

CHEM 07- 2018

# Book of Invited & Keynotes Lectures

*Organizing Committee CHEM 07  
Chemistry Department – Faculty of Science – Cairo  
University – Giza-Egypt.*



## Preface

*In 2000*, the Department of chemistry launched its very first scientific conference Chem01. When we first thought about it we set a goal to have these conferences more than just a scientific meetings; an event that involve not only faculty staff members but also graduate and post-graduate students too. Chem0x series of conferences kept this goal along the way from Chem01 to Chem06 in 2010. In Chem0x we tried our best to invite distinguished speakers from all over the world. This enriched the scientific discussions, kept us connected with the latest in chemistry and allowed us to make new friends. Along the scientific meetings and lectures we were able to launch several different workshops aimed at our students. Every one of the 6 Chem0x conferences had its own taste, advantages and memories which will never be forgotten.

*Egypt* went through a lot since our last conference Chem06 in 2010. But now it is the time to re-gain the momentum and start looking at the future. Chem07 come with a lot of expectations. We start organizing it from scratch. I tried to put together our old team ; three only accepted, *Profs. Hamed Ead, Faten Nour El-Dein* and *Azza Shoukry*. For whom I am really deeply indebted. A group of the younger generation having great enthusiasm and courage joined us, *Rabab El Sherif , Sahar Fadl Allah, Rasha El Nashare, Riham Rashad, Shymaa Medany* and *Randa Abdlahmeed*. Along the way, we got more momentum when *Profs. Hamdi Hassanen* and *Abdelgawad Fahmi* Joined us. Now we have a wonderful team which dedicates itself for Chem07.

*Chem07* will witness a lot of events. Three general lectures and more than 40 invited lectures and keynotes will bring to us the latest in all disciplines of chemistry. Chem07 is really international, thus in addition to the 50 Egyptian participants; colleagues from 11 different countries are joining us. Chem07 will start a new tradition, for the first time, it will organize tribute sessions dedicated to men and women who served and enriched our department and left us with their great Heritage. In Chem07 we will



pay tribute to three great scientists, *Prof. Schomberge, Prof. Ahmed Sami* and *Prof. Waheed Badawy*.

*A nanochemistry* and technology workshop will be organized. It will visit the nanotechnology center of Cairo University in 6<sup>th</sup> October City where participants will have the chance to see and hear from scientists about the latest instruments and research conducted and its applications.

*On the social side*, we always try to allow our guests to taste the Egyptian civilization; ancient, old and modern. Several site seeing tours and visits will be organized just after or along the conference days.

*We really hope* that Chem07 come as we would like it to be and more. A real addition to the department. We hope to boost a new spirit of cooperation, respect and love among us in our department.

*On behalf of the organizing committee*

*Rifaat Hilal*

*Conference Coordinator*

*Cairo Feb. 24<sup>th</sup> ,2018*



## CHEM 07 Committee

### Organizing Committee

**Prof. Hyman H. Rehan**

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**Prof. Rifaat H. Hilal**

*Conference Coordinator*

**Prof. Hamed A. Ead**

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Dr. Hadeer Mohamed Diab

Dr. Ibrahim Mostafa Zaki

Dr. Walaa Hamed

Dr. Sally El-Sayed

Dr. Marwa El-Badery

Dr. Ekram Hamdy El-Sayed

Dr. Fatma Saleh

Dr. Enas El-Hassan

Dr. Mohamed A. Sultan



**Prof. Roger M.  
Leblanc Cooper**

Chair Department of  
Chemistry University of  
Miami  
1301 Memorial Drive  
Coral Gables, FL, 33146  
USA

E-mail: [rml@miami.edu](mailto:rml@miami.edu)  
Tel: (+1)-305-284-2194

Roger M. Leblanc received his B. S. in chemistry in 1964 from Université Laval, Canada, and Ph. D. in physical chemistry in 1968 from the same university. From 1968 to 1970, he was a postdoctoral fellow in the laboratory of Prof. George Porter, FRS, in Davy Faraday Research Lab, the Royal Institution of Great Britain. He was a professor from 1970 to 1993 at Department of Chemistry and Biology in Université du Québec à TroisRivières, Canada. During this period, he was Chair from 1971 to 1975 at the same department, and Director from 1981 to 1991 at Photobiophysics Research Center. In 1994, he moved to University of Miami, where he has been a professor at Department of Chemistry since then to present. At University of Miami, he was Chair of Department of Chemistry from 1994 to 2002, and he is appointed as Chair from 2013 to present. He was also one of the three editors of Colloids and Surfaces B: Biointerfaces from 1998 to 2013. During his early career as a scientist, his research interest was on the photosynthesis and photoconductivity using surface chemistry and spectroscopy. His current research interest is to apply 2-dimensional (2-D) surface chemistry combined with spectroscopy and microscopy to investigate the properties of nanomaterials (graphene oxide, carbon dots and quantum dots) and the fibrillation process of amyloidogenic proteins (insulin, amyloid-beta peptide and islet amyloid polypeptide). He is also interested to design and develop biosensors with high sensitivity and selectivity for diseases diagnosis. He has published 505 scientific articles in peer-reviewed journals. As a professor, he has supervised more than 100 M.S. and Ph.D. students.

**Talk Title**  
Talk Date : Monday 5 March  
2018  
Place: Main Hall  
Time: 12:00-12:45

**Development and Bioapplications of  
Nontoxic Carbon Dots**



## Development and Bioapplications of Nontoxic Carbon Dots

Roger Leblanc

Department of Chemistry, University of Miami, 1301 Memorial Drive,  
Coral Gables, Florida, 33146, United States

### ABSTRACT

Carbon dots (C-Dots) with diameter smaller than 10 nm have recently attracted enormous attention in various fields due to their unique properties. In this talk, the synthesis, characterization and bioapplications of a new type of nontoxic, water-soluble C-Dots will be presented. A major medical challenge one faces to treat central nervous system (CNS) related diseases is to cross the tight junctions between endothelial cells, which are known as blood-brain barrier (BBB). Recently, our *in vivo* experimental observations suggested that the transferrin conjugated C-Dots could enter the CNS of Zebrafish while C-Dots alone could not. Thanks to the abundant presence of carboxylic acids on the surface, C-Dots are easily conjugated with transferrin and anticancer drug doxorubicin. The system was then applied as a drug delivery system for the delivery of doxorubicin into cancerous cells. Our *in vitro* study showed greater uptake of the conjugates compared to free doxorubicin, the conjugates at 10 nM was significantly more cytotoxic than doxorubicin alone, reducing viability by 14~45 %, across multiple pediatric brain tumor cell lines. Accidents, disease and aging compromise the structural and physiological functions of bones, and *in vivo* bone imaging test is critical to identify, detect and diagnose bone related development and dysfunctions. Here we show that C-Dots with low quantum yield ("dark") bind to calcified bone structures of live Zebrafish larvae with high affinity and selectivity. Binding resulted in a strong enhancement of luminescence that was not observed in other tissues, including non-calcified endochondral elements. Retention of Cdots by bones was very stable, long lasting, and with no detectable toxicity. These observations support a novel and revolutionary use of C-Dots as highly specific bioagents for bone imaging and diagnosis, and as a potential bone-specific drug delivery carrier.



### Prof. Oliver Kuhn

Professor on Institute of  
Physics, University of  
Rostock, Albert-Einstein-  
Str. 23-24 D-18059  
Rostock, Germany

oliver.kuehn@uni-rostock.de  
www.physik.uni-  
rostock.de/quantendynamik

#### Academic Record

2000 Habilitation, „Theoretical Chemistry“: Dynamics and Spectroscopy of Molecular Systems from Chemistry and Biology  
1995 PhD, „Theoretical Physics“: Theory of Dissipative Quantum Dynamics in Molecular Systems  
1990 Diploma, „Physics“, Theory of Resonant Tunneling Through Quantum Dots in the Presence of Electron-Phonon Interaction.

1985-1990 study of Physics, Humboldt University Berlin  
Professional Career

since 03/16 Vice Dean, Faculty for Mathematics & Natural Sciences.  
10/12 - 02/16 Managing Director, Institute of Physics, University of Rostock.  
since 01.01.08 Professor (W2) of Theoretical Physics, University of Rostock.

08/04 - 12/07 Oberassistent (C2), Institute for Chemistry, Free University Berlin.  
11/02 - 03/03 Visiting Professor, Institute for Molecular Science, Okazaki (Japan).

03/99 - 07/04 Researcher, Institute for Chemie, Free University Berlin.  
03/97 - 02/99 Habilitand, Institute for Chemistry, Free University Berlin (J. Manz).

05/96 - 12/96 Postdoc, Department of Chemistry, Lund University (V. Sundström).

04/95 - 05/96 Postdoc, Department of Chemistry, University of Rochester, New York. (S. Mukamel).

09/92 - 02/95 PhD student, Institute for Theoretical Physics, Humboldt University Berlin. (V. May).

10/91 - 08/92 Visiting Scientist, Stevens Institute of Technology, Hoboken, New Jersey.

10/90 - 09/91 Research Student, Institute for Theoretical Physics, Humboldt University, Berlin

08/89 - 12/89 Research Student, Petersburg Institute for Nuclear Physics of the Russian Academy of Sciences

#### Talk Title

#### First Principles Approach to X-ray Spectroscopy of Transition Metal Compounds

Talk Date : Wednesday 5

March 2018

Place: Hall A

Time : 10:00-10:45



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## First Principles Approach to X-ray Spectroscopy of Transition Metal Compounds

**Oliver Kühn**

Institute of Physics, Rostock University, Albert-Einstein-Str. 23-24, Rostock, Germany

X-ray spectroscopy has become a routine tool that can reveal highly local and element-specific information on the electronic structure of atoms in complex environments. Theoretical predictions for L-edge spectra of transition metal compounds are rather challenging due to the often pronounced multi-configurational character of the electronic wave function as well as strong spin-orbit coupling. Recently, we have developed an efficient and versatile theoretical methodology for the treatment of soft X-ray spectra of transition metal compounds mainly based on the multi-configurational self-consistent field (RASSCF) electronic structure theory combined with a perturbative LS-coupling scheme for spin-orbit coupling [1-7]. In this contribution, the developed protocol will be illustrated for the case of Fe(CO)<sub>5</sub> [4], which will also serve to demonstrate the shortcomings of standard density functional theory (ROCIS). Further, a wave function based approach adapted from exciton theory will be introduced as a means to quantify aggregation effects on X-ray absorption and scattering (RIXS) spectra [7].

- [1] S.I. Bokarev et al. *Phys. Rev. Lett.* 111, 083002 (2013).
- [2] R. Golnak et al. *Sci. Rep.* 6, 24659 (2016).
- [3] S.I. Bokarev et al. *J. Phys. Chem. C* 119, 19192 (2015).
- [4] E. Suljoti et al. *Angew. Chem. Int. Ed.* 52, 9841 (2013).
- [5] N. Engel et al. *J. Phys. Chem. B* 118, 1555 (2014).
- [6] K. Atak et al. *J. Phys. Chem. B* 117, 12613 (2013).
- [7] M. Preuße et al. *Struct. Dynamics* 3 062601 (2016).



**Prof. Marek  
Trojanowicz**

Professor of  
Chemistry in the  
Institute of Nuclear  
Chemistry and  
Technology in  
Warsaw, Poland.

[trojan@chem.uw.edu.pl](mailto:trojan@chem.uw.edu.pl)

**Marek Trojanowicz** received M.Sc., Ph.D. and D.Sci. (habilitation) degrees in Faculty of Chemistry, University of Warsaw. M.Sc. under supervision of Prof. Wiktor Kemula, Ph.D. under supervision of Prof. Adam Hulanicki. His post-doc one year stay was in Tohoku University in Sendai, Japan, in research group of Prof. Nobuyuki Tanaka. In years 1966-2014 his academic activity from research assistant position to full professorship was in Faculty of Chemistry, University of Warsaw. Currently he is employed as Professor of Chemistry in the Institute of Nuclear Chemistry and Technology in Warsaw, Poland. His expertise includes design of electrochemical sensors and biosensors, flow analysis, liquid chromatography and capillary electrophoresis, environmental analysis, application of ionizing radiation for water and waste treatment and application of chemical analysis in archaeometry. He is author of 340 scientific papers, 2 monographic books and editor of 1 book in the field of flow analysis and automation of analytical measurements. He is recipient of prestigious Świętosłowski Award of University of Warsaw for achievements in field of analytical chemistry, Kemula Medal of Polish Chemical Society and Scientific Honor Award of Japanese Society of Flow Injection Analysis. He was granted Visiting Professor positions in numerous universities all over the world including long-term appointments in University of Michigan, University of California at Riverside, University of Tasmania, Australia and University of Sao Paulo, Brazil. He is member of advisory boards of 10 international analytical journals and for 15 years he was a Scientific Secretary of Committee on Analytical Chemistry of Polish Academy of Sciences. His current number of citations according to ISI Web of Knowledge is about 5400, and Hirsch index 38.

**Talk Title**

**Occurrence, Analysis and Advanced Methods of Degradation of Selected Perfluorinated Surfactants for Environmental and Human Health Protection.**

Talk Date : Monday

5 March 2018

Place: Hall C

Session : 3

Time: 01:00 - 01:45



## Occurrence, Analysis and Advanced Methods of Degradation of Selected Perfluorinated Surfactants for Environmental and Human Health Protection

**Marek Trojanowicz<sup>1,2</sup>, Iwona Bartosiewicz<sup>1</sup>, Anna Bojanowska-Czajka<sup>1</sup>, Tomasz Szreder<sup>1</sup>, Krzysztof Kulisa<sup>1</sup>, and Krzysztof Bobrowski<sup>1</sup>**

### ABSTRACT

Wide interest in environmental role of perfluorinated surfactants (PFSs) since beginning of 2000-ties resulted from discovery of a common global presence of those anthropogenic compounds, mostly perfluorinated sulfonates and carboxylates, in human and animal organisms, and in the environment, even in the most remote places. It resulted in wide development of analytical methods of their determination, as well as toxicological studies. They are considered as a new class of persistent organic pollutants. The extraordinary chemical stability of PFSs results in insufficient efficiency of their removal from wastes, surface waters, and raw and drinking water sources by conventional treatment processes. This implies increasing interest in search for a new treatment technologies based on the use of strongly reactive free radicals produced in-situ in reaction medium. They include both methods based on reductive dehalogenation (employing *e.g.* sub-critical elemental iron reduction or UV-iodide photolysis), as well as advanced oxidation processes (AOPs), like electrochemical methods or Fenton reactions. The pulse radiolysis measurements indicate, that reactions of perfluorinated octanoic acid (PFOA), the most commonly occurring PFSs besides perfluorinated octanesulfonic acid (PFOS), with  $\cdot\text{OH}$  radical and hydrated electron  $e_{\text{aq}}^-$ , are much slower than with many other industrial and anthropogenic pollutants. The obtained rate constants are 2-3 orders of magnitude lower compared to reactions of different other organic pollutants. Therefore, there is need for application of especially efficient methods of advanced oxidation/reduction treatment such as photocatalysis with the use of specially designed nanocatalysts, ultrasonic treatment, or the use of ionizing radiation, employing both  $\alpha$ -rays from the radioisotope sources or beams of accelerated electrons. Authors developed a novel radiolytic method for the decomposition of PFOA employing ionizing radiation in reductive conditions, which can be efficiently employed in industrial treatment of waters and wastewaters.



**Prof. Mario Barbatti**

Professor of Chemistry,  
Chair of Excellence  
A\*MIDEX, Aix Marseille  
Univ, ICR, Marseille.

[mario.barbatti@univ-amu.fr](mailto:mario.barbatti@univ-amu.fr)  
[Website: barbatti.org.](http://barbatti.org)

**Contact:** Aix Marseille Université - Institut de Chimie Radicalaire (ICR) Avenue Escadrille Normandie-Niemen, Service D42 13397 Marseille cedex 20 – France Tel.: (office) +33 (0)4 84 52 92 00 (mobile) +33 (0)7 83 57 70 62 E-Mail: [mario.barbatti@univ-amu.fr](mailto:mario.barbatti@univ-amu.fr) Website: [barbatti.org](http://barbatti.org).

