

7th World Congress on Chemistry

November 13-15, 2017 Athens, Greece

Keynote Forum Day 1





Marc Gingras

Marseille-Aix-Marseille University, France

Sulfur-rich polyaromatic architectures: asterisks, dendrimers, polymers, and their metal interactions


Sulfur-rich polyaromatic architectures of various topologies will be presented, along with their synthesis, their opto-electronic properties and some applications in chemical-biology, in materials science and in nanoscience. They comprise asterisks, dendrimers, polymers and helicenes, which often incorporate a thiophenylene or a polyaromatic unit, leading to some molecular rigidity and restricted degrees of freedom. They represent an underexploited class of macromolecules with multivalent and attractive features for exalting supramolecular interactions, chiroptical and electronic properties. The latter features could be modulated from the coordination of divalent sulfur atoms to thiophilic metallic species, from some cation- π interactions, and from some π - π complexes. Additionally, polysulfuration often enhances some electronic, photophysical and biophysical properties, leading to exalted luminescence, stable redox states, metal-ion coordination ability, aggregation

or crystallization-induced phosphorescence or fluorescence emission (AIE or CIE). Some uses will be presented as asymmetric catalysts, as some of the most phosphorescent organic (nano)crystals (π ~100%), as cation-selective membranes, as cations/anions sensors (dual mode), as electrochromic molecular switches, as multivalent glycosylated biosensors, and as ligands for stabilizing metal alloys and bimetallic core-shell nanoparticles.

Biography

Marc Gingras chemistry at the University of Sherbrooke (1981-84). From 1985-89, he completed Doctorate at McGill University with Professor T H Chan and David N Harpp. He worked with Professor Edwin Vedejs (1989-92) and with Professor Laura Kiessling (1992-93) at the University of Wisconsin Madison. He then joined the Laboratory of Supramolecular Chemistry at the University of Strasbourg with Professor Jean Marie Lehn (1993-95). He occupied several faculty positions: Université Libre de Bruxelles (1995-99), University of Nice (1999-2007), and Aix-Marseille Université at the Interdisciplinary Center on Nanoscience of Marseille. He was Chairman of the Chemistry Department (2010-11). He guided 80 research trainees. He has a list of more 62 publications (~2000 cit.), 115 invited lectures and 30 short ones. He is a Board Member of Austin Journal of Biosensors and Bioelectronics, and a former one of the *Journal of Sulfur Chemistry* (2010-14) and *ISRN Organic Chemistry* (2010-12).

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 Notes:



Gerard Tobias

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Nanoengineering of inorganic and carbon materials

In this talk we will review some recent progress on the design and nanoengineering of inorganic and carbon nanomaterials for tailored applications. Special emphasis is paid in the group to exploit the synergies of both types of materials by the preparation of nanohybrids with novel or enhanced properties. We will mainly focus on the development of nanomaterials for application in the biomedical field, but we will also highlight work performed in other areas such as the isolation and template assisted-growth of rolled-up single-layered 2D materials. Among the different types of carbon nanomaterials, one advantage of using nanotubes is that their inner cavity can be filled with a chosen payload whilst the outer surface can be modified with biomolecules to improve their dispersibility, biocompatibility and even for targeting purposes. For instance, following this approach we have shown that by filling radioactive isotopes it is possible to achieve ultra-sensitive imaging and the delivery of an unprecedented amount of radiodose density. The presence of selected heavy elements allows even mapping of subcellular organelles via X-ray fluorescence imaging. Furthermore, functionalization of the external walls of these filled carbon nanotubes (CNTs) with monoclonal antibodies allows targeting the epidermal growth factor receptor (EGFR), over expressed by several cancer cells. We have also recently developed CNTs for dual imaging by radio-labelling iron oxide decorating the external surface of CNTs. The resulting hybrids allow single

photon emission computed tomography (SPECT) and magnetic resonance imaging (MRI). Worth noting is the enhancement of the MRI signal by modification of the nanocarrier (non-MRI active) rather than the magnetic nanoparticles themselves. The formation of such hybrid systems is not limited to the biomedical field. A large deal of attention is being devoted towards the isolation and growth of single layers of a wide variety of inorganic materials which is of interest for both fundamental research and advanced applications. When an individual layer is seamlessly wrapped into a cylinder, the resulting single-layered nanotube combines the characteristics of both two-dimensional (2D) and one-dimensional (1D) materials. Yet, despite their interest, reports on single-walled inorganic nanotubes are scarce because their multiwalled counterparts are generally favored during growth. We have reported on a versatile approach that allows the formation of high quality, single-crystalline single-layered inorganic nanotubes.

