochemicals industry: Feedstock price, electricity price, regulatory challenge, investment leakage. Debrief on the European Commission's cumulative costs assessment of its legislation on the European Petrochemicals industry. The performance of the European Petrochemicals industry in reducing GHG emissions.

Image of petrochemicals' most popular communication medium giving an overview from initial resources to downstream users



Biography

Dorothee ARNS, a German national, completed her university studies in Saarbruecken (Germany), Dublin (Ireland) and Granada (Spain) with two Master degrees: one in Applied Languages & Linguistics and the other one in Business Administration with special focus on Marketing, International Management and private law. Her professional career in the chemical industry started in 1995 when she joined the marketing & sales trainee programme of BASF in Ludwigshafen. In the course of the years she held senior management positions in various areas of BASF's chemicals business, notably in marketing, sales, eBusiness and controlling. On 1 July 2013 she was appointed Executive Director of Cefic's Petrochemicals and Plastic Additives Programme as well as of Petrochemicals Europe, the Association of Petrochemical Producers in Europe, formerly APPE. In a first assignment to Cefic from 2006 to 2011 she headed the solvents' cluster as Director General of ESIG, the European Solvents Industry Group.

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Transfer dehydrogenation of 1-phenylethanol over supported palladium nanoparticles under mild conditions

Reem AlBilali¹ * and Nikolaos Dimitratos²¹University of Dammam, Saudi Arabia²Cardiff University, UK

An interesting alternative to aerobic conditions for the production of oxygenated products, such as aldehydes and ketones, can be the use of unsaturated organic molecule as a hydrogen acceptor, instead of molecular oxygen. In this case, the oxidative dehydrogenation is changed to transfer dehydrogenation, which overcomes the safety limitations of aerobic oxidation. In the majority of reported works, researchers represent the catalytic activity of supported metals such as palladium and ruthenium on the transfer dehydrogenation of alcohols. This work demonstrated the catalytic activity of supported palladium nanoparticles and the influences of different parameters, such as controlling particle size, changing the stabilizer, thermal treatment of the catalyst on the liquid phase transfer dehydrogenation of 1-phenyl ethanol as a model reaction under mild conditions. Varying catalyst loading, stirring rate, and the 1-Phenyl ethanol/palladium molar ratio have determined the different regimes. The apparent activation energy of 5%Pd/C was determined. Moreover, the influence of varying the stabilizer type, and concentration, during the synthesis of palladium nanoparticles via sol immobilization technique on the resulted particles, and their catalytic activity on the liquid phase transfer dehydrogenation of 1-phenyl ethanol was investigated. The chemical composition and morphology of the catalyst were determined using XRD, XPS, TEM and SEM-EDX. The results illustrated that the two main parameters which can mainly control the catalytic activity of the liquid phase transfer dehydrogenation of 1-phenyl ethanol are the ratio between metallic palladium to palladium oxide, and the particle size of the catalyst.

Biography

Reem Khalid AlBilali is an assistant professor in physical chemistry at the University of Dammam, Saudi Arabia since 2012. Her research interests are the synthesis and characterisation of supported metal nanoparticles and their catalytic applications, corrosion and corrosion inhibitions of metals and the adsorption of photoactive materials on clay surfaces. In September 2015, she joined Cardiff Catalysis Institute at Cardiff University, UK, as a postdoctoral researcher associate as she is still working there. AlBilali has many publications in both Arabic and English language, and she is a (MRSC) member in the Royal Chemical Society (RSC) and a member in the American Chemical Society, Saudi Chemical Society and the National Association of Corrosion Engineers (NACE).

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Substituent effect on reactivity of β CCM: A computational study

Goncagul Serdaroglu

Cumhuriyet University, Turkey

β C compounds used in the treatment of many disease as a effective drug are obtained from both plants and marine organism as a secondary metabolism product. Here, all DFT calculations conducted with 3 basis set such as 631G(d,p), 631+G(d,p) and 6311++G(d,p) in both the gas phase and the water phase have been performed to predict the most reactive structure among the studied C1-substituted- N9-methyl- β CCM derivatives, which the substituent groups are that A (anthracen-9-yl), B (naphthalene-1-yl), C (naphthalene-2-yl), D (6-methoxynaphthalene-2-yl), E (phenanthrene-9-yl). The structure A is predicted as the most reactive structure in according to the quantum chemical descriptors such as the Energy Gap and global hardness values, that is, the Energy Gap of structure A has the lowest value than the other structures. Also it is determined as the soft molecule among the studied structures. As seem from Table 1, the calculated parameters are mostly compatible with each other to detemine the most reactive structure of the less reactive structure. This work is to aim to contribute to the future development of the new drug molecules using the computational tools based on the quantum chemical descriptors.