**Professional Appointments**

Since 2015 Professor of Chemistry, Chair of Excellence A\*MIDEX, Aix Marseille Univ, ICR, Marseille.

2010-Aug 2015 Professor of Chemistry, Chair of Excellence A\*MIDEX, Aix Marseille Univ, ICR, Marseille.

2004-2010 Postdoctoral associate at the Institute for Theoretical Chemistry, University of Vienna.

**Education and Titles**

2008 Habilitation for teaching Theoretical Chemistry, University of Vienna.

1997-2001 Doctor of Sciences (Physics). Institute of Physics, Federal University of Rio de Janeiro.

1995-1997 Master of Sciences (Physics). Institute of Physics, Federal University of Rio de Janeiro.

1991-1995 Bachelor of Sciences (Physics, *cum laude*), Institute of Physics, Fed. Univ. of Rio de Janeiro.

**Talk Title**

**Simulations of Organic Materials with Optical Activity: Advances, Appraisal, Applications**

Talk Date: Wednesday 7

March 2018

Place: Hall A

Session : 13

Time: 11:00-11:45



## Simulations of Organic Materials with Optical Activity: Advances, Appraisal, Applications

**Mario Barbatti**

Professor of the Chair of Excellence A\*MIDEX  
Aix Marseille Univ, CNRS, ICR, Marseille – France

### ABSTRACT

Organic materials with optical activity (OMOA) are central for diverse fields, including biology (photosynthesis, vision), health (phototherapy, imaging), and technology (photonics, photovoltaics, photocatalysis). Diversity, plasticity, and low cost make OMOA ideal for a variety of innovations, from solar cells, through sensors, to information storage and display. Photo-electronic processes in OMOA are highly complex and the development of a new OMOA targeting specific property goes through cumbersome and expensive processes of synthesis and characterization. Computational chemistry of excited states may help providing insights into physical-chemical phenomena, aiding deconvolution of experimental data, and predicting properties before synthesis. Using computational chemistry in this field faces, however, different challenges, including development of new functionalities, reliable research protocols, efficient computational methods, and integration with experimental analysis.

In this talk, I will present applications showing how computational chemistry can be used to investigate OMOA; recent methodological advances implemented by our group within the Newton-X platform ([www.newtonx.org](http://www.newtonx.org)); and a critical appraisal of excited-state computational chemistry.



**Prof. Brindaban C.  
Ranu.**

Professor on West  
Bengal Academy of  
Science & Technology,  
Indian Academy of  
Sciences, Bangalore and  
Indian National Science  
Academy, New Delhi.

Brindaban C. Ranu received his M.Sc. from Calcutta University (India) and obtained his Ph.D. from Jadavpur University (India) in 1982 working with Professor U.R. Ghatak at Indian Association for the Cultivation of Science. He did his post-doctoral work in Virginia Tech, USA with Prof. T. Hudlicky during 1982-85 and started independent research at the department of Organic Chemistry, IACS from 1985. He became Professor in 1996, senior Professor in 2006 and served as Head of the Organic Chemistry department during 2003-2008. He retired from regular job in 2013 and currently is continuing as INSA Senior Scientist in the same department, He is a fellow of West Bengal Academy of Science & Technology, Indian Academy of Sciences, Bangalore and Indian National Science Academy, New Delhi. He received the J C Bose fellowship from DST, Govt. of India. He received N.S. Narasimhan Award in 1993 and Chemical Research Society of India Bronze medal in 2001 and Silver medal in 2009 among others. His work primarily focuses on the issue of Green Chemistry. He has already published 270 papers in highly reputed international journals and currently his *h*-index is 58. He has supervised 33 students for Ph.D. degree (awarded). Professor Ranu's works received considerable appreciation all over the world and he has been invited to deliver key note, plenary and invited lectures in symposia in India and abroad. His research on green synthesis stimulated much interest and inspiration in the chemical community, at large. Professor Ranu has also edited a book entitled, 'Ball Milling Towards Green Synthesis – Applications, Projects, Challenges' published by Royal Society of Chemistry in 2015, which received great appreciation from the practicing chemists.

**Talk Title**  
Talk Date : Tuesday 6  
March 2018  
Place: Hall B  
Session : 11  
Time : 1:30-02:15

**Eco-acceptability and Economy – Two Vital  
Parameters for a Current Chemical Process**



## Eco-acceptability and Economy – Two Vital Parameters for a Current Chemical Process

**Brindaban C. Ranu**

Department of Organic Chemistry  
Indian Association for the Cultivation of Science  
Kolkata -700032

### ABSTRACT

The growing awareness of environmental implications and industrial acceptability of chemical processes lead to constant search for new green measures to reduce environment pollution and overall cost. With these objectives designing a chemical transformation in a minimum number of steps within a reasonable time is of current interest. In conventional reactions the energy used is heat from an electrical source. On the other hand electrical energy is produced mainly by the expense of fossil fuel. Thus concept of use of minimum energy and less toxic organic solvent both in reaction and purification of product is gaining momentum. The functionalization of a C-H bond in a molecule *via* C-H activation is of much importance as it reduces the number of steps and cost. This concept will be discussed. Ball milling (mechanical grinding) has emerged as a powerful tool in effecting various chemical reactions in a relatively green way by reducing the amount of solvent at ambient temperature by application of mechanical energy. Apparently, ball milling can be applied in a number of bond-forming processes and various standard chemical transformations benefit from the use of this mechano-chemical technique. The application of visible light photo-catalysis in organic synthesis has received considerable interest in recent years. These photocatalyzed reactions in the presence of suitable photosensitizers involve a single electron transfer process and the primary merits of these reactions are metal free protocol and mild generation of aryl radicals at room temperature. Several useful reactions have been accomplished by this green technique.

### Selected references

- 1) *Ball Milling towards Green Synthesis – Applications, Projects, Challenges* – ed. B. Ranu and A. Stolle, Royal Society of Chemistry, London, 2015.
- 2) N. Mukherjee, T. Chatterjee, B. C. Ranu, *J. Org. Chem.* 2013, 78, 11110.
- 3) T. Chatterjee, B. C. Ranu, *RSC Adv.* 2013, 3, 10680.
- 4) N. Mukherjee, S. Ahammed, S. Bhadra, B.C. Ranu, *Green Chem.* 2013, 15, 389.
- 5) D. Kundu, S. Ahammed, B. C. Ranu, *Org. Lett.* 2014, 16, 1814.
- 6) B. Majhi, B. C. Ranu, *Org. Lett.*, 2016, 18, 4162.
- 7) P. Maity, B. Paroi, B. C. Ranu, *Org. Lett.* 2017, 19, 5748.
- 8) P. Maity, B. C. Ranu, *Adv. Synth. Catal.* 2018, *In press.*



**Prof. Matthias  
Lehmann**

Professor of Organic  
chemistry  
*Institute of Organic  
Chemistry, University of  
Würzburg, Germany*

Matthias Lehmann is a Professor in Organic Materials – Soft Materials and Liquid Crystals – since 2011 at the University of Würzburg and held before the prestigious Heisenberg fellowship of the German Science Foundation. He studied Chemistry at the University of Mainz, and began his independent career as a Juniorprofessor at the Chemnitz University of Technology after Postdoc positions at the University of Zaragoza and the Free University of Brussels.

His research interest focus on the synthesis, self-assembly and application of complex soft matter with liquid-crystalline properties as new emerging materials. Special emphasis lays in the structural control, which is studied by comprehensive X-ray scattering methods, modelling and simulation.

**Talk Title**

**Fullerene-Filled Liquid-Crystalline Nanostructures  
A Possible Solution for LC Photovoltaics?**

Talk Date : Monday 5

March 2018

Place: Hall B

Session: 2

Time: 01:00-01:45



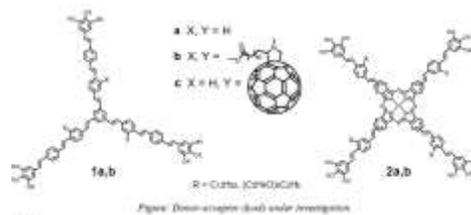
## Fullerene-Filled Liquid-Crystalline Nanostructures A Possible Solution for LC Photovoltaics?

Matthias Lehmann,<sup>1\*</sup> Moritz Dechant,<sup>1</sup> Markus Hügel<sup>1</sup>

<sup>1</sup>Institute of Organic Chemistry, University of Würzburg, Germany

### ABSTRACT

Liquid Crystals (LC) are well known materials for their application in display technologies (LCDs). They combine fluidity with anisotropic properties and can usually be well surface aligned in thin films. Although their application in photovoltaic devices offers various advantages over less ordered polymeric materials, LC compounds consisting of donor-acceptor dyads containing Fullerenes are much less explored. [1,2]



Recently, our group focused the research on star-shaped, shape-persistent LC molecules 1 and 2 with 1,3,5-benzene or Phthalocyanine cores and conjugated oligomers as arms decorated with either aliphatic or oligo(ethyleneoxy) chains (R).[3,4] The intrinsic void between the arms can be filled with Fullerenes, which are attached to one or more arms via spacers of various lengths (n). The stacking of these mesogens has been studied by comprehensive X-ray scattering methods and simulation. This contribution will present the beautiful hierarchical self-assembly in double-nanosegregated helical columns, which can be fine-tuned by the spacer length for molecules 1c. Even mixtures of Fullerene containing non-LC compounds (1b, 2b) with the parent stars without Fullerene (1a, 2a) self-organize in such donor-acceptor stacks. For the Phthalocyanine derivatives 2 a limited range of mixtures of components 2a and 2b can be aligned and result in  $\pi$ -stacked columns, in which the Fullerenes are nanosegregated at the periphery of the columnar stacks. The optimization of these mesogens for the development of possible new LC photovoltaic materials will be discussed.

### References

- [1] S. H. Park et al., *Nphoton*, 2009, 3, 297.
- [2] H. Hayashi, W. Nihashi, T. Umeyama, Y. Matano, S. Seki, Y. Shimizu, H. Imahori, *J. Am. Chem. Soc.* 2011, 133, 10736 – 10739.
- [3] M. Lehman, M. Hügel, *Angew. Chem. Int. Ed.* 2015, 54, 4110 –4114.
- [4] M. Lehmann, M. Dechant, unpublished results.



### Prof. Volker Abetz

Director of the Institute of  
Polymer Research Institute of  
Polymer Research, HZG  
Geesthacht.

Professor at the University of  
Hamburg  
Institute of Physical Chemistry.

[volker.Abetz@chemie.uni-hamburg.de](mailto:volker.Abetz@chemie.uni-hamburg.de)

His expertise is in design and synthesis of tailor-made polymers for special membrane-based separation processes, development of self-assembling membranes based on block copolymers for medical and environmental technology, "switchable" membranes, development and optimization of membranes and processes for the production of membranes for gas and liquid separation. He is a recipient of Grant the Research Training Group Polymer Sciences at the University of Freiburg (1987-1990), graduated grant from the Chemical Industry Association (VCI) (1990), travel grant under PROCOPE (1992-1993), scholarship under the "Human Capital and Mobility" program of the European Community (1993-1994), travel grant of the Section of Macromolecular Chemistry of the German Chemical Society (GDCh, 2000), research Grant by the VCI in conjunction with the BMBF (since 2001) He participates in "Polymer Bulletin", Springer Verlag GmbH & Co KG- 1995 - 1998: Assistant to the Editor for Europe and Africa, **e-Polymers** Co-initiation (1999) and participation (advisory board) for *e-polymer*, an "open access" Internet journal for polymer science, **Macromolecules** (ACS) From 2006 to 2008 member of the "Advisory Editorial Board" of *Macromolecules*.

#### Talk Title

#### Development of Polymer Membranes for Gas and Liquid Phase Separations

Talk Date: Monday 5 March  
2018

Place: Hall B

Session: 5

Time: 2:45 - 03:30



## Development of Polymer Membranes for Gas and Liquid Phase Separations

Volker Abetz

Institute of Polymer Research, HZG Geesthacht.

### ABSTRACT

Membrane technology is present in everyday life but its potential for energy and resource efficient cleaning and processing of water, air, and chemicals is not fully exploited. Besides process engineering also membrane development and especially material development are important parameters on the way to develop competitive membrane processes. Polymers are very attractive candidates for membranes in many separation tasks, as they are much cheaper, easier to upscale and easier to handle in applications as compared to ceramic or metallic membranes. Polymers fail, however, if separations have to be carried out at very high temperatures or under chemically very harsh conditions. In this contribution a few highlights in the material development of polymer membranes will be presented. On one side these will be block copolymers as candidates for a new generation of ultrafiltration membranes and on the other side novel dense and very fast membranes for gas separation will be presented. While in the case of the ultrafiltration membranes a big challenge is the processing of tailor-made block copolymers in order to produce regular, isoporous membranes in flat sheet or hollow fibre geometry with controlled pore size and pore properties, a big challenge in the case of novel gas separation membranes based on so-called thermally rearranged polymers is a well chosen polymer chemistry allowing the necessary thermal rearrangement reactions at temperatures compatible with the requirements of membrane production.



**Prof. Samy El-Shall**  
Mary Eugenia Kapp  
Endowed Chair in  
Chemistry,  
Commonwealth  
Professor and the  
Chairman of the  
Chemistry Department  
at Virginia  
Commonwealth  
University (VCU).  
[mshelshal@vcu.edu](mailto:mshelshal@vcu.edu)

He received his B.S. and M.S. degrees from Cairo University, and a Ph.D. from Georgetown University. He did postdoctoral research in nucleation and clusters at UCLA. His research interests are in the general areas of cluster ions, ion mobility, nucleation phenomena, nanostructured materials, graphene and nanocatalysis for energy and environmental applications.

He has published over 250 refereed papers and review chapters, and he holds eight US patents on the synthesis of nanomaterials, nanoalloys, nanoparticle catalysts, graphene, and graphene-supported catalysts.

Dr. El-Shall received the *Exxon Education Award* in 1994 and 1995; the *Outstanding Faculty Award* of the State Council of Higher Education of Virginia (SCHEV), Virginia's highest faculty honor in 1999; *Jabir IbnHyyan Award* from the Saudi Chemical Society for "Advances in Nanomaterials & Nanotechnology" in 2007; the *Distinguished Research Award* from the Virginia Section of the American Chemical Society in 2009; the *Innovative Research Award* from the Society of Automotive Engineering (SAE) in 2009; the *VCU Distinguished Scholarship Award* in 2011, and the *VCU Award of Excellence* in 2016. He was selected as a *Jefferson Science Fellow* and worked as a Senior Science Advisor at the U.S. Department of State in 2012-2013. He is an elected Fellow of both the American Physical Society (APS) and the American Association for the Advancement of Science (AAAS).

**Talk Title**

**Graphene-based Materials for Applications in Heterogeneous Catalysis, Water Treatment and Solar Water Desalination**

Talk Date : Tuesday 6  
March 2018  
Place : Hall A  
Session: 10  
Time: 1:30-2:15



## Graphene-based Materials for Applications in Heterogeneous Catalysis, Water Treatment and Solar Water Desalination

M. Samy El-Shall

Departments of Chemistry

Virginia Commonwealth University, Richmond, Virginia 23284-2006, USA

### ABSTRACT

The combination of highest carrier mobility, thermal, chemical and mechanical stability of graphene with its high surface area offers many interesting applications in a wide range of fields including heterogeneous and photocatalysis where metallic and semiconductor nanoparticles can be efficiently dispersed on or within the graphene nanosheets. This talk will address the development of three classes of graphene-based materials as (1) support for metal nanoparticle catalysts in heterogeneous catalysis, (2) sorbent materials for the removal of heavy metal ions from polluted water, and (3) photothermal energy converter materials for efficient solar water desalination. In heterogeneous catalysis, we will discuss the superior catalytic activity of Pd nanoparticles supported on reduced graphene oxide (RGO) nanosheets for carbon-carbon cross-coupling reactions. Second, the enhanced catalytic activity for the Fe-based nanoparticle catalysts supported on graphene in the *Fischer-Tropsch Synthesis* of liquid transportation fuels will be presented. Finally, the superior catalytic activity and selectivity of Pd nanoparticles supported on a sandwich-type nanocomposite consisting of Metal-Organic Frameworks (MOFs) wrapped with thin RGO nanosheets for the biomass-refining of liquids derived from lignocellulosic sources will be presented. For the removal of heavy metals from water, we will discuss the development of chemically modified graphene-based adsorbents containing highly efficient chelating groups such as diamine, imino and thiourea for the effective extraction of the toxic metal ions mercury (II), copper (II), lead (II), chromium (VI), and arsenic (V) from wastewater. For photothermal energy conversion, we will discuss the development of a new generation of highly efficient, flexible, low weight, highly porous and cost effective *Plasmonic Graphene Polyurethane (PGPU)* nanocomposite materials for solar steam generation through the efficient evaporation of water surface pools. The PGPU nanocomposites contain metallic nanoparticles that exhibit very strong solar absorption. The polyurethane (PU) foam provides a hydrophilic surface with abundant microporous structure, excellent thermal insulation properties, and facile and scalable synthesis. The high solar thermal evaporation efficiency, excellent stability and long-time durability make the PGPU nanocomposites excellent candidates for practical solar-steam-generation applications and seawater desalination.