Biography

Gerard Tobias obtained the degree in Chemistry (with Honours) from the Autonomous University of Barcelona (2000), Master in Materials Science and Ph.D. with European mention (UAB, 2004). He was a research visitor at Ames Laboratory (United States) and at the Electron Microscopy for Materials Science center (EMAT, Belgium). Between 2004-2009 he was a postdoctoral Fellow at the Inorganic Chemistry Laboratory, University of Oxford (UK). Since 2009 he leads research on "Nanoengineering of Carbon and Inorganic Materials" at the Materials Science Institute of Barcelona (ICMAB-CSIC). Dr. Tobias has been a member of the European COST Action TD1004 on "Theragnostics Imaging and Therapy", has coordinated the FP7 European project RADDEL involving 11 groups (2012-2016) "Nanocapsules for Targeted Delivery of Radioactivity" and has been recently granted an ERC Consolidator Grant (NEST, 725743).

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Junrong Zheng
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Electron/hole transformation between two atomic layers

Electron/hole transformations on interfaces determine fundamental properties of opto-electrochemical devices, but remain a grand challenge to experimentally investigate and theoretically describe. Herein combining ultrafast VIS/NIR/MIR frequency-mixed micro-spectroscopy and state-of-the-art two-dimensional atomic device fabrications, we are able to directly monitor the phase transitions of charged quasiparticles in real time on the ultimate interfaces – between two atomic layers. On type II semiconductor/semiconductor interfaces between two transition metal dichalcogenide (TMDC) monolayers, interfacial charge transfers occur within 50fs and interlayer hot excitons (unbound interlayer e/h pairs) are the necessary intermediate of the process for both energy and momentum conservations. On semiconductor/conductor (graphene) interfaces, interlayer charge transfers result in an unexpected transformation of conducting free carriers into insulating interlayer excitons between the conducting graphene and the

semiconducting TMDC. The formation of interlayer excitons significantly improves the charge separation efficiency between the two atomic layers for more than twenty times.

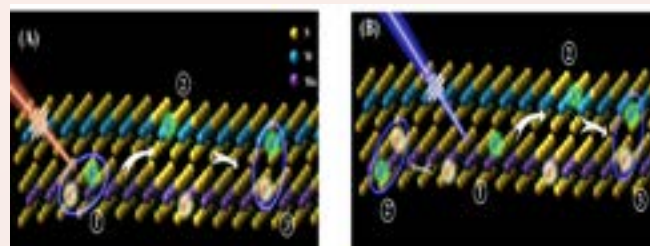



Figure 1. Interlayer charge transfers between MoSe₂/WS₂ atomic layers. The interlayer charge transfers (<50fs) result in the formation of interlayer hot excitons, much faster than the formation of intralayer excitons (~600fs).

Biography

Junrong Zheng completed his PhD and postdoctoral studies from Stanford University. He is professor of chemistry at Peking University, and a co-founder of Uptek Solutions, a Long-Island-based laser company. He is a recipient of numerous prestigious awards including the Sloan Fellowship, and the Packard Fellowship.

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Philippe C Gros

SRSMC - University of Lorraine-CNRS, France

Bimetallic reagents for synthesis of functional heterocyclic compounds

Functional heterocyclic derivatives are compounds of great importance with a wide spectrum of applications in e.g. biology, catalysis, supramolecular chemistry or energy conversion. The development of emerging technologies increases the need for more and more sophisticated heteroaromatic compounds drawing the synthetic chemist to design selective and applicable functionalization routes. Pyridine derivatives belong to one of the most important family and our group is focussing on chemo and regioselective routes to pyridyl organometallics (lithium [1] and ate complexes [2]). These intermediates are subsequently used in coupling reactions or enantioselective additions. The conference will focus on the preparation of a range of pyridyl organometallics from lab-made metalation reagents, their characterization and use for the synthesis of functional poly- and chiral heteroaromatic compounds.