Biography

Goncagul Serdaroglu has completed his PhD from Cumhuriyet University (2008) and postdoctoral studies from Auburn University (2013). Her major research interests are on structural properties and chemical behavior of biologically and pharmacologically important molecules by using computational tools.

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DFT studies on copolymers of 3,4-Ethylenedioxythiophene/3-methylthiophene and pyrene

Nevin Kaniskan

Anadolu University, Turkey

Conducting polymers, superior electrical, electronic, magnetic, and optical properties of compounds are very important in the industry. They are named as the "synthetic metal" or "organic metal". Thiophene can be prepared easily and have high conductivity. Therefore, too much theoretical work has been done until now. However, it is very little theoretical work about derivatives of these compounds. Since the interaction between alternating donors and acceptors results in a diminished band gap, a low band gap (<1.8 eV) will be expected in polymers containing donor-acceptor (D-A) repeating units. In order to predict the band gaps for guiding the synthesis of novel materials with low band gaps, we apply quantum-chemical techniques to calculate the band gaps in several polythiophene homo- and copolymers: poly{3-methylthiophene} (P1), poly{2,3-dihydrothieno[3,4-b][1,4]dioxine}, EDOT (P2) and polypyren (P3), poly{5-(4-methylthiophen-2-yl)-2,3-dihydrothieno[3,4-b][1,4]dioxine} (P3), poly{3-methyl-2-(pyren-1-yl)thiophene} (P4), and poly{5-(4-methyl-5-(pyren-1-yl)thiophen-2-yl)-2,3-dihydrothieno[3,4-b][1,4]dioxine} (P5). The geometries of the oligomers were optimized using semi-empirical PM6 method. The band gap calculations on these oligomers were performed by density functional theory (DFT) (B3LYP/6-31G(d,p)). Band gaps of the corresponding polymers were obtained by extrapolating oligomers gaps to infinite chain lengths. The results indicate that calculated band gaps are in good agreement with the experimental values. In addition, depending on the type of substituent and the substitution pattern, large differences in the delocalization pattern are observed between the substituted and unsubstituted oligomers. It is found that the band gaps critically depend on the chemical structures.

Biography

Nevin Kaniskan has completed her PhD in 1989 from Anadolu University. She is associated professor of Anadolu University at Chemistry Department.

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DNA N6-methyladenine modification from unicellular eukaryotes to mammals

Hailin Wang

Chinese Academy of Sciences, China

The same genomic sequences of four nuclear DNA bases, A, T, G, and C, code all heritable gene information required for various types of cells in mammalian individuals. Essentially, the methylation of Cytosine at the C-5 position in genome provides a biochemistry-based plasticity required for establishing functionally varying cells in mammals. By this modification, the gene expression can be comprehensively or specifically regulated and chromatin structures be dynamically manipulated. Meanwhile, the methylation of the other nuclear base adenine at the N-6 position (N6-methyladenine, 6mA), which is the dominant DNA modification in genomes of bacteria and shows diverse functions (e.g., regulation of DNA replication initiator factors, control of transposon activity, regulation of DNA gene expression, host-pathogen interactions and guiding DNA repair), is absent in high eukaryotes. Intriguingly, 6mA was also found in unicellular eukaryotes. Until recently we and other groups discovered this 6mA modification predominated in *Drosophila melanogaster* and *Caenorhabditis elegans*, respectively. These observations compulsively prove the presence of 6mA in high eukaryotes. Interestingly, in addition to the functions revealed in bacteria, 6mA may mark active transcription start sites and transposon activity and regulates embryonic development. These findings suggest that 6mA is a potential epigenetic mark in eukaryotes. However, it is not clear whether 6mA DNA modification is conservatory and present in mammalian genomes. These recent findings further prompted us to search 6mA modification in mammals again. If so, how 6mA distributes in various tissues and how 6mA distributes in genome. Consistent with previous work, recent work show very low levels of 6mA DNA modification in genomes of frogs, mice, and human cells (approximately 1 6mA for every 1.2×10^6 deoxyadenosine residues). We speculated that 6mA DNA modification can dynamically function in certain cells or stage in a meaningful abundance. Now we showed the prevalence of 6mA in genomes of mice and human cells by developing a unique analytical technology.