**Prof. Wilhelm Schwieger**

Institute of Chemical  
Reaction Engineering,  
Friedrich-Alexander  
University, Erlangen-  
Nuremberg  
Egerlandstraße 3, 91058  
Erlangen, Germany  
Phone: +49-9131-85  
28910,  
[www.crt.fau.de](http://www.crt.fau.de)

Since 1998 Professor for Technical Chemistry at the Institute of  
Chemical Reaction Engineering, Friedrich-Alexander-  
University Erlangen-Nuremberg, Germany,  
1994-1998 Assistant professor at the Martin-Luther-University  
Halle-Wittenberg, Halle, Germany, Institute of  
Technical Chemistry  
1994 Habilitation at the Martin-Luther-University Halle-  
Wittenberg  
1993-1994 Visiting scientist, Department of Chemistry,  
1993-1995 University of British Columbia  
1987-1989 Head of the joined Molecular Sieve Research Center at  
the Chemiewerk Bad Köstritz (CWK) and the University  
Halle  
1980-1987 Member of inorganic research division at the  
"ChemiekombinatBitterfeld", head of the 'Molecular-  
Sieve-Group'  
1980 PhD thesis: Preparation and characterisation of  
aluminium-free layered silicates and their related silicic  
acids, (summa cum laude)  
1974-1979 Research assistant at the Institute of technical  
Chemistry, University of Halle-Wittenberg, advisor  
Prof. Dr. F. Wolf  
1970-1974 Study of Chemistry, Martin-Luther-University  
1970-1975 Halle-Wittenberg, Halle Germany  
The Research interests are widespread in the field of heterogenous  
catalysis and porous materials in general. W.S. focused is the structure  
formation and the application of porous systems. In particular: (i) Surface  
chemistry on and in crystalline porous materials (layered silicates, zeolites  
or zeolite-like materials, aluminum phosphates); (ii) structure-working  
relationships of porous materials in respect to their of different  
applications; (iii) development of new porous inorganic materials; (iv)  
reaction on and in porous materials and development of composite  
materials with hierarchical pore structures for the development of new  
reactor concepts. Member of the Synthesis Commission of the  
International Zeolite Assoziation (IZA), Member of the eolithgesellschaft  
within ProcessNet, Member of the Cluster "Engineering of Advanced  
Materials" (EAM) funded by the German, Excellence Initiative and the  
Energy Campus Nürnberg (EnCN), Member of ECRC, SPP1517, Vertec,  
Coordinator and Member of BFS-ProjectsReferee to leading national and  
international journals and institutions. *Selected Awards*  
'Leopoldina-Förderpreis' (1992) / Feodor-Lynen-Stipendium der  
Alexander v. Humboldt-Stiftung (1993) / Research and Innovation Prize  
of the Martin-Luther-University Halle-Wittenberg (1997)

**Talk Title**  
Talk Date: Tuesday 6  
March 2018  
Place: Hall A  
Time: 10:00-10:45

**Zeolitic Materials with Hierarchical Porosity:  
Preparation Concepts and Applications**



## Zeolitic Materials with Hierarchical Porosity: Preparation Concepts and Applications

Wilhelm Schwieger

Lehrstuhl für Chemische Reaktionstechnik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Egerlandstr. 3, 91058 Erlangen, Germany

### ABSTRACT

In recent years, major progress had been made in the preparation of highly ordered porous materials with tailored porosities and different structure, controlled surface functionality and their adjustable structure related applications. Advances have been made in the synthesis and structural characterization of so-called hierarchical material, which combine porosity features of different scale lengths, micro-, meso- and/or (sometimes) macropores, in one material. This contribution will give an overview about the ongoing research activities in the field hierarchically organized porous materials covering both, the synthesis strategies and the potential application, mainly in the field of catalysis. A special focus will be laid on the design options of hierarchical zeolites. Such hierarchical zeolitic systems do not only offer the possibility of reducing mass transfer limitations, but they also allow the catalytic conversion of large molecules over zeolites. However, the extra porosity in hierarchical zeolites often leads to a loss of selectivity of the products. Thus, introducing additional pores with an optimal size has to be combined with a tailoring of the surface properties at the different pore scales in such hierarchical system. Therefore, novel synthesis routes are required to prepare hierarchical zeolites. Thus, such preparation pathway will be described and classified. Special preparation routes to two catalytically important and hierarchically zeolites, zeolites of the MFI and FAU type, will be highlighted. This includes in particular pathways to layered like zeolites assemblies and a new zeolite material with micro/macropore network. The effect of different experimental conditions like the influence of silica and aluminum source as well as the kind and the content of heteroatoms like aluminum or boron in tuning the textural will be in the focus of the talk. Finally, the results of some catalytically test reactions to characterize the effect of the hierarchy in the system will be shown.

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He received his BS (1994) , MS (1996) , and PhD (1999) degree from The University of Tokyo. After 2 years as a research associate at The University of Tokyo, he started a faculty career as an assistant professor in Keio University in 2001. He was promoted to associate professor in 2003, and to professor in 2011. He was also a research director of JST-CREST (2011-2014), and JST-ACCEL (2014-present). His research interests include functional materials science, photochemistry, electrochemistry, and diamond electrodes.

**Prof. Yasuaki  
Einaga**

Professor in the  
Department of  
Chemistry at Keio  
University, Japan.

[einaga@chem.keio.ac.jp](mailto:einaga@chem.keio.ac.jp)

**Talk Title**

**Recent Development on Electrochemical Application on  
Boron-Doped Diamond Electrodes**

Talk Date :

Wednesday 7

March 2018

Place: Hall A

Session: 16

Time: 1:30-2:15



## Recent Development on Electrochemical Application on Boron-Doped Diamond Electrodes

Yasuaki Einaga

Department of Chemistry, Keio University Hiyoshi, Yokohama 223-8522, Japan

### ABSTRACT

Boron-doped diamond (BDD) electrodes are very attractive material, because of their wide potential window, low background current, chemical inertness, and mechanical durability[1]. In these years, we have reported several examples for electrochemical sensor applications[2]. Here, we report some recent examples of electrochemical sensor application of BDD such as influenza virus, oxytocin, which is known as a simple cuddle chemical using BDD microelectrodes. As other applications such as organic synthesis, ozone generation, and CO<sub>2</sub> reduction are also shown. Furthermore, one of the main problems for waste water treatment application is an electrolytic corrosion of BDD electrodes. Here, we have studied on the mechanisms of the corrosion, and then, proposed conditions required to prevent them during the electrolysis of organic compounds in aqueous solutions.

#### Highly sensitive detection of influenza virus

Several dozen plaque-forming units (pfu) of influenza virus (IFV) could be detected using a boron-doped diamond (BDD) electrode terminated with a sialic acid-mimic peptide. The peptide was used instead of the sialyloligosaccharide receptor—the common receptor of influenza A and B viruses required during the early phase of infection—to capture IFV particles. The peptide, which was previously identified by phage-display technology, was immobilized by click chemistry on the BDD electrode. Electrochemical impedance spectroscopy revealed that H1N1 and H3N2 IFVs were detectable in the range of 20–500 pfu by using the peptide-terminated BDD electrode.

#### Continuous and selective measurement of oxytocin

Oxytocin, which is known as a simple cuddle chemical, is a nonapeptide with many important biological functions. In addition to its functions as a hormone in facilitating uterine contractions and mammalian milk ejection, it was also discovered that oxytocin works as a neurotransmitter and is considered to mediate social behavior, such as pair bonding and instinctive maternal aggression. Cyclic voltammetry of oxytocin in a phosphate buffer solution exhibits an oxidation peak at +0.7 V (vs. Ag/AgCl), which is attributable to oxidation of the phenolic group in the tyrosyl moiety. The linearity of the current peaks obtained in flow injection analysis (FIA) using BDD microelectrodes over the oxytocin concentration range from 0.1 to 10.0 μM with a detection limit of 50 nM (S/N = 3) was high (R<sup>2</sup> = 0.995). Furthermore, a clear distinction between oxytocin and vasopressin was observed with anodically-oxidized BDD electrodes due to the attractive interaction between vasopressin and the oxidized BDD surface.

#### Microsensing system for in vivo real time detection of local drug kinetics

Recently, we have developed a microsensing system for in vivo real time detection of local drug kinetics and its physiological relevance. The system consists of two different sensors of both a micro-sensor composed of BDD microelectrodes with tip diameter ~40 μm and a glass microelectrode. By using the system, we have first tested bumetanide, a diuretic that is ototoxic but applicable to epilepsy treatment.

#### References

[1] *Diamond Electrochemistry*, Elsevier, 2005. [2] *Nature Biomed. Eng.*, 1, 654 (2017).



**Prof.  
Swapandeeep  
Singh Chimni**

Professor of Chemistry  
at Guru Nanak Dev  
University, Amritsar,  
India

[sschimni@yahoo.com](mailto:sschimni@yahoo.com);  
[sschimni.chem@gndu.ac.in](mailto:sschimni.chem@gndu.ac.in)

Swapandeeep Singh Chimni received a B.Sc. (Hons. Sch.) (1984), M.Sc. (Hons. Sch.) (1985) and Ph.D. (1991) degrees in Chemistry from Guru Nanak Dev University, Amritsar. From 1990 to 1992, he was Lecturer in Applied Chemistry at N. I. T. Jalandhar, Jalandhar where he initiated his research on Biocatalysis. From 1992 to 1997, he was a Lecturer in Chemistry at Guru Nanak Dev University and was promoted as Senior Lecturer in 1997 and subsequently as Reader in 2000. In 2009 he was promoted as Professor of Chemistry. His research interests include enantioselective synthesis of small molecules using biocatalytic and organocatalytic methods. He has authored more than 110 publications with his students and collaborators. Two of his publications received Most Cited Paper Awards from Tetrahedron Letters (2005-2008) and Tetrahedron Asymmetry (2005-2008, 2006-2009). His two research papers were highlighted as Inside Cover (2013, 2014) in Asian Journal of Organic Chemistry and another two highlighted in Chemistry Views (2012, 2013). One of his research papers has been highlighted on the Front Cover of Organic & Biomolecular Chemistry (2015). Professor Chimni was awarded INSA-RSC Bilateral Exchange Fellowship in 1996 to visit the laboratory of Professor Stanley M. Roberts, Robert Robinson Laboratory, University of Liverpool, U.K. He also visited the laboratory of Professor D. Basavaiah, School of Chemistry, Central University, Hyderabad as UGC Visiting Fellow (2000-2002). He visited Institute of Organic Chemistry, Warsaw, Poland under PAS-INSA bilateral exchange of scientists in 2017 and delivered seven lectures in different Institutes/Universities in Poland. He has delivered over 25 invited talks in National and International Conferences and gave a keynote address in a National Conference at GJUS&T, Hisar and has chaired sessions in many Conferences/Symposiums. He was bestowed with Costal Chemical Research Society Award for the year 2014.

**Talk Title**  
Talk Date : Tuesday 6  
March 2018  
Place: Hall B  
Session 8  
Time: 11:00 - 11:45

**Nature Inspired Organocatalytic  
Antioselective Carbon-Carbon Formation via  
Decarboxylative Addition Reaction.**



## Nature Inspired Organocatalytic Antioselective Carbon-Carbon Formation *via* Decarboxylative Addition Reaction.

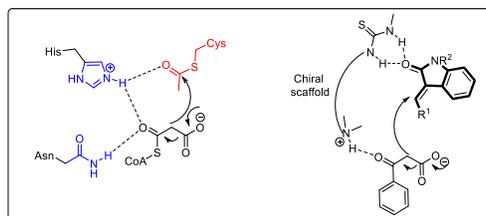
Swapandeep Singh Chimni

Department of Chemistry, U.G.C. Centre of Advance Studies in Chemistry, Guru Nanak Dev University, Amritsar, 143005, India

### ABSTRACT

The decarboxylative carbon-carbon bond formation has emerged as a very important tool for the synthesis of natural products and biologically active compounds.<sup>1</sup> In Nature, polyketides synthases utilizes malonic acid half thioesters (MAHTs) as thioesterenolate equivalents for the biosynthesis of complex polyketides. In the active site of PKSs, the amino acid residues histidine, cysteine and asparagines are involved in activation of MAHTs for decarboxylation *via* hydrogen bonding.<sup>2</sup> Inspired by the natural decarboxylative generation of an enolate, organic chemists have used malonic acid half thioesters (MAHTs) as thioesterenolate equivalents in various decarboxylative addition reactions. Several metal based approaches towards the decarboxylative addition reaction of MAHTs to different electrophiles have been developed.

In order to mimic the Nature's activation of MAHTs, it was envisaged that a bifunctional organocatalyst, providing both a hydrogen bonding unit and a basic moiety, could be a key for efficient catalysis.<sup>3</sup> In this context, it was planned to explore the application of *Cinchona* alkaloid organocatalysts for various decarboxylative addition reactions.<sup>4</sup> We have developed an organocatalytic asymmetric synthesis of chiral molecules using this approach. The 3-substituted-3-aminoindole derivatives have been synthesized with up to 91% yield and 98% *ee* *via* reaction of  $\beta$ -ketoacids derivatives with isatin imine catalyzed by quinine squaramide. The reaction of  $\beta$ -ketoacid derivatives with methyleneindolinones derivatives catalyzed by chiral *Cinchona* derived squaramide affords adduct in up to 87% yield, up to 98% enantiomeric excess and up to 3:1 dr.