Recent Publications

1. P C Gros, Y Fort (2002) nbuli/lithium aminoalkoxide aggregates: new and promising lithiating agents for pyridine derivatives. *Eur. J. Org. Chem.*, 2002(20):3375-3383.
2. P C Gros, Y Fort (2009) Title of the Article. *Eur. J.*

Org. Chem. Volume. 4199-4209.

3. H K Khartabil, P C Gros, Y Fort, M F Ruiz López (2010) Metalation of pyridines with nbuli–li–aminoalkoxide mixed aggregates: the origin of chemoselectivity. *J. Am. Chem. Soc.* 132(7):2410-2416.
4. Francos J, Gros P C, Kennedy A, O'Hara C (2015) Structural Studies of (rac)-BIPHEN organomagnesiates and intermediates in the halogen–metal exchange of 2-bromopyridine *Organometallics.* 34(11):2550-2557.
5. Tilly D, Chevallier F, Mongin F, Gros P C (2014) Bimetallic combinations for dehalogenative metalation involving organic compounds. *Chem. Rev.* 114(2):1207-1257.

Biography

Philippe C Gros studied Chemistry at the University of Lyon (France) and obtained his PhD in 1992. After two years as a Postdoctoral Fellow, he entered CNRS in 1994 and became Research Director in 2006. He is now first-class Research Director and Head of CNRS UMR SRSMC in Nancy, France (120 persons). He has published more than 100 peer-reviewed papers (h index 26) and coordinated several research programs. His research interests include the design of new metallating agents for functionalization of heterocycles, transition metal-catalyzed cross-couplings for ligand synthesis, and the design of photo- and electroactive organometallic materials.

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Keynote Forum Day 2





Bilge Sener

Gazi University, Turkey

Quality control and regulatory issues of phytomedicines for global health care

Herbal medicinal products have been playing an important role in the primary health care of the people around the world, specially in the developing countries. In order to treat health problems with the modern medicines, the production of safe and effective herbal medicinal products in a standardized way is essential. Assessment of the quality, safety and efficacy of herbal medicinal products are an important issue. Standardization of raw materials, intermediates and final product of herbal medicines are the main issue for the quality control of herbal medicinal products. All of the supporting evidence behind the use of phytomedicines has been on use of standardized extracts of the plant material to ensure reproducibility in the clinical setting. With the growing interest for alternative approaches in treating diseases, herbal medicinal products have also an important role for the development of new therapeutic agents. For this issue, researches should focus on: 1. characterization of phytomedicines in terms of chemical composition and biofunctional activity. 2. studying the effects of certain processing and extraction methods and parameters on the chemical characteristics of phytomedicines source materials. 3. development of chemo-based and bio-based standardization methods for phytomedicines. Herbal medicinal products named as "Phytomedicines" exhibit a variety of biological

activities on human health. These range from the control of regulatory processes by Health Authorities is essential for human life. Therefore, herbal medicinal products are also subject to the same legislative controls as other medicines. The overview of the herbal medicinal products worldwide along with current registration guidelines and criteria for the control and market situation of herbal medicinal products in Turkey will be highlighted.