Biography

Hailin Wang has his expertise in epigenetics, in particular, DNA methylation and demethylation. He developed ultrasensitive analytical technologies (UHPLC-MS/MS, qPCR, genome-wide sequencing) for characterization and functional study of DNA 5-methylcytosine and its oxidation intermediates. He for the first time showed the enhancement of genome-wide 5-hydroxymethylcytosine by nutrient vitamin C, revealing a role of vitamin C in the regulation of DNA modification, and his study established a direct link among vitamin C, Tet dioxygenases, and DNA methylation. He further extended these technologies for study of other DNA modifications, and as a world-wide seminal work, he discovered new DNA modification (N6-methyladenine) in high eukaryotes (Cell, 2015). He also has his expertise in ultrasensitive analytical technologies (e.g., capillary electrophoresis-laser induced fluorescence polarization, single molecule fluorescence imaging, and UHPLC-MS/MS) for detection of carcinogenic DNA adducts and for study of DNA-repair proteins interactions. He published 100 peer-reviewed papers on leading journals, including Cell, Cell Stem Cell, Mol Cell, Proc. Natl. Acad. Sci. USA, J. Am. Chem. Soc., Nucleic Acids Research, Analytical Chemistry.

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Influence of different parameter in air gap membrane distillation for seawater desalination

Rochd Sanaa, Zerradi Hicham, Mizani Sofia, Lahlou Souad and Dezairi Aouatif

Ben Msik Université Hassan2 Casablanca, Morocco

Access to drinking water and resource management are major challenges of the coming decades. In a social and industrial purpose, it seems therefore vital for some people, particularly, in remote site to develop new facilities for drinking water production. Membrane distillation is one of the latest developments in the distillation desalination. It is based on the principle of vapor migration of water through a hydrophobic microporous membrane by a vapor difference between a heated solution and the air in a cold channel (the condensation channel) cooled by the initial temperature solution. Air gap membrane distillation (AGMD) is considered one of the five configurations of the Membrane distillation. Our contribution is to study the effect of NaCl concentration, porosity, and membrane pore size on the production of the flux. The results have been carried using polynomial approximations through MATLAB and the results show a good agreement with the experience.

Biography

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Notes:

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First principles study on the reaction mechanisms of hydrolysis reaction of PCl_3 and POCl_3

Hyunwook Jung
Yonsei University, Korea

Lethal accidents caused by explosive reactions of toxic chemicals should be prevented and once happened, fast and safe control is of importance. An accurate understanding of thermodynamic properties and kinetic rates is the first step toward accomplishing the purpose. Using first principles density functional theory (DFT) and ab-initio molecular dynamic (AIMD) simulations we study hydrolysis reactions of two archetype chemicals, PCl_3 and POCl_3 , to unveil potential energy surface over reaction coordinates. By calculating the intermediates and Gibbs free energy diagrams reaction mechanism and activation barriers. Our results indicate that H_2O molecules nearby the chemical species play a key role in catalyzing the hydrolysis reaction as a proton donor or acceptor. The catalytic mechanisms is explained as more water molecules attach the charge separation at the transition state is enhanced, leading to higher polarity and stabilization via hydrogen bonding network. It could dramatically reduce the activation energy of reactant complex. The effect is, however, mitigated by disordering entropic effect resulting in only slight reduction of activation energy upon increasing H_2O molecules. It is noteworthy that PCl_3 react with H_2O molecule by interplay of the proton transfer and dissociation of chlorine, while POCl_3 first forms a six-coordinated complex and then, quickly decomposes to HCl. Reaction rate constants are calculated from calculated activation energy using a transition state theory.

Biography

Hyunwook Jung has completed his BS at Department of Chemical & Biomolecular Engineering in Yonsei University. After serving as marine for two years he joined graduate program of Yonsei University. He was invited to the 10th International Conference on Computational Physics (ICCP10) held at Macao in China, January, 2017.