Design of organocatalyst mimicking the active site of enzyme PKS

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## Dr. Ing. Doris Segets

Institute of Particle  
Technology (LFG)  
Friedrich-Alexander-  
Universität Erlangen-  
Nürnberg (FAU)

[doris.segets@fau.de](mailto:doris.segets@fau.de)

URL for web site:

[www.nanoprocessing.forschung.fau.de](http://www.nanoprocessing.forschung.fau.de)

### ACADEMIC CAREER

Since 07/2015 Scientific coordinator of the Center for Functional Particle Systems (FPS, [fps.fau.de](http://fps.fau.de)) of Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)

Since 11/2014 Habilitate of the Faculty of Engineering of FAU

Since 04/2013 Leader of the Nanoparticle Processing group (NanoPro, [nanoprocessing.forschung.fau.de](http://nanoprocessing.forschung.fau.de))

04/2013 PhD in Chemical Engineering: "Fundamental Aspects during the Processing of Semiconductor Nanoparticles", with distinction

2008 – 2013 Research assistant at Institute of Particle Technology (FAU) with research visits in Japan (Prof. Yasushige Mori, Doshisha University Kyoto), France (Prof. Lubomir Spanhel, University Rennes), and USA (Prof. A. Paul Alivisatos, Lawrence Berkeley National Laboratory)

2002 – 2008 Studies of Chemical and Biological Engineering at FAU

### AWARDS AND FELLOWSHIPS

04/2016 Friedrich-Löffler-prize for young scientists awarded by VDI-GVC

11/2015 Research Grant of the Alfred-Kärcher Foundation

09/2015 Starting Grant of the Erlangen Cluster of Excellence 'Engineering of Advanced Materials'

07/2015 Max-Buchner Research Fellowship, DECHEMA

11/2013 Doctoral prize of the Faculty of Engineering of FAU

**Talk Title**  
Talk Date: Monday 5  
March 2018  
Place: Hall A  
Session: 4  
Time: 2:45-03:30

**How in-Depth Understanding of Colloidal Interfaces Paves the way Towards Efficient Photocatalysis, Wastewater Reuse and Lightning**



## How in-Depth Understanding of Colloidal Interfaces Paves the way Towards Efficient Photocatalysis, Wastewater Reuse and Lightning

Doris Segets

Institute of Particle Technology (LFG) and Interdisciplinary Center for Functional Particle Systems (FPS), Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)

### ABSTRACT

The in-depth understanding of colloidal interfaces is of major importance for the development of future sustainable technologies. During photocatalysis for air purification, i.e. removal of volatile organic compounds (VOCs), interfaces govern the adsorption of pollutants, which is the first step in degradation. In wastewater reuse, highly efficient filter media with large pore diameters and low pressure loss potentially reduce the energy consumption during prefiltration for reverse osmosis. Finally, for lightning applications based on inorganic semiconductor nanoparticles (quantum dots, QDs) interface design is important for achieving so-called straddling-type band alignment to confine electron and hole within the core particle. Afterwards QDs have to be formulated, i.e. embedded in a continuous phase like a polymer, without agglomeration, a critical step that is again strongly governed by surface chemistry. Thus, interface characterization on both, the molecular and the particle level is of vital importance towards tailored colloidal surfaces for sustainable technologies. Herein, a widely-applicable strategy to study the thermodynamics of ligand adsorption to colloidal surfaces is presented [1]. The derived toolbox was applied to tailor the surface of ZnO nanoparticles by catechol derivatives (CAT) with different functionalities. To unambiguously order different CAT molecules along their binding strength, a new, fitting free approach which combines isothermal titration calorimetry (ITC) as heat-based technique with a mass-based method was developed. It turned out that the binding enthalpies of the CAT molecules follow the electron-donating/withdrawing properties of the tail groups. Finally, with the efficiency of quenching visible emission of ZnO due to the binding of different CAT molecules was investigated by photoluminescence (PL) spectroscopy which resulted in the same order as found for the binding enthalpy and the electron-donating/withdrawing properties [2]. In the next step, these molecular findings will be linked with a novel approach for knowledge-based formulation by introducing a new, standardized scoring method for the determination of Hansen parameters of colloidal systems using analytical centrifugation (AC). Based on AC profiles, a fully non-subjective ranking of NPs in different liquids was developed. Noteworthy, in contrast to other approaches the final discrimination of “good” and “poor” liquids is not based on preset arguments but derived automatically within the Hansen evaluation procedure. Finally, these mesoscopic findings on dispersibility and colloidal stability will be linked with interface properties at the molecular level. The derived methods for interphase understanding and design are now being used, e.g. for photocatalysis, the understanding of deep bed nanoparticle filtration by diffusion deposition and lightning applications. Thus, they are a key step towards the development of sustainable nanotechnologies.

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[2] H. Lee, D. Segets, S. Süß, W. Peukert, S.-C. Chen, and D.Y.H. Pui, *J. Membr. Sci.*, 524 (2017) 682-690



**Prof. M. Soror El-Shahawy**

Professor of Analytical and Environmental Chemistry  
Department of Chemistry,  
Faculty of Science, King Abdulaziz University, Saudi Arabia

[mohammedsoror@mans.edu.eg](mailto:mohammedsoror@mans.edu.eg)

His expertise is about preparation and fully characterization of a series of optically active and non-active transition complexes of biological and industrial applications, developing dual-wavelength  $\beta$ -correction spectrophotometric methods for analysis of trace concentrations of ions in industrial wastewater effluents and total determination and speciation of trace metal ions and some selected inorganic ions in air aerosols.

He is the consultant at the Centre of Excellence in Environmental Studies (CEES), King Abdulaziz University, Jeddah, Saudi Arabia since 2009 till present. He is an external reviewer of scientific merits of projects submitted to the Deanship of Scientific research, King Saud University since 2008 till present.

**Talk Title**

**A Promazine Derivative Oriented Chemical Sensor for Ultra-Sensitive Chemical Speciation and Total Determination of Chromium(III, VI) Species**

Talk Date: Wednesday 7

March 2018

Place: Hall C

Session: 15

Time: 11:00-11:45



## A Promazine Derivative Oriented Chemical Sensor for Ultra-Sensitive Chemical Speciation and Total Determination of Chromium(III, VI) Species

Z.M. Saigl<sup>1</sup>, W. Ahmad<sup>1</sup>, G.I. Mohammed<sup>2</sup>, H. Alwael<sup>1</sup>, D. A. Al-Eryani<sup>1</sup>, M.S. El-Shahawi<sup>1†</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, King Abdulaziz University, P. O. Box 80203, Jeddah, 21589, Saudi Arabia

<sup>2</sup>Department of Chemistry, Faculty of Science, Umm Al Qura University, Makkah, Saudi Arabia

### ABSTRACT

This study reports a simple and highly selective spectrofluorometric method for precise determination and speciation of trace concentrations of chromium species(III & VI) in water using 10-(3-dimethylaminopropyl) phenothiazine hydrochloride namely promazine hydrochloride (PMH) as a fluorescence tagging reagent. The method was based on the formation of colored chromium(III) complex species [Cr(III)-PMH] as a result of the initial redox reaction between PMH with chromate in aqueous H<sub>3</sub>PO<sub>4</sub> followed by fluorescence quenching at  $\lambda_{\text{ex}}^{\text{max}}/\lambda_{\text{em}}^{\text{max}}=300/449$  nm of the resultant chromium(III)-PMH complex species. A wide linear range (0.1-2000  $\mu\text{g L}^{-1}$ ) was achieved under the optimized analytical parameters with exceptional limit of detection (LOD)  $5.7 \times 10^{-10}$  M (0.03  $\mu\text{g L}^{-1}$ ). A coefficient of variation (CV) of  $\pm 2.05\%$  (n=5) was obtained at 2.0  $\mu\text{g L}^{-1}$  level of chromium(VI). Trace speciation of chromium(III & VI) species were also achieved successfully after oxidation to chromium(VI) with H<sub>2</sub>O<sub>2</sub> in KOH solution. The method was validated in environmental water samples with satisfactory recovery percentages (> 97.7%) using inductively coupled plasma-optical emission spectrometry (ICP-OES). The proposed and reference methods were subjected to statistical treatment (student's *t* and *F* tests) with no significant difference at 95 % confidence indicating the precision and accuracy of the proposed optical probe.

**Keywords:** Chromium(III & VI) speciation; Fluorescence quenching; Promazine hydrochloride; Redox reaction; Chromium(III) complex species; Environmental water samples.



**Prof. V. Narayana  
Kalevaru**

Leibniz Institute for Catalysis,  
Rostock, Germany

[narayana.kalevaru@catalysis](mailto:narayana.kalevaru@catalysis)

Dr. Narayana Kalevaru awarded Ph.D. degree in Chemistry (Heterogeneous Catalysis) from Indian Institute of Chemical Technology, India in 1998.

He joined as a scientist at the Institute for Angewandte-Chemie (ACA), Berlin, Germany in April 2000.

From 2000 to 2006, he worked as a scientist at the same institute, but from 2007, the name of ACA has been changed to Leibniz-Institute for Catalysis (LIKAT), Rostock, Germany.

He became the group leader in 2009 at LIKAT in the department of Heterogeneous Catalytic Processes and is leading the "gas phase oxidations" group since then.

His research interests include selective oxidation, ammoxidation and acetoxylation of aromatics, biogas and methane conversion to oxygenates, oxidative coupling of methane, oxy-chlorinations, CO<sub>2</sub> utilisation, oxidative dehydrogenation of lower alkanes etc. To his credit, he has > 30 patents, published ca. 110 papers in various journals of international repute.

**Talk Title**

**Industrially Important Oxidation Reactions  
Using Heterogeneous Catalysts**

Talk Date: Tuesday 6

March 2018

Place: Hall A

Session: 7

Time: 11:00 – 11:45



## Industrially Important Oxidation Reactions Using Heterogeneous Catalysts

V. Narayana Kalevaru

Leibniz-Institut für Katalyse e.V. an der Universität Rostock, Albert-Einstein-Str.29a,D-18059 Rostock, Germany

### ABSTRACT

Oxidation reactions constitute an important class of heterogeneous catalysis with good commercial significance. It is known that the catalytic properties are significantly influenced by various factors such as acidity characteristics, redox properties, particle size, surface composition, nature of support, method of catalyst preparation and so on. Among them, particle size and surface composition are found to be very crucial parameters that largely impact the catalytic activity and selectivity. In this contribution, we present an overview on the industrial importance of some selected oxidation reactions and also the key properties that need to be considered for the development of highly active and selective catalyst compositions. For instance, one step oxidation of cyclohexane to adipic acid using gold nanoparticles will be discussed. In this case, good correlation between Au size, dispersion and catalytic activity will be presented. Other oxidations of this contribution include oxidative dehydrogenation of ethane to ethylene, direct oxidation of benzene to phenol and oxidative coupling of toluene with methane to styrene. Furthermore, development of green and sustainable approach for synthesis of benzyl acetate via acetoxylation using Pd catalysts will also be described. It has been observed that dynamic changes are being occurred at different stages of the reaction concerning the Pd particle size, distribution of different Pd species, surface composition, coke deposition and so on. These properties in turn have shown tremendous impact on the catalytic activity and long-term stability. As a result of coke deposition, deactivation has become the major problem of Pd based catalysts. The differences in the size of Au and Pd particles and their impact on the catalytic performance will also be clearly addressed. In order to gain deeper insights on the mechanistic aspects of acetoxylation reaction, particularly to investigate the role of lattice oxygen, formation of CO<sub>2</sub> and coke, some isotopic transient experiments were also carried out using SSITKA set up. Such results provide hints that the acetic acid decomposition is the main source of carbon deposition and CO<sub>2</sub> formation, while the lattice oxygen takes part in the formation of H<sub>2</sub>O and then the lattice oxygen vacancies are replenished by the gas phase oxygen. On the whole, it can be stated that the metal particle size and its composition have shown remarkable influence on the catalytic performance. Results also revealed strong evidences that the surface composition and distribution of different Pd species on the catalyst surface play a key role on the catalytic activity and selectivity.



**Prof.  
Carsten Tschierske**

Professor of Organic  
Chemistry/Supramolecular  
Chemistry at the Martin  
Luther University Halle-  
Wittenberg, Halle, Germany.

*Carsten Tschierske* received his PhD in Organic Chemistry in 1985 at the university of Halle. After habilitation and several visitor professorships His primary research interests are focussed on the design of new materials forming complex self organised soft-matter structures, fluid ferroelectrics and the spontaneous mirror symmetry breaking in fluid systems.

**Talk Title**

**Dynamic Mirror Symmetry Breaking in  
Liquids and Liquid Crystals**

Talk Date: Wednesday 7

March 2018

Place: Hall B

Session: 14

Time: 11:00 – 11:45



## Dynamic Mirror Symmetry Breaking in Liquids and Liquid Crystals

C. Tschierske<sup>1</sup>, C. Dressel<sup>1</sup>, T. Reppe<sup>1</sup>, M. Alaasar<sup>1</sup>, M. Prehm<sup>1</sup>, X. B. Zeng<sup>2</sup>  
and G. Ungar<sup>2</sup>

<sup>1</sup>*Institute of Chemistry, Martin Luther University Halle-Wittenberg, Halle(Saale), Germany*

<sup>2</sup>*Department of Materials Science and Engineering, University of Sheffield, Sheffield, U. K.*

### ABSTRACT

Chiral segregation of enantiomers and chiral conformers of achiral molecules during self-assembly in crystalline or other well ordered assemblies has fascinated scientists since Pasteurs ground breaking resolution experiment. In recent years interest in mirror symmetry breaking extended into soft matter systems. In this talk observation of spontaneous mirror symmetry breaking in isotropic liquids and bicontinuous cubic phases of achiral molecules will be discussed.[1] In these soft matter systems, the classical concepts of achiral symmetry breaking, where formation of well ordered crystalline structures favours the homochiral packing of “frozen” enantiomeric molecules or conformers, cannot be applied. The new concept of “dynamic symmetry breaking” is proposed, which only requires that the energy gain of packing of chiral conformers in homochiral domains exceeds the entropic penalty of the demixing process. It can be achieved for molecules with a sufficient conformational helicity and low enantiomerization barrier, sufficiently strong intermolecular interactions favouring homochiral packing, a sufficiently large molecular size to reduce the entropic penalty of mixing, and a locally ordered structure, allowing a preorganization of the individual molecules (cooperativity). This dynamic and autocatalytic mode of stochastic symmetry breaking allows strong chiral amplification of traces of chiral information, leading to uniform chirality. This represents a new chirogenesis process providing chiral fluids, ensuring the development, preservation, and enhancement of uniform chirality, as required for prebiotic fluids and development of life. Focus of this talk will be on the implications of dynamic symmetry breaking for the understanding of achiral symmetry breaking in liquids and on the phase structures in complex liquid crystalline phases.

[1] C. Dressel, T. Reppe, M. Brautzsch, C. Tschierske, *Nat. Chem.* 6, 971 (2014); C. Dressel, F. Liu; M. Prehm, X. B. Zeng, G. Ungar, C. Tschierske, *Angew. Chem. Int. Ed.* 53, 13115 (2014); C. Tschierske, G. Ungar, *ChemPhysChem* 17, 9 (2016).



**Prof. Hans Georg  
Breitinger**

Professor at Department of  
Biochemistry, Faculty of  
Pharmacy and  
Biotechnology, German  
University in Cairo, New  
Cairo, Egypt

[hans.breitinger@guc.edu.eg](mailto:hans.breitinger@guc.edu.eg)

Dr. Breitinger obtained a M.Sc. (Diplom) in Chemistry from Heinrich-Heine Universität Düsseldorf. He then joined the laboratory of George P. Hess, Cornell University, Ithaca, NY, USA, where he worked on the synthesis of light-activated (caged) neurotransmitters and studied rapid chemical kinetics and mechanisms of ion channel receptors. He then joined the University of Erlangen and continued to work on ion channel receptors in the laboratory of Cord-Michael Becker. In 2003 he completed his cumulative habilitation on regulatory domains of the inhibitory glycine receptor. In 2004 he joined the German University in Cairo as Full Professor of Biochemistry where he established the first Patch-Clamp recording unit in Egypt. He is the coordinator of the Biotechnology program at the GUC, and serves as Associate Editor for the Journal *Frontiers in Molecular Neuroscience*. Dr. Breitinger received a DAAD Fellowship as an exchange student to King's College, London, UK, and a Swiss Academy of Sciences Postdoctoral Fellowship for his work at Cornell University. He was awarded research grants from the German Research Council (DFG), the Egyptian STDF, as well as grants from DAAD, the Wilhelm-Sander foundation, and a cooperation ZIM grant from the German Federal Ministry of Economics (BMWi). His research interests are mechanisms of activation and modulation of ligand-gated ion channel receptors, viral ion channels as pharmaceutical targets, mechanisms of drug synergies, and the identification and isolation of novel pharmaceuticals from marine organisms.