Biography

Bilge Sener graduated from Ankara University, Faculty of Pharmacy in 1974. She has completed her PhD awarded by the Turkish Scientific and Technological Research Council (TUBITAK) at the Department of Pharmacognosy in 1977. In 1981, she became an Associate Professor. She was involved within the process of establishing Department of Pharmacognosy, Faculty of Pharmacy, Gazi University in 1982. She became a Full Professor in 1988. She achieved some researches at the Department of Chemistry, The Pennsylvania State University (USA) between 1986 and 1988 as Visiting Scientist awarded by National Science Foundation. She was also involved in several administrative works at Gazi University; as Director at the Department of Pharmacognosy, Faculty of Pharmacy, Gazi University between 1982 and 2002, as Chair at Division of the Professional Sciences of Pharmacy, as Co-Director at the Institute of Health Sciences (1988-1994) and as Dean at the Faculty of Pharmacy, Gazi University (1994-1997). She was given the degree of Adjunct Professor by University of Karachi, Pakistan. She worked as Director in 48 projects supported by NATO, NSF, IUPAC, Soctrates-Grundtvig, TUBITAK and University Research Funds by now. She has authored or co-authored 7 books, 85 chapters and 658 research articles published in leading international journals. She has also given 68 conferences and 313 plenary and invited lectures at the international symposia in the field of natural product chemistry. She has supervised 5 PhD, 12 MSc at Gazi University as well as co-supervised 17 PhD thesis at the University of Karachi. She is a member for 14 international and national professional societies.

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Yifat Miller

Ben-Gurion University of the Negev, Israel

Investigating neurodegenerative diseases by computational biophysical chemistry


Protein aggregation of amyloids is associated with numerous incurable diseases, including amyloid β ($A\beta$) in Alzheimer's disease (AD) and α -synuclein in Parkinson's disease (PD). Clinical studies have shown that patients with AD can develop PD and vis-à-versa. Experimental evidence led to the hypothesis that cross-amyloid interactions (e.g., interactions between $A\beta$ and α -synuclein) also play a critical role in protein aggregation. Structure-based characterization of the interactions between two types of amyloids is fundamental to understanding the self-assembly mechanism that exists between them and may pave the way to elucidate the link between two diseases (e.g. PD and AD). Computational biophysical chemistry

tools are critical techniques to investigate the molecular mechanisms of these proteins. The Nobel prize in Chemistry 2013 was awarded jointly to Martin Karplus, Michael Levitt and Arieh Warshel for the development of these techniques to investigate the chemistry behind the biological systems. The lecture will demonstrate how these computational tools assist us to investigate neurodegenerative diseases.

Biography

Yifat Miller has completed her PhD in Chemistry from the Hebrew University of Jerusalem (Israel) in 2007. She did her Postdoc in the National Institute of Health (MD, USA) and was awarded the prestigious HFSP and NIH grants. She has published more than 60 papers in several journals, among which are Nature Comm., JACS, PNAS, Angew. Chem. Int. Ed., Chem. Comm. She is serving as an editor in Scientific Report of Nature publishing. She was awarded prizes such as Toronto prize for excellence of young faculty member. She is currently an Associate Professor in the Chemistry Department at BGU.

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Udo Schwingenschlögl

King Abdullah University of Science and Technology, Saudi Arabia

Substrate effects on silicene and how to exploit them


Silicene is the Si analogue of graphene with the same honeycomb structure and linear dispersions of the π and π^* bands at the K point of the Brillouin zone. It is predicted to realize a buckled structure, due to sp^2 - sp^3 hybridization, and is compatible with the current Si-based nano-electronics. Silicene yet has not been achieved by mechanical exfoliation but can be deposited on metallic substrates such as Ag(111), Ir(111), and $ZrB_2(0001)$. Regrettably, strong interaction to these substrates destroys the Dirac physics. For this reason, semiconducting substrates, including Si(111) and SiC(0001), have been explored theoretically to evaluate whether they lead to a Dirac cone with reasonable band gap (which is essential for

applications). However, surface passivation is inevitable for these and similar substrates, due to their dangling bonds. Layered materials such as $MgBr_2(0001)$, MoX_2 , and GaX_2 ($X = S, Se, \text{ and } Te$), on the other hand, might preserve the characteristic electronic states of silicene and additionally simplify the preparation procedure as passivation is not required. The predicted effects of different substrates on silicene will be compared and evaluated with respect to technological requirements.

Biography

Udo Schwingenschlögl is a Professor of Materials Science & Engineering at King Abdullah University of Science and Technology. His research interests in condensed matter physics and first-principles materials modeling focus on two-dimensional materials, interface and defect physics, correlated materials, thermoelectric materials, metal-ion batteries, nanoparticles, and quantum transport.

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