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Notes:

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Physical and chemical characterisation of captagon tablets seized in dubai in 2016

Samar Gewily, Khalid Alsumaiti and Saif and Eldin Abdelrahim
Dubai Police Forensic Laboratory, UAE

Illicit production of Captagon tablets has become widely spread in the Middle East recently. Around 5% of cases of seized drugs in Dubai in 2016 were Captagon. Originally Captagon is the trademark name of Fenethylline, however studies and chemical analysis of seized tablets has proven the absence of Fenethylline, rather it showed different combinations of Amphetamine, Caffeine and other compounds. In this study, total of 20 representative samples from different cases were analysed chemically using Gas Chromatography coupled with Mass Spectroscopy (GC-MS), and Micro X-Ray Fluorescence (μ XRF) to determine organic and inorganic content. In addition, samples were physically characterised using 3D microscope. Based on results, comparisons were made between samples and linked to information on originality as a first step towards Captagon Profiling.

Biography

Samar Gewily has completed her Bsc of science in Chemistry and Ecology from Monash University, AUS. She worked for WWF-UAE in environmental education program, a leading organization in environmental education and conservation work. She has published on Wadi Wurayah National Park, UAE. Also participated in two research projects with Earth Watch, AUS. She has joined a UNESCO program for Young Ecologist in Ethiopia and UAE for Biosphere Reserves. Currently works as Expert in Chemistry at Dubai Police Forensic Laboratory, UAE. Presented a scientific paper at Hemaya 12th Annual Conference, Dubai, UAE in 2016, for Narcotics.

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4th European Chemistry Congress

May 11-13, 2017 Barcelona, Spain

Scientific Tracks & Abstracts Day 3

Euro Chemistry 2017

Medicinal Chemistry | Materials Chemistry | Petro Chemistry | Multi-disciplinary Chemistry

Session Chair

Tuanli Yao

Shaanxi University of Science and Technology, China

Session Introduction

Title: **Increasing affinity and selectivity for target proteins by peptide conjugation to small molecule ligands – extending interactions just outside of the binding pocket**
Lars Baltzer, Uppsala University, Sweden

Title: **Prussian blue analogues as battery materials for energy science**
Yutaka Moritomo, University of Tsukuba, Japan

Title: **Palladium catalyzed domino heck/aryne carbopalladation/c-h functionalization: Synthesis of heterocyclefused 9,10-dihydrophenanthrenes**
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Title: **Tensinometry as a conceptually innovative tensiometric versus skin pathway (TVS) for non-invasive evaluation of surface energy phenomena related to the epidermal functional state and its aging critical level**
Antonio Bettero, University of Padova, Italy

Title: **Sensors based on biomimetic porphyrin derivatives & their hybrid combinations with photonic nanoparticles**
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Title: **Characterization of lamb flavor using selected ion flow tube mass spectrometry (SIFT-MS)**
Hardy Z Castada, The Ohio State University, USA

Title: **Application of vegetable oils for extraction of rare-earth elements from water solutions**
Denis L, Saint-Petersburg Mining University, Russia

Title: **CO₂ utilisation: Waste or resource for chemical industry**
Ozge Yuksel Orhan, Hacettepe University, Turkey

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Increasing affinity and selectivity for target proteins by peptide conjugation to small molecule ligands – extending interactions just outside of the binding pocket

Lars Baltzer and Aleksandra Balliu
Uppsala University, Sweden

Organic synthesis has reached a level of proficiency that allows the efficient preparation of molecules of high complexity but the design of small organic molecules and peptides with sufficient affinities and selectivities for proteins in biomedical applications lags behind. We have developed a technology where polypeptide conjugation to small organic molecules or peptides provides affinities increased by as much as four orders of magnitude in comparison to those of the small molecules. Selectivities between highly homologous proteins, measured as ratios of dissociation constants, have been shown to increase by between one and two orders of magnitude. The aspect of the technology that appears to be the most surprising, while it at the same time makes it the most attractive to use, is that a single sixteen membered set of polypeptides is enough to improve affinities and selectivities for essentially any protein. We have recently begun to focus our attention on problems related to *in vivo* applications, addressing a) the risk of elicitation of immune responses and b) the problem of fast renal clearance. To this end, chemical modifications were introduced that allowed us to reduce the size of the polypeptides from the original 42-residue scaffolds to 11-mers without loss of affinity. We have identified a small molecule ligand that will provide tight binding of peptides to human serum albumin, a carrier protein present in human blood at a concentration of 0.6 mM. HSA binding will keep peptides in circulation thus reducing the problem of fast renal clearance and, in addition, the rate of proteolytic degradation. The peptide conjugates to be discussed may be used e.g. in clinical imaging or as radiotherapeutic agents, but also as guides for the redesign of small molecule drugs or for target validation purposes.