**Talk Title**

**Glucose – Industrial Mass Product and  
Major Nutrient Finds a New Role as  
Neuronal Modulator**

Talk Date: Tuesday 6 March  
2018

Place: Hall C

Session: 9

Time: 11:00 ~ 11:45



## Glucose – Industrial Mass Product and Major Nutrient Finds a New Role as Neuronal Modulator

Ulrike Breiting<sup>1</sup>, Rama A. Hussein<sup>1</sup>, Marwa A. Abdelhalim<sup>1</sup>, Heinrich Sticht<sup>2</sup>, Hans-Georg Breiting<sup>\*1</sup>

<sup>1</sup>Department of Biochemistry, Faculty of Pharmacy and Biotechnology, German University in Cairo, New Cairo, Egypt

<sup>2</sup>Department of Bioinformatics, Institute for Biochemistry, Friedrich-Alexander-University Erlangen-Nuremberg, Germany

### ABSTRACT

Glucose is one of the most important nutrients in human physiology. Glucose is also one of the world's major industrial products with a production of 3.1 billion tons estimated for 2015. The development of starch liquefaction that allowed production of glucose from starch led to a dramatic reshape of agricultural production, with significant amounts of starch produced for the production of glucose and sweeteners. Glucose is a major metabolite in humans, yet still new roles and implications for its use are discovered. Here, an overview of industrial production and use of glucose is presented, leading to a novel role of glucose as a modulator of neuronal transmission. Ligand-gated ion channels mediate fast synaptic signaling between neurons in the central and peripheral nervous system. Among these, glycine receptors mediate neuronal inhibition, and are essential for the control of muscle tone, movement, nociception and pain-related signaling. We identified glucose and related sugars as positive modulators of the inhibitory glycine receptor, leading to a 3 – 5 – fold increase in apparent affinity of the receptor for its activating ligand, glycine, and stabilizing a high-activity state of the receptor. Action of glucose was specific for glycine-mediated signaling. Kinetics of modulation agree with non-enzymatic glycation as mechanism of receptor potentiation by sugars. A key lysine residue in the extracellular domain of the receptor was identified by mutagenesis and structure modeling as possible attachment point for glucose. These findings suggest a role for glucose as modulator of neuronal synaptic signal transmission which may be a relevant parameter for altered pain sensitivity in diabetes and other clinical situations where blood glucose levels escape control.



**Dr. R. Puchta**

Organization: Department of  
Chemistry and Pharmacy

Working group: Inorganic and  
Organometallic Chemistry

Address: Egerlandstr. 1  
91058 Erlangen Room A2.12

[ralph.puchta@fau.de](mailto:ralph.puchta@fau.de)

**Current Research Interests:**

Investigations of potentially pharmaceutically-  
biologically or catalytically relevant transition metal  
complexes Studies on ligand and solvent exchange  
on Mn<sup>+</sup> ions {2} (metallo) cryptands and {2}  
(metallo) cryptates Huckeland

Möbiusaromaticity Aktuelle Forschungsinteressen:

Untersuchungen an potentiell pharmazeutisch-  
biologisch bzw.

katalytisch relevanten Übergangsmetallkomplexen Stu-  
dien zum Liganden-

zw. Lösungsmittelaustausch an Mn<sup>+</sup>-Ionen {2}-

(Metallo) Cryptanden und {2}-(Metallo) Cryptate

Hückel- und Möbiusaromatizität

**Publication**

[1] Begel S., Puchta R., Sutter J., Heinemann F.,  
Dahlenburg L., van Eldik R.: Studies on the Reaction  
of Iron(II) with NO in a Noncoordinating Ionic  
Liquid In: Inorganic Chemistry 54 (2015), p. 6763-  
6775; ISSN:0020-1669

DOI: 10.1021/acs.inorgchem.5b00595.

[2] Alzoubi B., Weber I., Walther M., van  
Eikema Hommes N., Puchta R., van Eldik R.:

HCN exchange on [Cu(HCN)(4)](+): a quantum  
chemical investigation

In: Journal of Coordination Chemistry 67 (2014), p.  
2185-2194, ISSN: 0095-8972.

DOI: 10.1080/00958972.2014.941828.

**Talk Title**

Talk Date: Tuesday 6

March 2018

Place: Hall C

Session: 12

Time: 01:30-02:15

**Ligand Exchange at Metal Centers Investigated  
by Quantum Chemistry – Green, Sustainable  
and Complementary**



## Ligand Exchange at Metal Centers Investigated by Quantum Chemistry – Green, Sustainable and Complementary

R. Puchta

Department of Chemistry and Pharmacy, University of Erlangen-Nürnberg,  
Egerlandstr. 1, 91058 Erlangen, Germany.

[Ralph.Puchta@fau.de](mailto:Ralph.Puchta@fau.de)

Detailed knowledge of the reactivity of solvated metal cations is a necessity since they play a crucial role in catalysis and in bio-inorganic chemistry.[1,2] While solvent exchange reactions are the most fundamental substitution processes that a solvated metal ion can undergo and do not necessarily lead to a chemical conversion, they contribute fundamentally to our understanding of reactivity and substitution mechanisms. Experiments will lead to knowledge about reactions under realistic conditions, in contrast to quantum chemical calculations that permit detailed investigations unbiased by external effects. Therefore quantum chemistry offers



complementary investigations - without chemicals and a lab.[2] The focus of this contribution will be on the quantum chemical (mainly DFT: B3LYP/6-311+G\*\*) investigated reaction mechanism of ligand or solvent exchange on tetrahedral coordinated cations like *e.g.* Be<sup>2+</sup> [3] and on octahedral coordinated metal ions like *e.g.* Zn<sup>2+</sup>. [4].

[1] R. van Eldik, *Chem. Rev.* 2005, 105, 1917.

[2] L. Helm, A. E. Merbach, *Chem. Rev.* 2005, 105, 1923.

[3] F. P. Rotzinger, *Chem. Rev.* 2005, 105, 2003.

[4] *e.g.* M. Walther, R. Puchta, *RSC Adv.* 2012, 2, 5815

[5] *e.g.* B. M. Alzoubi, M. Walther, R. Puchta, R. van Eldik, *Eur. J. Inorg. Chem.* 2013, 2059.



**Prof. Ibrahim M. El-Sherbiny**

Professor of nanomaterials and nanomedicine at the University of Science and Technology, and he is the Founding Chairman of nanoscience program, and the J. Director of the Center for Materials Science (CMS) at Zewail City.

[ielsherbiny@zewailcity.edu.eg](mailto:ielsherbiny@zewailcity.edu.eg)

El-Sherbiny earned his Bachelor of Science degree, with honors, in chemistry (top scholar) and his Master of Science degree in Organic (polymer) chemistry from Mansoura University, Egypt. He was awarded a graduate scholarship from the Egyptian government and a second from Massey University, New Zealand to study for his Doctor of Philosophy degree abroad. He earned his PhD degree in drug delivery from Massey University in 2007. El-Sherbiny's academic acumen was recognized by being offered a Fulbright Fellowship at the School of Biomedical Engineering, University of Michigan (U.S.) in 2009. He was also awarded several awards including the Prize of late Prof. Abdou Salam in the field of pharmaceuticals and bioproducts, the prestigious Egyptian State Incentive Award in Science, and the Venice Kamel Goda Award for Scientific Creativity for Young Researchers in the field of materials science and its applications. El-Sherbiny was selected among a group of top 40 European Union professors to form the new COST action committee, "Simm-Inhale", which focuses on the pulmonary drug delivery's research. He was also honored by some national and international universities and academies including the Academy of Scientific Research and Technology (ASRT), and Texas University, USA. El-Sherbiny's research focuses on the design and development of new classes of intelligent nano- and nano-in-micro-polymeric matrices using advanced techniques, and evaluating these new structures as potential candidates in various environmental, biotechnological, and biomedical applications including targeted and controlled drug delivery, tissue engineering, regenerative medicine, and biosensing. Dr. El-Sherbiny has more than 100 scientific papers published in high impact peer-reviewed journals over the last ten years in addition to many more papers in the pipeline. He also has more than 90 participations in international conferences in different countries including for instance, Germany, France, New Zealand, England, the United Arab Emirates, Jordan, Australia, Saudi Arabia, Singapore, Turkey, Malaysia, Spain, Canada, and the United States. Dr. El-Sherbiny is the author of three books plus contribution to more than other 18 books, and more than fifteen review articles. He is also a named inventor on 24 patents and patent applications in the U.S., U.K., Japan, Europe and Egypt. El-Sherbiny has contributed as a principal investigator and co-principal investigator for more than 17 funded applied research projects in Egypt, Europe and the U.S. In addition to El-Sherbiny's professional experience, he cofounded the Egyptian Organization for Scientific Research and Technology in 2012. He is a member of different societies and associations including the American Association of Pharmaceutical Scientists, the Biomedical Engineering Society (U.S.), the American Chemical Society, the New Zealand Institute of Chemistry, the Egyptian Chemical Society, the Egyptian Society for Polymer Science & Technology, and the Materials Research Society (U.S.).

**Talk Title**

**Smart Nanomaterials for Better Health**

**Date: Monday 5 March 2018**

**Place: Hall A**

**Session: 4**

**Time: 03.30 - 04:00**



## Smart Nanomaterials for Better Health

Ibrahim M. El-Sherbiny

Zewail City of Science and Technology, 6th October City, 12588 Giza, Egypt.

### ABSTRACT

Smart (stimuli-responsive) soft polymeric nanomaterials, a very favorable class of nanomaterials, are three-dimensional networks that are able to dramatically change their size and other characteristics in response to specific environmental stimuli such as pH, temperature, magnetic field, light, electricity or certain chemicals. More recently, the ability to manage the size in the nanoscale, shape, porosity and surface morphology of materials has created new opportunities to avoid various challenges in various applications. Besides, the concurrent fast and considerable stimuli-response of these nano-structured smart soft nanomaterials may magnify the scope of their applications, and suggest improved performance in their uses especially in the biomedical fields. The talk describes the development, *in-vitro* and *in-vivo* evaluation of several new series of smart nano and nano-in-micro systems for advanced biomedical applications with focus on the controlled drug delivery, tissue engineering and highly controllable and accurate biosensing applications.



**Prof. Mohamed  
Mokhtar**

Professor of Physical Chemistry,  
Chemistry Department, Faculty  
of Science, King Abdul-Aziz  
University, Jeddah 21589,  
P.O.Box 80203, Saudi Arabia.

mmokhtar2000@yahoo.com /  
[mmoustafa@kau.edu.sa](mailto:mmoustafa@kau.edu.sa)

Date of Birth: 11.11.1966  
Nationality: Egypt

I am Interested in advanced materials, nanomaterials with special interest in their application in heterogeneous catalysis. Solid acids and solid bases for liquid phase and gas phase reactions. In addition, I am specialist in catalyst and adsorbent characterization with particular expertise in adsorption measurements. I have published over 92 refereed publications and many international patents in these and related topics. I have numerous collaborative projects with public and private sector organizations. My *h-index* according to ISI-Thomson Reuters is 20.

**Distinctions (Awards)**

- Cambridge Certificate for outstanding scientific achievement, 22nd December 2016.
- Cited in Marquis Who's Who in Science in 2013
- The Award of Excellence of Scientific Publication for the staff members 2016,2015,2014,2013,2012, 2011 2010 and 2009 deanship of Scientific Research, King Abdulaziz University, Jeddah, Saudi Arabia
- The Award of Excellence of Citation on the Scientific Publication for the staff members 2016,2015,2014,2013,2012 and 2011 deanship of Scientific Research, King Abdulaziz University, Jeddah, Saudi Arabia.

**Talk Title Cu/Co- Layered Double Hydroxides Supported Carbon Nanotubes and Graphene Oxide as Enhancing Catalysts for Carbon-Carbon Coupling *via* Aldol and Ullmann Reactions**

Talk Date: Monday 5 March 2018

Place: Hall A

Session: 1

Time: 01:45 ~ 02:15



## Cu/Co- Layered Double Hydroxides Supported Carbon Nanotubes and Graphene Oxide as Enhancing Catalysts for Carbon-Carbon Coupling *via* Aldol and Ullmann Reactions

Mohamed Mokhtar<sup>1,2</sup>

<sup>1</sup>Chemistry Department, Faculty of Science, King Abdulaziz University, P.O. Box 80203, Jeddah 21589, Saudi Arabia

<sup>2</sup>Physical Chemistry Department, National Research Centre, El Buhouth St., Dokki, Cairo 12622, Egypt.

### ABSTRACT

Plentiful attempts have been made to develop heterogeneous catalysts for C-C bond coupling reactions due to their growing importance in pharmaceutical, agrochemical and fine chemical industries. There are several approaches to synthesize symmetrical biaryls; one of the foremost routes is the classic Ullmann coupling reaction. Another one is the base-catalyzed aldol condensation to produce diacetone alcohol (DAA). Overall, the C-C homocoupling classical synthesis of biaryls takes place using homogeneous catalytic routes. The homogenous catalytic procedures described in the literature suffer from drawbacks, such as discarding of waste and struggle in recovering the catalyst from the products, therefore these processes are not considered to be environmentally friendly. Conversely, heterogeneous catalysts can be separated from products easily and reprocessed, therefore manufacture processes “greener” since the waste stream is reduced. Therefore, the application of such catalysts has fascinated much consideration in the fine chemicals industry. Amongst the solid base catalysts studied for the catalysis of self-condensation of acetone and Ullmann reactions, layered double hydroxides (LDHs), especially Mg-Al-LDH and their copper, cobalt exchanged cations are considered to be promising candidates. Nevertheless, the catalytic activity of LDHs is always limited by their tendency to aggregate and poor mechanical properties, therefore nanocarbons, having 2D geometry such as graphene oxide (GO) is noticeably compatible with the layered structure of LDHs with their charge compatibility among the positively charged LDH and negatively charged GO. The large size of GO sheets associated to LDH platelets suggests that it could be possible to form an open network with large pores permitting access of the reactants to the active LDH sites which is supportive for the high rate conversion of the reactants. When combining LDH with GO, the heat and mass transfers during a reaction can be greatly improved.



Fig.1 Cu/Co LDHs -GO hydride catalyst for C-C homocoupling Ullmann reaction



# PHYSICAL CHEMISTRY

## KEYNOTES



**Prof. Rifaat Hilal**

Professor of Theoretical  
and Computational  
Chemistry Cairo  
University, Egypt.  
BSc, MSc, PhD, DSc  
rifaat.hilal@gmail.com

**Visiting Research Associate:** University of New South Wales Australia  
**Visiting Research associate:** State University of New York , Buffalo, NY, USA.  
**Visiting Professor:** Project SERAFIM, American Chemical society, , Computer Aided Chemistry Education. **Eastern Michigan University**  
**Awards:** -Egypt class 1 Max for Science and Arts 1981. -Fulbright Fellow 1989. -The Egyptian National Science Award 1981. -Shield of dedication, Egyptian Society of information and Tech.2003. -The Contribution to Science Award. International Science Institute, (ISI) ,USA, 2004. - Cairo University Award for Distinguish Scientific Research" 2007. - Cairo University Award for Excellence Scientific Achievement" 2010. -[Order of Merit Chevalier](#) (knight) for Significant contribution to the enrichment of science and cultural" French Government 2011.

**Membership of National and International Committee**

-Secretary General, National Council for Scientific Culture and Knowledge, Academy for Scientific research and Technology 2009-2011// -Scientific Culture committee, Supreme council for culture 2010-2012.// -National Committee for the History and Philosophy of Science 2006-2009.// - National UNISCO committee for the memory of the world register 2009-2010.// - Regional Executive committee for the Memory of the Arab World 2006-2011.// -Co-Chair of the content selection committee of the world digital Library 2010 -2012.// -International Advisor Board of King Abdullah university for Science and Technology (KAUST) for the history of Science 2007-2010.

**Research Interest:** My research interest is concerned with the application of quantum chemical methods to investigate the electronic structure and dynamics of molecules. Emphasis was and still is on molecules of biological interest. Computational methods, techniques and strategies have evolved into a mature state within the forty years of research which, our work covers. This is reflected in recent publications which utilize state-of-the art methodologies in solving chemical problems of practical interest. **Contribution to science / Computer Software:** 1) Development of a complete module (few subroutines) to the ab initio program package HONDO, now widely distributed under the commercial name "Gamess". This is a configuration interaction calculation module. 1979. 2) Development of a semi-empirical ZINDO/s computer program package. This program was designed to run on PC's very fast and efficiently. This program was made available to all colleagues at the time. 1987. 3) "Dot Density Graphs for Atomic and Hybrid Orbitals Program". Project SERAPHIM Am. Chem. Soc., Catalogue Div. of Chemical Education (1989). 4) "Huckel MO Demonstrator and Aided-Instructions Program". R. Hilal, Project SERAPHIM Am. Chem. Soc., Catalogue Div. of Chemical Education (1989). 5) DFT-B interface to Newton-nx computer program in collop ration with prof. Mario Barbatti's group. ©-version is already released. (2016). **Books:** A total of 11 books . Three of them have been widely published and distributed. Two books, published in the Arabic language, are of special interest in the present context. 1) Quantum Chemistry I. Atomic structure. 2) Quantum Chemistry II. Molecular electronic structure and Spectroscopy. These two books are widely distributed and present the foundation of the quantum theory in simple self-explanatory fashion. These books provide the underlying mathematics in detailed simple way to overcome the inherent weakness of the mathematics background for students. 3. History of Chemistry. Alchemie , Published in three languages (Arabic, English and French). Published by the UNISCO 2010. **Publications:** Over 150 papers in international Journals (see publication list).