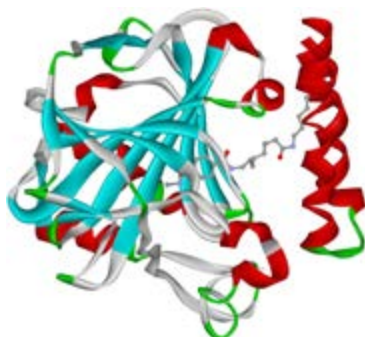


Illustration of concept. Conjugate formed from small molecule ligand and 42-residue polypeptide binds target protein due to small molecule-protein interactions supplemented by those between peptide and protein in close proximity to the small molecule binding site. Protein is human Carbonic Anhydrase II and small molecule ligand is benzenesulphonamide.

Biography

Lars Baltzer is Professor in Organic chemistry at Uppsala University since 2004. He has a well-documented and longstanding interest in research topics related to catalysis and molecular recognition based on fundamental principles of physical-organic chemistry. He has introduced catalytic sites, demonstrated rate enhancements of several orders of magnitude and proven the formation of enzyme-substrate complexes in proteins he has designed from scratch. More recently he has become engaged in research on the molecular recognition of proteins by polypeptide conjugates, for the purpose of increasing affinities and selectivities for proteins of biomedical interest. Affinity enhancements due to peptide conjugation of four orders of magnitude, increased selectivities as well as improved pharmacokinetic and pharmacodynamic properties have been demonstrated. He has expertise in molecular design and the quantitative evaluation of structure and activity relationships especially those related to protein recognition. Aleksandra Balliu obtained her Ph D in the laboratory of Lars Baltzer, working on aspects of the polypeptide conjugate technology.

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Prussian blue analogues as battery materials for energy science

Yutaka Moritomo

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Prussian blue analogues (PBAs: $\text{Na}_x\text{M}[\text{Fe}(\text{CN})_6]_y$, where M is a transition metal) have three-dimensional (3D) jungle-gym-type host framework and cubic nanopores, 0.5 nm at the edge. PBAs are promising cathode materials for lithium ion (LIBs) and sodium ion (SIBs) secondary batteries, [1-3] reflecting their nanoporous host framework. Actually, thin film of $\text{Na}_x\text{Co}[\text{Fe}(\text{CN})_6]_{0.90}$ shows high capacity of 135 mAh/g, [3] which is comparable to the value (= 140mAh/g) of actually-used LiCoO_2 . The thin film electrode exhibits a high capacity of 121 mAh/g (90 % of the OCV value) even at 60 C. The discharge curve exhibits two plateaus at 3.8 and 3.4 V. By means of ex situ X-ray diffraction and absorption measurements, we have ascribed them the redox processes of Fe and Co. [3]

The thin film battery electrode is a nice platform for energy science, because the electrode is free from carbon-based conducting material and polymer-based binder. With use of an optical battery cell and microscopy, we clarified the structural dynamics in the charge process (Li intercalation process) of $\text{Li}_x\text{Co}[\text{Fe}(\text{CN})_6]_{0.90}$. [4] We clearly observed phase separation into the Li-rich and Li-poor domains of order of 10,000 nm. With use of the inelastic X-ray scattering technique, we clarified that local structures around CO^{2+} and Co^{3+} in $\text{Na}_x\text{Co}[\text{Fe}(\text{CN})_6]_{0.90}$.

- [1] T. Matsuda and Y. Moritomo, Appl. Phys. Express 4 (2011) 047101
- [2] T. Matsuda, M. Takachi and Y. Moritomo, Chem. Comm. 49 (2013) 2721.
- [3] M. Takachi, T. Matsuda, and Y. Moritomo, Jpn. J. Appl. Phys. 52 (2013) 090202.
- [4] M. Takachi and Y. Moritomo, Sci. Rep. in press.

Biography

Yutaka Moritomo has completed his PhD in physics at the age of 27 years from University of Tokyo and postdoctoral studies from University of Tokyo. Now, he is the director of division of materials for energy storage and conversion, Center for Integrated Research in Fundamental Science and Engineering (CiRfSE), University of Tsukuba. He has published more than 300 papers (total citation is more than 20,000).

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Palladium catalyzed domino heck/aryne carbopalladation/c-h functionalization: Synthesis of heterocycle-fused 9,10-dihydrophenanthrenes

Tuanli Yao

Shaanxi University of Science and Technology, China

Arynes generated from the corresponding *o*-(trimethylsilyl)aryl triflates have emerged as powerful synthons in organic synthesis. Aryne annulation reactions with intramolecular C-H functionalization can be a powerful method for the synthesis of polycyclic compounds. We developed a novel palladium-catalyzed domino Heck/aryne carbopalladation/C-H functionalization reaction using in situ generated arynes, in which three new C-C bonds and a carbon quaternary center are formed. This methodology affords moderate to excellent yields of heterocycle-fused 9,10-dihydrophenanthrenes.

Biography

Tuanli Yao has completed his PhD from Iowa State University and postdoctoral studies from University of California, Berkeley. He worked as Senior Scientist at Deciphera Pharmaceuticals and Associate Researcher at University of Kansas before beginning his career in academy. Currently, he is professor at Shaanxi University of Science & Technology. His research interests include aryne chemistry, electrophilic cyclization and palladium catalysis. He has published more than 30 papers in reputed journals.

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4th European Chemistry Congress

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Tenskinmetry as a conceptually innovative tensiometric versus skin pathway (TVS) for non-invasive evaluation of surface energy phenomena related to the epidermal functional state and its aging critical level

Antonio Bettero and Camilla Dal Bosco

University of Padova, Italy

Tenskinmetry is a conceptually innovative Tensiometric Versus Skin (TVS) pathway for non-invasive evaluation of surface energy phenomena closely related to the epidermal functional state. The TVS modeling: (i) exploits the structure-surface correlations which are characteristic of all systems; (ii) applies the principle of permutability of the tensiometric technique, according to which unknown solids can be characterized by their known surface characteristics, and vice versa; (iii) applies the contact angle method, with only water as reference liquid; (iv) is carried out by a suitable mobile tensiometer (*tenskinmeter*) directly in contact with the skin in a non-invasive way; (v) measures and correlates the surface free energy reflex induced by inter- and intra-molecular and particle forces acting on underlying epidermic layers; (vi) allows the epidermal hydration directly from the polar surface energy fraction.

Biography

Antonio Bettero is a professor in Università di Padova, Italy.

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4th European Chemistry Congress

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Sensors based on biomimetic porphyrin derivatives & their hybrid combinations with photonic nanoparticles

Eugenia Fagadar-Cosma

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Most synthetic porphyrins are hydrophobic π -conjugated macrocycles and as a consequence organic building blocks for supramolecular chemistry, providing in this way the required optoelectronic and morphological properties for a plethora of novel sensors. Besides, porphyrins possess huge capacity for chemical modifications by peripheral substitution and by using them in hybrid combination with photonic, electronic and magnetic compounds. Wide band absorption hybrid materials were prepared from different A_3B porphyrins and cobalt, manganese and zinc metalloporphyrins and silver or gold nanoparticles with the purpose to develop optical and electrochemical detection of hydrogen peroxide or other compounds showing potential in early medical diagnosis. The synthesized materials were characterized by UV-vis, fluorescence, FT-IR, AFM, SEM TEM and CV. STEM investigation of the porphyrin-gold hybrids revealed some dendritic structures produced mainly by porphyrin H- and J-type helicoidal self-aggregation due to their interaction with gold nanoparticles. Layer-by-layer assembly of gold colloid nanoparticles and cobalt porphyrins on GC electrodes generated electroactive thin films capable to electrochemically detect minute quantities of H_2O_2 that are relevant for early diagnosis in medicine. The Co-porphyrin-gold hybrid was exposed to increased amounts of H_2O_2 and the changes of the absorption spectra were monitored by UV-vis spectroscopy, proving the same quality of sensing capacity.