**Structure and Dynamics of Molecular Systems.  
Unconventional H-bonds and Renewable Energy Sources. A  
Theoretical Perspective**

**Rifaat Hilal**

Chemistry Department, Faculty of Science, Cairo University, Cairo, Egypt

**ABSTRACT**

For over a century, theoretical chemistry become an integrated part of all chemistry disciplines and will be so in the future. Its success in providing a common ground for chemistry was celebrated few days ago in the STC 2015 conference in Potsdam\*. In my talk, I will present some of our recent work which would shade light onto the capabilities, accuracy and perspective of theoretical quantum chemistry with especial emphasis on compounds of biochemical relevance. Quantum Dynamics (QD) is and will continue to be a very powerful tool to explore chemistry in a different dimension viz. the evolution of structure or reaction in the time domain. Example of its relevance will be detailed. Unconventional H-bonds involving ionic species will be discussed and examples are detailed. Our contribution to chemical technological advances is presented. viz., dye-sensitized solar cells (DSSC) will be discussed.

.B. Friedrich, The rise of physical and theoretical chemistry, 51<sup>th</sup> symposium on Theoretical chemistry, Sept 20-24,2015, Potsdam, Germany

Talk Date: Wednesday 7 March 2018

Place: Hall A

Session: 13

Time: 11:45-12:10



**Prof. M.S. Abdel  
Mottaleb**

*Professor at Department of  
Chemistry, Faculty of Science,  
Ain Shams University, Cairo,  
Egypt*

[m.s.abdelmottaleb@sci.asu.edu.eg](mailto:m.s.abdelmottaleb@sci.asu.edu.eg)

Professor M. S. A. Abdel-Mottaleb, Dr. rer. nat., Friedrich-Schiller Uni., Jena. Winner of the Egyptian State Appreciation Award with the order of Merit, 2013, and holder of the State Decoration of Science and Arts, 1<sup>st</sup> order; two times (1985 and 2014). He founded the Photoenergy Centre at Ain Shams University in Cairo, 1996. Founder and ex Editor-in-Chief of the International Journal of Photoenergy (Hindawi Limited, UK). He organized and chaired the famous series of international conferences on Solar Energy and Applied Photochemistry since 1991 in Egypt. He established research groups of photochemistry that spread over several Egyptian scientific institutions. He has numerous publications, particularly in photo-, solar-, nano- and computational-chemistry, and spectroscopy. ORCID: 0000-0003-3462-2396

**Talk Title Computational Chemistry: Important Dry Tool  
Examples in Flexible Molecules and Complexes of Technological,  
Medicinal and Renewable Energy Potentials**

Talk Date: Wednesday 7 March 2018

Place: Hall A

Session: 13

Time: 12:10~12:35



## Computational Chemistry: Important Dry Tool Examples in Flexible Molecules and Complexes of Technological, Medicinal and Renewable Energy Potentials

M.S.A. Abdel-Mottaleb

Nano-Photochemistry, Solarchemistry and Computational Chemistry Labs,  
Department of Chemistry, Faculty of Science, Ain Shams University, 11566  
Abbassia, Cairo, Egypt

### ABSTRACT

Computational chemistry and modelling field is concerned, in a dry way, with the solution of interesting chemical problems in all topics of chemistry (Organic, Inorganic, Analytical, Organometallic and Physical Chemistry). Nowadays, it even uses the widely spread computers to generate information such as properties of molecules or simulated experimental results. Examples of results obtained in our dry laboratory, which are related to materials of potential applications such as organic light emitting diodes (OLED), solar Cell fabrications, acidities (proton transfer, PT), molecular flexibility, photochromism, inclusion complexes and more, will be lively presented. These includesome topics (computational chemistry language) of interest such as: - molecular reactivities (quantitative descriptors). //electronic structure determinations of molecules. // geometry optimizations // frequency calculations (IR and Raman)

- transition structures (during a chemical reaction) and reaction pathways.
- electron and charge distributions in the ground and excited states
- potential energy surfaces (PES) and maps.// rate constants for chemical reactions (kinetics)
- thermodynamic calculations- heat of reactions, energy of activation etc.
- excited state computations (UV-VIS, Fluorescence, etc.)

The lecture will shed light onthe link needed to bridge the rift between experiment and theory. *References: M. S. A. Abdel-Mottaleb, et. al.*

*Excited state intramolecular proton transfer (ESIPT) in the Photoresponsive Prototropic Schiff-Base N'-(2-hydroxybenzylidene)-4-hydroxybenzohydrazide: Computational Modeling Study, Journal of Molecular Structure, vol. 1144, pp. 545–551, 2017.*

*Novel Thiazole Derivatives of Medicinal Potential: Synthesis and Modeling, Journal of Chemistry, vol. 2017, 2017.*

*DFT Studies of Caffeic Acid Antioxidant: Molecular Orbitals and Composite Reactivity Maps Correlation with Photophysical Characteristics and Photochemical Stability, Journal of Chemistry, vol. 2016, 2016.*

*A New Approach for Studying Bond Rupture/Closure of a Spiro Benzopyran Photochromic Material: Reactivity Descriptors Derived from Frontier Orbitals and DFT Computed Electrostatic Potential Energy Surface Maps, International Journal of Photoenergy, vol. 2016, 2016.*

*Molecular modeling studies of some uracil and new deoxyuridine derivatives, Journal of Chemistry, vol. 2016, 2016.*

*J-aggregates of amphiphilic cyanine dyes for dye-sensitized solar cells: A combination between computational chemistry and experimental device physics, International Journal of Photoenergy, vol. 2014, 2014.*

*Lanthanide Complexes of Spiropyran Photoswitch and Sensor: Spectroscopic Investigations and Computational Modelling, Photochemical & Photobiological Sciences, RSC, Submitted 2017.*



**Prof. Maher Z.  
Elsabee**

Professor of Physical  
Polymer at Chemistry  
Department, Faculty of  
science, Cairo University,  
Egypt.

[mzelsabee@yahoo.com](mailto:mzelsabee@yahoo.com), or,  
[mzelsabee43@gmail.com](mailto:mzelsabee43@gmail.com)

Date of Birth: 10/2/1943 Egypt  
Marital status: Married 1974, (two sons, Karim and Ramy)  
Education  
Cairo University: B.Sc. 1963 Chemistry (distinction with Honors)  
American University in Cairo: M. Sc. 1965 Solid State Chemistry  
Leningrad Institute of Textile and Light Industry: Ph. D. 1970 Polymer Chemistry.  
Professional Experience:  
University of Massachusetts Amherst, MA, USA 1976-1977 Post doctorate, Polymer Science. Dept.// Carnegie-Mellon Institute of Research, Pittsburgh, PA, USA 1977-78 Research Associate. Institute of Macromolecular Chemistry, Freiburg, Germany 1981, (two months), DAAD, Scholar.// Institute of Macromolecular Chemistry, Freiburg, Germany 1983-1984 Fellow Alexander Von Humboldt Stiftung.// University of Sterling, Scotland 1986 (one month), British council. // University of Hamburg, Germany 1988 (two months), Alex. Von Humboldt stiftung.// University of Florida, FL, USA 1989 (three months) Fulbright Scholar.// University of Florida, FL, USA 1990-1992 Visiting Professor of Chemistry University of Kuwait Kuwait 1993-1998.// Visiting Professor of Chemistry University of Halle, Institute of 2002, and 2003, two months each year, Physical Chemistry, Halle Alexander von Humboldt stiftung Germany.// Hillsbrough Community College 2014-2015 Adjunct Professor.

Professional Recognition:

- DAAD Fellowship Freiburg, and Braunschweig, March-April 1981 Germany.
- Alexander von Humboldt Freiburg, 1983-84 and 1988, Hamburg Fellowship
- Third World Academy of Trieste, Italy April 1987 Science Symposium of Macromolecules
- Fulbright Fellowship 3 months, Gainesville, Florida, USA 1989
- Member of the Central Committee of Promotion Egypt

Publications: 135 Published Papers.

**Talk Title**            **Chitin and Chitosan the Amazing Materials, Extraction, Modification and Applications**

**Talk Date:** Wednesday 7 March 2018

**Place:** Hall B

**Session:** 14

**Time:** 12:10 -12:35



## **Chitin and Chitosan the Amazing Materials, Extraction, Modification and Applications**

**Maher Z. Elsabeé**

**Chemistry Department, Faculty of Science, Cairo University, Cairo, Egypt**

### **ABSTRACT**

Chitosan [poly-( $\beta$ -1/4)-2-amino-2-deoxy-D-glucopyranose] is an amazing polymer, it can be easily modified to yield a huge array of very interesting materials which can be used in a great number of applications and area of technologies, in agriculture, biomedical, paper, medicinal chemistry and others. The main source of chitosan is chitin which is found in abundance in nature, actually it is considered as the second most abundant natural polymer after cellulose it is also considered as a polysaccharides. Sea food industry is probably the main provider of chitin mainly from the exoskeleton of shrimps and crabs which contain chitin among other ingredients. Chitin is obtained by a sequence of reactions starting by decarboxylation, deprotonation and then chitosan can be obtained finally by deacetylation. Chitin is found also in many insects [2], fungi and algae. Chitin/chitosan (CH/CS) have become a very versatile area of research due to their, antimicrobial activity, biocompatibility, total biodegradability and non-toxicity of the degradation by products which is extremely important for biomedical and medicinal applications. The ease of modifying chitin/chitosan, due to the presence of the highly reactive OH and NH<sub>2</sub> groups, has led to the appearance of huge number of derivatives which found a variety of applications in a vast area of industry and academic research. In addition to the direct chemical modification of CH/CS several other routes were exploited to the production of extremely interesting materials by for example grafting, blending, electrospinning and nanoparticles and nanofibers formation. The literature contains huge number of references addressing these topics. This talk is a trial to shed some light on applications of chitosan in Food, agriculture, active packaging, antimicrobial and antioxidant fields. Blending of chitosan with essential oils has also been an active field which warrant mentioning.



**Prof. Mostafa M.  
Emara**

Director of Science  
Center for Detection  
and Remediation of  
Environmental Hazards  
Professor of physical  
chemistry, Faculty of  
Science (Boys), El-  
Azhar University,  
Naser City, Cairo,  
Egypt.  
[scdreh@yahoo.com](mailto:scdreh@yahoo.com)

Dr. Emara is an Expert in the field of solution chemistry especially in the kinetics, thermodynamics, catalysis of chemically and diffusionally controlled reactions. He applied his background to the area of environmental chemistry (air, water, soil, food). Long a leader in the international science field, he supervised more than 106 graduated students (M.Sc and ph.D). He and his students has authored more than 120 scientific articles and presented more than 60 articles in international conferences, symposium, and workshops. Also he is authored and co-authored 14 Arabic text books. In various field of chemistry. And authored 19 essays in several periodical journal in Arabic language. He worked as visiting scientist at Michigan state university, east lancing Michigan USA (1977), and visting profrrsor at university of Oklahma, Norman, Oklahma, USA (1973- 1975). Also as visiting professor at king abdaziz university, jaddah, Saudi Arabia during 1978-1982 and during 1987-1992. He served a member in excutive boards scientific-sociable, spoorts, educational. Dr Emara received his bachor's degree from the UV of Alexandria, Egypt (june 1962), his M.Sc. Degree from polythehechnic institute of Brooklyn, N.Y., USA (June) (1967), and his ph.D Degree from University of Maryland college Park, USA(January 1971).

**Talk Title The Role of Universities in Maintaining Green Environment**

Talk Date: Monday 5 March 2018

Place: Hall C

Session: 3

Time: 01:45-02:15



## The Role of Universities in Maintaining Green Environment

**Mostafa M. Emara**

Director of Science center for Detection and Remediation of Environmental Hazards (SCDREH)

Al-Azhar University, Cairo, Egypt.

### ABSTRACT

The Concepts of Green Chemistry will be discussed as part of the green university. How can the universities be the basic grounds of having green environment from all different aspects. A study case at Al-Azhar university can offer the services and role of being green and helping to attain sustainable development both on the university level as well as environment and eco-system as a whole. Water, Air and Soil are taken as part of the eco-system of Egypt and how to make it as green as possible. Also few tips will be given to our university structures to help living and making their school and environment as green as they can different ways will be offered to make a college campus greener and eco-friendly tips for college students. Also green initiatives for college campuses will be discussed. Hope this all will have its impacts on quality of life of our Egyptian society in large.



### **Prof. Ahmed Galal**

Professor at Chemistry  
Department, Faculty of  
Science, Cairo  
University, Egypt.

Prof. Galal earned his BSc and MSc degrees in Chemistry from Cairo University, Egypt; and MSc and PhD degrees from the University of Cincinnati, OH, USA. He joined the chemistry department of Cairo University as assistant professor on 1992 where he is currently a full professor. Professor Galal worked at several universities where he assumed Professor visit-ship including: Ulm, Erlangen, Ilmenau, and Free Universities (Germany); Cincinnati and Texas A&M Universities (USA); University of Liverpool (UK); Polytechnic University of Turin (Italy); United Arab Emirates and Kuwait Universities. Professor Galal served as member of Strategic Planning and Technical Support Centre, a member of Board of Research for the Ministry of Higher Education & Scientific Research (Egypt); Development and Innovation Program, a Program funded by the European Union of the Ministry of Higher Education of Egypt. Professor Galal also served as Dean of Faculty of Science, Cairo University and as Interim Head of Center of Hazardous and Environmental Mitigation of the University.

Professor Galal earned several honors: Graduate Fellowship Award, Quantum Chemical Corporation (USA); Fellowship award of the "Alexander von Humboldt Stiftung," Germany. He also acted as member in National Committee on New and Advanced Materials, the committee of Basic Sciences both of the Academy of Science and Technology of Egypt. Professor Galal was the Egyptian delegate to: International Science Technology and Innovation Centre for South-south Cooperation under the Auspices of UNESCO, (Malaysia); The inauguration of the Euro-Mediterranean University (EMUNI) (Slovenia); The Centre for Science and Technology of the Non-Aligned and other Developing Countries (NAM S&T), Cochin - (India); The RussNano Forum (Russia); COMEST meeting on Ethics of Science and Technology under the Auspices of UNESCO (Qatar). Professor Galal is a member of the Advisory Board for International Institute for Multifunctional Materials for Energy Conversion (IIMEC), Texas A&M University (USA). Professor Galal earned State and University of Cairo University Prizes in Excellence in Research in the area of Advanced Materials for Technological Applications. He authored and co-authored over 140 research papers in international renowned journals and delivered over 60 lectures in international conferences and institutes. He supervised several theses that led to both Master and PhD degrees. His research covers a wide spectrum of interests including surface tailoring with nano-structured materials for energy conversion, storage and sensing applications. Synthesis and modification of carbon based nano-structures with emphasis on graphene and carbon nanotubes, and perovskites. His research deals with the application of conducting polymers and composites in electronic and display materials. Another area of research interest is corrosion prevention and control using smart coating and studies of newly developed super-alloys for advanced applications. Professor Galal acted as member of the editorial board of "Talanta" published by Elsevier and is reviewer for several international journals.



## The Wonder of Electrochemistry at The Interface – From Monolayer Assembly to Nanostructures and Functionalization

Nada F. Atta, Ekram H. El-Ads, Hagar K. Hassan, Dina A. Abd El-Hakeem, Yousef M. Ahmed, Asmaa R.M. El-Gohary, Samar H. Hassan, Dalia M. El-Said, Asmaa H. Ibrahim, Mahmoud A.A. Khalil, Ahmed Galal\*

Department of Chemistry, Faculty of Science, University of Cairo  
Giza 12613, Egypt.