Biography

Eugenia Fagadar-Cosma has completed her PhD in 1997 at Polytechnical University of Timisoara. She is senior scientist, doctoral advisor and coordinator of Organic Chemistry –Porphyrin Programmes in Institute of Chemistry Timisoara of Romanian Academy. She has published more than 250 peer-reviewed full-papers, 93 papers in prestigious ISI journals, 8 books and 2 chapters in international volumes, 7 patents and has been serving as an editor to a special issue (Bentham). She was involved in managing of many FP6, FP7 and national granted projects. She is reviewer of more than 20 ISI indexed ELSEVIER, SPRINGER and ACS Journals.

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4th European Chemistry Congress

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Characterization of lamb flavor using selected ion flow tube mass spectrometry (SIFT-MS)

Hardy Z Castada

The Ohio State University, USA

Volatile 4-alkyl-branched fatty acids and 3-methylindole are characteristic flavor compounds associated with lamb. The partitioning behavior of these volatile organic compounds (VOCs) between the gas and condensed phase is important for their effective characterization especially during high throughput screening and quantitative analysis. Selected ion flow tube-mass spectrometry (SIFT-MS) was used for the headspace concentration analysis of the compounds associated with lamb flavor. Standard solutions of 4-ethyloctanoic acid, 4-methyloctanoic acid, 4-ethylnonanoic acid and 3-methylindole were prepared in an oil-based matrix, equilibrated for an hour at 4 different temperatures (80, 100, 110 and 125°C), prior to headspace sampling and quantification. Further linear regression analyses and calculations of Henry's law constants were carried out at each specified equilibration temperature. The Henry's law constants of the lamb flavor compounds were calculated with a high degree of confidence ($p < 0.05$) based on direct proportionality with a very good fit of linearity ($R^2 > 0.99$) between the headspace and solution concentration of the standard solutions. The detected headspace concentrations increased with elevated equilibration temperature resulting to increased volatility of the compounds. Therefore, the calculated temperature-dependent Henry's law constants for these volatile compounds decreased with increasing temperature. We have established the temperature-dependent Henry's law constants for the volatiles 4-alkyl branched-chain fatty acids and 3-methylindole in air-oil matrixes. As the equilibration temperature is increased, volatility increases and Henry's law constant decreases with increasing molecular weight. The partitioning behavior of the compounds is necessary for their high throughput characterization and approximation of their concentrations in situ.

Biography

Hardy Castada is a post-doctoral food scientist and analytical chemist with research interest in the fundamental and applied volatile compound analysis using SIFT-MS. He studies physico-chemical changes and behavior of volatile, semi-volatile, aroma and flavor volatiles in various matrixes and systems.

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Application of vegetable oils for extraction of rare-earth elements from water solutions

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Various types of vegetable oil-based organic solvents (VOS), i.e. vegetable oils (corn, canola, sunflower and soybean oils) with and without extractant (pure oleic acid), were investigated into their potentiality as greener substitutes for the conventional petroleum-based organic solvents to extract REM from aqueous solutions [1, 2]. The pH-extraction isotherms of Ce (III) using various vegetable oils loaded with oleic acid were investigated and the percentage extraction of Ce (III) achieved by different types of VOS was determined. Vegetable oils without extractants showed a poor extractability for Ce (III). Vegetable oils loaded with oleic acid were found to be the most effective VOS for Ce (III) extraction and, thus, are potential greener substitutes for the conventional petroleum-based organic solvents. It was shown that all vegetable oils investigated such as olive and sunflower, either with or without naphthenic acid exhibited a similar trend of extractability for Ce (III) from aqueous solutions. A sigmoid curve was obtained for all the pH-extraction isotherms of Ce (III) investigated with various types of vegetable oils loaded with 500 mM of naphthenic acid as VOS. The extraction was the lowest at pH of 4.0, but increased sharply from 4.7 to 5.5, and achieved its maximum from 5.5 to 6.0. Vegetable oils without extractants were poor VOS for Ce (III) wherein only about 10% of Ce (III) was extracted. Hence, vegetable oils functioned more as diluents than as additional extractants in Ce (III) extraction. Vegetable oils loaded with 500 mM naphthenic acid, however, were effective VOS where more than 90% of Ce (III) was extracted from aqueous solutions. Therefore, naphthenic acid functioned as an effective extractant in Ce (III) extraction by various types of VOS.