### ABSTRACT

The modification of the surface of electrodes targets the control of reactions taking place at the interface. In the early stages of electrochemical science, research work predominantly dealt with the electrolyte side with limited interest in processes at the electrode surface. More attention was directed towards interfacial phenomena as mercury electrodes were introduced. At the beginning of the 70s of the last century, a wide variety of “solid” electrodes were used that encouraged the scientific community to explore electrochemistry at the interface at the atomic and molecular level. The passion even increased using different approaches to modify the electrode surfaces that provided a powerful route to tune their performance for targeted applications. In this presentation, a brief description will be given for the different modes of modification of the electrode surfaces. Three surface modifiers will be illustrated: polymeric films, nanoparticles and carbon-based materials (carbon nanotubes and graphene). Since the architect of the electrode surface dictates its relevant property and consequent application, some examples will be given including: sensors for biological molecules, electrocatalysis, energy storage, electrochromism and others.

#### References\*\*

- Nada F. Atta, Ahmed Galal, Ersin A. Karagozler, Hans Zimmer and Harry B. Mark, Jr., *Biosensors & Bioelectronics*, 6, 333-341, (1991).
  - Ahmed Galal, Nada F. Atta, Soher A. Darwish, Shima M. Ali, *Topics in Catalysis*, 47, 73-83, (2008).
  - A. Galal, Nada F. Atta, Soher A. Darwish, Ahmed Abdel Fatah, Shima M. Ali, *J. Power Sources*, 195, 3806-3809, (2010).
  - Nada F. Atta, Ekram H. El-Ads, Yousef M. Ahmed, Ahmed Galal. *Electrochim. Acta*, 199, 319-331 (2016).
  - Hagar K. Hassan, Nada F. Atta, Maher M. Hamed, Ahmed Galal, TimoYacob, *RSC Advances*, 7, 11286-11296, (2017).
- \*\* More literature will be cited in the presentation

Talk Date: Tuesday 6 March 2018

Place: Hall A Session: 7

Time: 11:45-12:15



*Prof. El-Deab* received his PhD from Cairo University (1999) and was promoted as full Professor of Physical Chemistry-Cairo University on 2010. He received the prestigious JSPS post doc fellowship for two years (2001-2003) and JSPS long-term invitation fellowship in the Department of Electronic Chemistry - Tokyo Institute of Technology (TIT), Japan. In 2008, he got the prestigious Alexander von Humboldt (AvH) fellowship to Ulm University-Germany. He is the author of 82 international publications which receives more than 2200 citations with an h-index of 25. The major research topics include: Electrocatalysis by nanoparticles, energy conversion systems (FCs), waste water treatment, Biodiesel production.

**Prof. Mohamed  
S. El-Deab**

Professor of physical  
chemistry, Chemistry  
Department, Faculty  
of Science, Cairo  
University, Egypt.

**Talk Title**

**Electrocatalysis by Nanoparticles**

Talk Date: Wednesday 7 March 2018

Place: Hall A

Session: 13

Time: 02:15 – 02:45



## Electrocatalysis by Nanoparticles

Mohamed S. El-Deab

Department of Chemistry, Faculty of Science, Cairo University, Cairo,  
Egypt

### ABSTRACT

Catalysis and electrocatalysis at nanoparticles' surfaces is a subject of continuously growing interest due to its diverse applications. The incentive behind this interest is attributed to the fascinating physical, chemical, optical as well as structural properties of the nanoparticles in addition to the use of minute amounts compared to the bulk material. Metal (or metal oxide) nanoparticles are usually dispersed and confined onto a relatively inert substrate, e.g., glassy carbon (GC). For instance, Au nanoparticles-based catalysts are widely applicable in many vital processes, e.g., reduction of NO with propene, CO or H<sub>2</sub>, removal of CO from H<sub>2</sub> streams, selective oxidation, e.g., epoxidation of olefins as well as selective hydrogenation of CO and CO<sub>2</sub>. Au nanoparticle-based electrodes showed an extraordinary catalytic activity for the oxygen reduction and have been efficiently utilized for the hydrogenation of unsaturated organics as well as low-temperature oxidation of CO.

This study addresses our recent achievements in the field of preparation, characterisation and application of metal/metal oxide nanoparticle-based catalysts as efficient electrodes for reactions of direct relevance to fuel cells applications, e.g, formic acid oxidation, methanol oxidation, oxygen reduction and evolution reactions.

#### *References:*

- [1] M. S. El-Deab et al., Applied Catalysis B: Environmental, Volume 213, 15 September 2017, Pages 118-126.
- [2] M. S. El-Deab et al., Electrochimica Acta, Volume 180, 20 October 2015, Pages 268-279.
- [3] M. S. El-Deab et al., Journal of Power Sources, Volume 286, 15 July 2015, Pages 504-509.
- [4] M. S. El-Deab et al., International Journal of Hydrogen Energy, Volume 37, Issue 1, January 2012, Pages 68-77



### Prof. Ahmed Abd El-Moneim

Head of Materials Science and  
engineering department  
Egypt-Japan University of Science and  
Technology, New Borg El-Arab,  
Alexandria 21934,  
Egypt.

ahmed-abdelmoneim@ejust.edu.eg.

Prof. Abd El-Moneim is a Professor of materials Science and engineering at Egypt- Japan University of Science and Technology. He obtained his Ph.D. in materials Science and Engineering from institute of materials research, Faculty of engineering, Tohoku University, Japan, 1998. Received fellowships at; i) IMR-Tohoku University, Japan; ii) IFW- Technical University, Dresden, Germany; iii) TIT- Sendai, Japan; iv) visiting scholar to MSE and Micromechanical Engineering Departments, Kyoto University, Kyoto, Japan. He has 4 international patents, 75 International per-reviewed journal publication and 35 conference proceeding. Supervising/supervised 9 M.Sc and 14 Ph.D. students. PI of 3 grants from the industry, 5 research grants from STDF in collaboration with NSF and JSPS. He is currently a consultant for international Worley Parsons, Energy and, Resources and member in the editorial board of African Corrosion Journal and Journal of Energy and Power Engineering. He received several recognized national and international awards. He is also founding member in many scientific societies and NGO that contribute to public services and national awareness of science and technology.

**Talk Title**                      **Graphene Based Materials for Energy Applications**

Talk Date: Tuesday 6 March 2018

Place: Hall A

Session: 10

Time: 02:15-02:45



## Graphene Based Materials for Energy Applications

**AHMED ABDEL-MONEIM**

Department of Materials Science and Engineering,  
Egypt-Japan University of Science and Technology, New Borg El-Arab,  
Alexandria 21934, Egypt.

### ABSTRACT

The Bi-Sb material is regarded as a potential thermoelectric (TE) material for low temperature cooling applications and doping is a commonly used way to modulate the thermoelectric performance of this materials. In the present study, graphene (Gr) dopant was introduced into the Bi<sub>85</sub>Sb<sub>15</sub> powder by ball milling and fully densified (Bi<sub>85</sub>Sb<sub>15</sub>)<sub>1-x</sub> Gr<sub>x</sub> (x= 0.0, 0.02, 0.1, 0.5, 1.0 wt. %) solid composites were prepared by spark plasma sintering and extrusion. The microstructure of the tailored composites was characterized by XRD, SEM, FIB, TEM, and TEM techniques and their transport properties, including the electrical and thermal conductivities, Seebeck coefficients and calculated power factor and figure of merit, were investigated and their variations with regard to Gr fraction and sintering mode in the temperature range of 173 -373 K were discussed.



# ORGANIC CHEMISTRY

## KEYNOTES



**Prof. Abdou  
Osman  
Abdelhamid**

Professor at Chemistry  
Department, Faculty of  
Science, Cairo  
University,  
Egypt.

Born on 17 February , 1945 in Monoufia, Egypt.  
Graduated B.Sc. degree from Cairo University, Faculty  
of Science in 1976.

M. Sc, on 1971, Ph. D. 1978. From Cairo University  
Postdoctor fellowship on 1982-1984 in USA  
(University of Texas at El Paso),.

Visiting Professor at King Khalid Academy, KSA 1987-  
1993.

I award State Encouragement Award in Chemistry  
1987 and First Class Excellence Award 1995

229 Scientific papers (Publication from 1972- 2017),  
(Citations 2236, h-index 22, i10-index 72).

Interest: Heterocyclic Chemistry field and reaction  
mechanism

Supervisor: 30 M.Sc. thesis and 32 Ph.D. thesis)

Member of the Promotion Committee of the Professors  
and Assistant Professors in Organic Chemistry 2013-  
2016.

**TalkTitle Chemoselectivity in 1,3-Dipolar Cycloaddition Reactions of  
Nitrilimines with Multifunctionalized Dipolarophiles**

Talk Date: Tuesday 6 March 2018

Place: Hall B

Session 11

Time: 02:15-02:45



## Chemoselectivity in 1,3-Dipolar Cycloaddition Reactions of Nitrilimines with Multifunctionalized Dipolarophiles

Abdou O. Abdelhamide

Chemistry Department, Faculty of Science, Cairo University, Cairo, Egypt.

### ABSTRACT

It is clear that chemo-selectivity plays an important role in synthetic design. Literature data revealed that both site- and peri-selectivities are controlled by the molecular structures of the reactants. The ready availability of the reactants together with the generally good yields of the products make the reactions outlined above very attractive to synthetic chemists. In addition, there are reasons to believe that the chemo-selectivity of some reactions reported needs further refinement.

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**Prof. Magdy  
W. Sabaa**

Professor of Polymer  
Chemistry, at the  
Faculty of Science,  
Cairo University,  
Egypt.

Since August 2010, I was appointed as Emeritus Professor of Polymer Chemistry, at the Faculty of Science, Cairo University. I got my B.Sc. degree in Applied Chemistry in 1971 with grade Distinction and Honor degree from Cairo University. After completing my Ph.D. degree in 1979, in the field of Polymer Chemistry, I was appointed as lecturer of polymer chemistry at the Faculty of science, Cairo university, then associate professor and finally as professor of polymer chemistry in 1991. During my scientific career , I attained two postdoctoral fellowship, the first at Prague Institute of Chemical Technology (1981-1982) and the second at Tokyo Institute of Technology (1983-1984). Moreover, I attained a training course in polymer physics at Trieste, Italy during April-May 1987. I published 130 research articles and one review article in international Journals, five book chapters along with 18 publications in proceeding of National and International conferences. Moreover, I was a co-editor for a book , published by Springer in 2013. I have supervised more than 63 M.Sc. and Ph.D. theses all in the field of polymer chemistry. I am a reviewer in more than 20 international scientific journals, I am a member in the Arab Society of Material Sciences and in the Egyptian Society of Polymer Science and Technology. I was a member of the Promotion Committee for the job of Professors and Assistant Professors for the Atomic Energy Authority (2014 - 2017) and I got the Cairo University Award for Scientific Excellence in the field of Basic Sciences for the year 2014.

My main research activities are in the field of polymer degradation and stabilization, graft copolymerization, preparation of polymer hydrogels and SI-hydrogels, super absorbing materials, water treatment, biodegradable polymers, synthesis of novel powder coatings, synthesis and characterization of rubber/clay nanocomposites and in the synthesis of polymers with antimicrobial and antitumor activities.

**Talk Title Chemically Modified Chitosan for Water treatment and as Antimicrobial agents**

**Talk Date: Monday 5 March 2018**

**Place: Hall B**

**Session: 5**

**Time: 03:30 - 04:00**



## Chemically Modified Chitosan for Water treatment and as Antimicrobial agents

Magdy W. Sabaa

Chemistry Department, Faculty of Science, Cairo University, Giza, Egypt

### ABSTRACT

Chitosan (Ch), which is the result of the alkaline hydrolysis of the naturally occurring chitin biopolymer is considered to be one of the highly versatile polymeric materials due to its active functional groups (-NH<sub>2</sub> and -OH groups), biodegradability, biocompatibility and non-toxic property. The outstanding properties of Ch will be presented in details, and its chemical modification either through grafting with a variety of vinyl or acrylate polymers or through carboxymethylation to form carboxymethyl chitosan or through Schiff base reaction on its amino functional group will be discussed in detail. Various applications of the modified chitosan for sewage water treatment, and as antimicrobial agents will be also discussed.

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## Effect of Including Extra Phenylazo Moiety on The Mesophase Behavior of Three-Ring Azo/Ester Molecules

Nesma E. Mahmoud, Abdelgawad A. Fahmi, Magdi M. Naoum\* & Gamal R. Saad  
Chemistry Department, Faculty of Science, Cairo University, Giza, Egypt

**Prof. Magday M. Naoum**

Professor of physical Chemistry,  
Chemistry Department,  
Faculty of Science,  
Cairo University, Egypt.  
[magdinaoum@yahoo.co.uk](mailto:magdinaoum@yahoo.co.uk)

### ABSTRACT

Five homologous series of the four-ring 4-substituted phenylazo phenyl 4'-(4''-alkoxy phenylazo) benzoates ( $I_{n_{a-e}}$ ) were prepared and their mesophase behavior investigated by differential scanning calorimetry (DSC) and identified by polarized light microscopy (PLM). Compounds prepared were structurally characterized via infrared,  $^1\text{H-NMR}$ , mass spectroscopy, thermogravimetric and elemental analyses. Transition temperatures were first correlated with the alkoxy-chain length ( $n$ , that varies between 6, 8, 10, 14, and 16 carbons) within each homologous series, and again with the polarisability anisotropy ( $\Delta\alpha_x$ ) of the Ar-X bond, where X changes between  $\text{CH}_3\text{O}$ ,  $\text{CH}_3$ , H, Br, and CN groups.

Comparative studies were made to investigate the effect of introducing an extra phenyl azo moiety into the previously investigated three-ring compounds, 4-substituted phenyl 4'-(4''-alkoxyphenylazo) benzoates ( $II_{n_{a-e}}$ ), 4-substituted phenylazo 4'-(4''-alkoxy phenyl) benzoates ( $III_{n_{a-e}}$ ), and 4-(4'-alkoxy phenylazo) phenyl 4''-substituted benzoates ( $IV_{n_{a-e}}$ ), each bear the same polar group, X, and the alkoxy group,  $n$ .



**Prof. Ahmed H. M.  
Elwahy**

Professor of Organic  
Chemistry  
Chemistry Department,  
Faculty of Science,  
Cairo University, Egypt.

[aelwahy@hotmail.com](mailto:aelwahy@hotmail.com)  
[elwahy@sci.cu.edu.eg](mailto:elwahy@sci.cu.edu.eg)

Professor Ahmed H. M. Elwahy was born in 1963 in Giza, Egypt. He was graduated from Cairo University, Egypt in 1984 with accumulative grade of excellent with honor then he carried out his M.Sc. and Ph.D. studies in 1988 and 1991, respectively, at Cairo University in the field of organic synthesis.

He was awarded the Alexander von Humboldt research fellowship in 1998–2000 as well as short visits in 2003, 2005, 2009, 2010 and 2012 with Prof. Klaus Hafner, at TU Darmstadt, Germany. In 2017 he joined Prof. Holger Butenschön in hannover University for a short visit. In 2002 he was appointed as a full Professor of Organic Chemistry at Cairo University. In 2001 he received Cairo University Incentive Prize in Basic Science as well as State Prize in Chemistry from academy of Egyptian Scientific Research. In 2013 and 2016 he got Cairo University Prize for Merit in Basic Science and Cairo University Prize for Appreciation in Basic Science, respectively. Professor Elwahy published mor than 100 scientific papers in distinguished international journals. Under the supervision of Professor Elwahy 25 students have awarded their M. Sc. and Ph.D. Degrees.