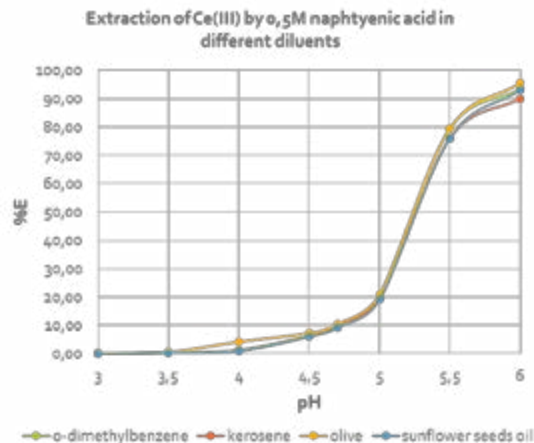


Figure. 1: Degree of extraction Ce (III) from the equilibrium pH of the aqueous phase in the extraction solution of oleic acid in o-xylene, paraffin, olive oil and sunflower.

Biography

Denis Lutskii graduated St. Petersburg State Mining Institute (Technical University) on a specialty "Metallurgy of ferrous metals", qualification "engineer". In 2011, after graduate school, defended his thesis for the degree of candidate of technical sciences, specialty 05.16.02 "Metallurgy of ferrous, non-ferrous and rare metals", thesis - "Recovery and separation of lanthanides hydrometallurgical methods for complex processing of raw low-concentration"

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4th European Chemistry Congress

May 11-13, 2017 Barcelona, Spain

CO₂ utilisation: Waste or resource for chemical industry

Ozge Yuksel Orhan and Erdogan Alper
Hacettepe University, Turkey

CO₂ emissions into atmosphere is a global concern and a recent theoretical model provides a quantitative approach for its connection with global warming and climate change. CO₂ is potentially a suitable resource of carbon which can partially replace oil and gas in many synthetic applications. Benefits can also extend to safety considerations since it is not toxic. It can replace certain toxic building blocks such as CO and phosgene in several commercially important processes, such as methanol or polyurethane manufactures. In addition, it can be used as a viable technological fluid with distinct advantages over other possible solutions in applications such as enhanced oil recovery and supercritical solvent. In near future, the use in carboxylation processes (synthesis of carbonates, carbamates and carboxylates, including cyclic compounds in both monomeric and polymeric forms) appears to be the most likely synthetic applications. In these cases, CO₂ serves as both carbon and oxygen sources. Replacing CO for making acrylic acid and use as a mild oxidant are other interesting applications. Reduction by catalytic and electrocatalytic hydrogenation necessitates energy from non-fossil fuels and solar and renewable energy resources should then be incorporated. The photocatalytic reduction of CO₂ in water under solar light irradiation, which is known as artificial photosynthesis, is a potential option that would increase carbon recycling. A unique aspect of this paper is the exploitations of reactions of CO₂ which stems from existing petrochemical plants-with the commodity petrochemicals (such as, methanol, ethylene and ethylene oxide) produced at the same or nearby complex in order to obtain value-added products while contributing also to CO₂ fixation simultaneously. Exemplifying worldwide ethylene oxide facilities, it is recognized that they produce about 3 million tons of CO₂ annually. Such a CO₂ resource, which is already separated in pure form as a requirement of the process, should best be converted to a value-added chemical there avoiding current practice of discharging to the atmosphere.

Biography

Ozge Yuksel Orhan obtained her Ph.D. in Chemical Engineering from Hacettepe University, Turkey, in December 2014. Her thesis is entitled "The Absorption Kinetics of CO₂ into Ionic Liquid-CO₂ Binding Organic Liquid Hybrid Solvents". Currently, she is a Research and Teaching Assistant at Chemical Engineering Department of Hacettepe University. Her research topics have dealt with the study of carbon dioxide capture by novel solvents. Erdogan Alper is a Professor at the Chemical Engineering Department of Hacettepe University in Ankara, Turkey. He obtained his BSc (Honours) (First Class) from Birmingham University, England (1968), and earned his PhD from Cambridge University (1972). In 1977-1978, he was an Alexander von Humboldt fellow at Hannover University, Germany, and received Turkish Scientific and Technological Research Council prize in Engineering in 1982. His research areas include carbon dioxide capture by innovative solvents, fuel cell modelling by CFD, petroleum refining and petrochemical technologies. He published 4 books and around 150 research papers in cited journals.

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