**Talk Title**

**Synthesis of Multi-Armed Molecules**

Talk Date: Monday 5 March 2018

Place: Hall B

Session: 2

Time: 01:45-02:15



## Synthesis of Multi-Armed Molecules

Ahmed H. M. Elwahy\*

Chemistry Department, Faculty of Science, Cairo University, Giza, Egypt

### ABSTRACT

Multi-armed molecules began to draw interest of chemists and physicists in the last decades due to distinctly different properties as compared to their linear analogues. Some derivatives were synthesized as promising molecules and building blocks for application in (opto)electronics and electrochromic devices.<sup>1</sup>The structure of such molecules makes them versatile building blocks for the formation of mesophases of interesting mesomorphic and photophysical properties studied. The applications of multi-armed molecules as building units for dendrimers as well as in supramolecular host-guest chemistry have been also reported.<sup>2</sup>The interesting biological activity of some diverse multivalent scaffolds have also recently investigated. Some of these compounds are designed to study their promising photovoltaic application organic solar cells OSCs. In this respect we recently studied the synthesis of some interesting multi-armed compounds.<sup>3</sup>

### References

1. J. W. Steed and J. L. Atwood, *Supramolecular Chemistry*, John Wiley & Sons, 2013.
- A. L. Kanibolotsky, I. F. Perepichka, P. J. Skabara. *Chem Soc Rev.* 2010, 39, 2695–2728.
3. a) Ahmed H. M. Elwahy, *Tetrahedron Lett.* 2001, 42, 5123–5126. b) Ismail A. Abdelhamid, Ahmed F. Darweesh, Ahmed H. M. Elwahy, *Tetrahedron Lett.* 2015, 56, 7085–7088. c) Mostafa E. Salem, Ahmed F. Darweesh, Ahmad M. Farag, and Ahmed H. M. Elwahy, *J. Heterocyclic Chem.* 2017, 54, 586. d) Nesma A. Abd El-Fatah, Ahmed F. Darweesh, Adel A. Mohamed, Ismail A. Abdelhamid a, Ahmed H.M. Elwahy, *Tetrahedron*, 2017, 73, 1436-1450. e) Mostafa E. Salem, Ahmed F. Darweesh, Ahmad M. Farag, Ahmed H. M. Elwahy, *Tetrahedron* 2016, 72, 712-719. f) Ahmed H. M. Elwahy, Radwan M. Sarhan and Mohamed A. Badawy, *Current Organic Synthesis*, 2013, 10, 786-790. g) Magda F. Mohamed, a Ahmed F. Darweesh, b Ahmed H. M. Elwahy and Ismail A. Abdelhamid, *RSC Adv.*, 2016, 6, 40900.



**Prof. Ismail  
Abdelshafy  
Abdelhamid**

Professor of Organic  
Chemistry, Chemistry  
Department,  
Faculty of Science,  
Cairo University,  
Egypt.

[ismail\\_shafy@yahoo.com](mailto:ismail_shafy@yahoo.com)

[ismail@sci.cu.edu.eg](mailto:ismail@sci.cu.edu.eg)

**Prof. Abdelhamid** was born in Egypt in December 1978 in Giza, Egypt. He obtained his B.Sc. (2001) and M.Sc. (2005) degrees from the Faculty of Science at Cairo University. He received a Ph.D. degree in 2007 from the same university.

In December 2017 he was appointed as a full Professor of Organic Chemistry at Cairo University.

**Prof. Abdelhamid** was awarded the Alexander von Humboldt research fellowship in 2008-2010 as well as short visits in 2014, and 2016 with Prof. Holger Butenschön, at Hannover University, Germany.

**Prof. Abdelhamid** was awarded the Cairo University Award for Scientific Excellence in Basic Science 2016. He also was awarded the Cairo University Incentive Prize in Basic Science 2012. He received the Cairo University award for the best Ph.D. thesis in 2007. In 2016 he was awarded the Egyptian Association of heterocyclic chemistry prize for the best research paper 2016. Two of his students obtained Cairo University award for the best Ph.D. thesis in 2011 and 2012.

**Prof. Abdelhamid** supervised more than 20 M. Sc. and Ph.D. dissertations.

**Prof. Abdelhamid** specializes in heterocyclic chemistry and has published more than 70 papers and review articles in distinguished international Scientific journals in the field of Synthetic Organic Chemistry.

**Talk Title Synthesis of Heterocycles via C-C Bond Formation Reactions:  
Michael Addition, Hantzsch, Biginelli, Baylis-Hillman and  $\pi^4+\pi^2$   
Cycloaddition Reactions.**

Talk Date: Tuesday 6 March 2018

Place: Hall B

Session: 8

Time: 11:45 – 12:15



## Synthesis of Heterocycles *via* C-C Bond Formation Reactions: Michael Addition, Hantzsch, Biginelli, Baylis-Hillman and $\pi^4+\pi^2$ Cycloaddition Reactions

Ismail Abdelshafy Abdelhamid

Chemistry Department, Faculty of Science, Cairo University, Giza, Egypt.

### ABSTRACT

The most generally used approach for the synthesis of heterocycles include carbon-heteroatom bond formation. The synthesis through carbon-carbon bond formation is little bit more difficult, multistep and usually occurs using the transition metals as catalysts for C-H bond functionalization. In our work we managed to achieve this target using the simple reactions including Michael addition, Hantzsch, Biginelli, Baylis-Hillman and  $\pi^4+\pi^2$  Cycloaddition Reactions.



**ANALYTICAL & INORGANIC  
CHEMISTRY  
KEYNOTES**



**Prof. Yousry  
Moustafa Issa**

Professor at Chemistry  
Department, Faculty of  
Science, Cairo  
University, Giza,  
Egypt  
[yousrymi@yahoo.com](mailto:yousrymi@yahoo.com)

**EDUCATION**

- D. Sc. Analytical Chemistry, Cairo University (2015)
- Ph. D. Analytical Chemistry, Cairo University (1974)
- M. Sc. Applied Chemistry, Cairo University (1971)
- B. Sc. Applied Chemistry, Cairo University (1968).

**WORK EXPERIENCE**

- Professor (Emeritus) (2005) till now.
- Professor (1984-2005).
- Associate professor (1979-1984)
- Lecturer (1974-1979).
- Instructure-Assistant lecturer (1968-1974)

**AWARD**

- State encouraging award in Analytical Chemistry (1989).
- Medal and diploma of excellency, Egypt Arab Republic (1995).
- Cairo University Award of Appreciation (2005).
- Arab award of Chemistry (Saudi Chemical Society) (2010)

Publications **457**

Theses Supervision M. Sc. **59** Ph. D. **61**.

**Talk Title                      Ion-Selective Electrodes @ Our Laboratory**

Talk Date : Wednesday 7 March 2018

Place : Hall C

Secission : 15

Time: 11:45 - 12:15



## Ion-Selective Electrodes @ Our Laboratory

**Yousry M. Issa**

Chemistry Department-Faculty of Science-Cairo University, Giza, Egypt.

### ABSTRACT

This presentation deals with the story and success of ion-selective electrodes in our laboratory in Chemistry Department-Faculty of Science-Cairo University, Giza, Egypt. How did it start? Who started this discipline? (Three musketeers with the theme, *Unus pro omnibus, omnes pro uno*, "One for all, all for one").

The achievement made by the group of analytical chemistry and the success made during more than 30 years. 98 Publications, 13 M. Sc. and 12 Ph. D. theses were the final results.

Our work was based on using plastic membrane (PVC), chemically modified carbon paste, coated wire, and screen printed electrodes.



**Prof. M. A.  
ZAYED**  
(D.Sc. Analytical and  
Inorganic Chemistry)

Professor of Analytical  
and Inorganic Chemistry  
Chemistry Department,  
Faculty of Science,  
Cairo University,  
Egypt.

He received his B.Sc. 1969 (Honors), M.Sc. Analytical Chemistry 1972, then completed his Ph.D. Analytical and Inorganic Chemistry 1975, Under supervision of Prof. Dr. H. Khalifa and M.M. Khater Demonstrator, Faculty of Science, Cairo University. Then finally he got D.Sc. (Analytical Chem.), 2010.

#### Fields of Interest

- Air analysis and air quality.
- Analysis of major and minor elements, rare earths in geological ores and minerals
- Toxicity of organic and inorganic substances in its sources.
- Water quality in resources, mathematical modeling of pollution problems.
- Analysis of pharmaceutical materials and in preparations.
- Soil analysis, analysis of natural and synthetic solid state materials (simple compounds and complexes) using different physicochemical methods
- Transition metals
- Coordination chemistry
- Synthesis and spectroscopic characterization of metal complexes
- Schiff-base ligands
- Charge transfer complexes
- Biological activity of simple and complex materials
- Thermal analyses techniques
- Cytotoxicity of materials to Cancer cells.

#### Talk Title

**Chemistry of Biodiesel as Biomass Energy Source in  
Egypt, It is a Hope and Target**

Talk Date: Monday 5 March 2018

Place: Hall C

Session: 6

Time: 02:45 – 03:15



## Chemistry of Biodiesel as Biomass Energy Source in Egypt, It is a Hope and Target

Prof. Dr. M.A. ZAYED,

Chemistry Department, Faculty of Science, Cairo University.

### ABSTRAT

#### 1- Biodiesel Definition:

Biodiesel is a fuel made from vegetable oil that runs in any unmodified diesel engine. It can be made from any vegetable oil including oils pressed straight from the seed (virgin oils) such as soy, sunflower, canola, coconut and jatropha. Biodiesel can also be made from recycled cooking oils from fast food restaurants. Even animal fats like beef tallow and fish oil can be used to make biodiesel fuel. Biodiesel is a clean, renewable and domestically produced diesel fuel, which has many characteristics of a promising alternative energy resource. The most common process for making biodiesel is known as *transesterification*. This process involves combining any natural oil (vegetable or animal) with virtually any alcohol, and a catalyst. There are other thermochemical processes available for making biodiesel, but transesterification is the most commonly used one due to the simplicity and high energy efficiency. The high energy efficiency of transesterification is an important aspect of Biodiesel, which makes it favorable in the competitive energy market. The following is a transesterification reference guide that can be used to process Biodiesel on an experimental scale for classroom demonstrations. It can be done with basic equipment and common chemicals. Be sure to use extreme caution when carrying out this procedure, the methanol and catalyst are toxic, and give off potentially harmful vapors. Proper personal protection is imperative, including thorough ventilation. Links will also be given for more information on building more sophisticated small-scale (“homebrew”) biodiesel processors.

#### 2-Biodiesel Benefits:

The simple process allows the diesel engine to run on thick fuels. Since biodiesel is chemically similar to petroleum diesel fuel it can replace it into the fuel tank of any diesel vehicle. Biodiesel has advantages as a transport fuel. It has lower emissions, it is made domestically (which increases national security), it does not affect engine performance and is produced from plants. Since plants are a product of solar energy, it is called “liquid solar fuel”.

#### 3- Biodiesel Production in Egypt (Hope and Target)

The basis is the production of biodiesel oil on large national economic and strategic purposes from *Jatropha* plant and waste restaurant used oil. The aim is to produce 106 m<sup>3</sup> of biodiesel / year. Each plant is to treat seeds at a capacity of 555.5 tons / day. (noting that 555.5 tons seeds correspond to 555.5 tons × 2 = 1111.0 tons / d of raw seeds before peeling).

#### 4- Jatrova in Egypt:

Egypt imported seeds from India few years ago, Plantation was initiated in Luxor on a demonstration area of 200 feddans; Wastewater is used for irrigation, Plantation is considered to be very successful under the prevailing conditions.

5- **Biodiesel preparation in our lab:** Biodiesel was produced by transesterification of various types of waste cooking oil of (oil mixture of 25% sunflower + 75% Soybean, sunflower oil and cotton oil) at different conditions (50C°, 60C° and 70C° heating for 1h, 1.5h and 2h) with methanol using NaOH catalyst. The prepared biodiesel samples by the suggested procedures were compared with the European Standard Specifications.



**Prof. Azza A.  
Shoukry**

Professor of Inorganic  
Chemistry, Faculty of  
Science -University of  
Cairo, Egypt.

[sazza@sci.cu.edu.eg](mailto:sazza@sci.cu.edu.eg)

**Dr. Shoukry** obtained M.Sc (Diplome) in Chemistry from Cairo University. She then received a DAAD Ph.D Fellowship at the University of Erlangen-Nurnberg, Germany, and joined the scientific research group of **Prof. Rudi van Eldik**, Institut of Inorganic und Analytical Chemistry, where she studied kinetics and mechanisms of ligand substitution reactions of model antitumor palladium(II) complexes with biorelevant ligands, and received her Ph.D in Chemistry in (1999). She continued her research work in the field of bio-inorganic chemistry in Cairo University. She received DAAD Post doctoral Fellowship at the University of Erlangen-Nurnberg, Germany in (2002), (2004) and in (2006). She was promoted as full Professor of Inorganic Chemistry in Cairo University in (2013). She joined King Abdulaziz University, Saudi Arabia, as Professor of Inorganic Chemistry (2011-2015). Her research interests cover the elucidation of inorganic and bioinorganic reaction mechanisms, with special emphasis on the application of thermodynamic and kinetic techniques. Currently her interest is directed to DNA-Binding behavior, and DNA-Cleavage studies of bioactive transition metal complexes to Calf-Thymus DNA. She is the author of many international publications which receives many citations with an h-in-dex of 23. She is a member of the advisory editorial board of : Journal of Information and Computer Security, EnPress Publishing. Journal of Materials Science: Materials Review, Whioce publishing PTE. LTE.

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**Talk Title DNA- Cleavage studies, Spectroscopic and Binding behavior of some selected bioactive Transition Metals Complexes with Calf-thymus DNA . Antitumor and Antimicrobial Evaluation.**

Talk Date: Tuesday 6 March 2018

Place: Hall C

Session 9

Time: 11:45 ~ 12:15

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## DNA- Cleavage studies, Spectroscopic and Binding behavior of some selected bioactive Transition Metals Complexes with Calf-thymus DNA . Antitumor and Antimicrobial Evaluation.

Azza A. Shoukry

Department of Chemistry, Faculty of Science, Cairo University, Egypt.

### ABSTRACT

In this study two new complexes [Cu(bpy)(Gly)Cl]·2H<sub>2</sub>O (1) and [Cu(dpa)(Gly)Cl]·2H<sub>2</sub>O (2) (bpy = 2,2'-bipyridine; dpa = 2,2'-dipyridylamine, Gly = glycine) have been synthesized and characterized by elemental analysis, IR, TGA, UV-vis and magnetic susceptibility measurements. The binding properties of the complexes with CT-DNA were investigated by electronic absorption spectra. The intrinsic binding constants ( $K_b$ ) calculated from UV-vis absorption studies were  $1.84 \times 10^3 \text{ M}^{-1}$  and  $3.1 \times 10^3 \text{ M}^{-1}$  for complexes 1 and 2 respectively. Thermal denaturation has been systematically studied by spectrophotometric method and the calculated  $\Delta T_m$  was nearly 5 °C for each complex. All the results suggest that the interaction modes between the complexes and CT-DNA were electrostatic and/or groove binding. The redox behavior of the two complexes was investigated by cyclic voltammetry. Both complexes, in presence and absence of CT-DNA show a quasi-reversible wave corresponding to Cu<sup>II</sup>/Cu<sup>I</sup> redox couple. The change in  $E_{1/2}$ ,  $\Delta E$  and  $I_{pc}/I_{pa}$  ascertain the interaction of complexes 1 and 2 with CT-DNA. Further insight into the binding of complexes with CT-DNA has been made by gel electrophoresis, where the binding of complexes is confirmed through decreasing the mobility and intensity of DNA bands. In addition, the antitumor activity of the complexes was tested on two cancer cell lines; the breast cancer (MCF7) and the human hepatocellular carcinoma (HEPG2), as well as one normal cell line; the human normal melanocytes (HFB4). The results showed that complex 1 was more potent antitumor agent than complex 2. The in-vitro antimicrobial activity of the two complexes was carried out using the disc diffusion method against different species of pathogenic bacteria and fungi. The activity data showed that complex 2 was more active in inhibiting the growth of the tested organisms.



## The philosophy of Symmetry in the dictionary of Chemistry

Mohsen M. Mostafa

Talk Date: Tuesday 6 March 2018

Place: Hall C

Session: 12

Time: 02:15-02:45

### ABSTRACT

The main goal of this talk is to go inside the meaning of symmetry and through the light to know if it is true or not according to the definition in the text books. Also, we try to prove that the symmetry is false meaning using x-ray single crystal for some complex compounds.



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