



# 3rd Polish-Taiwanese Conference

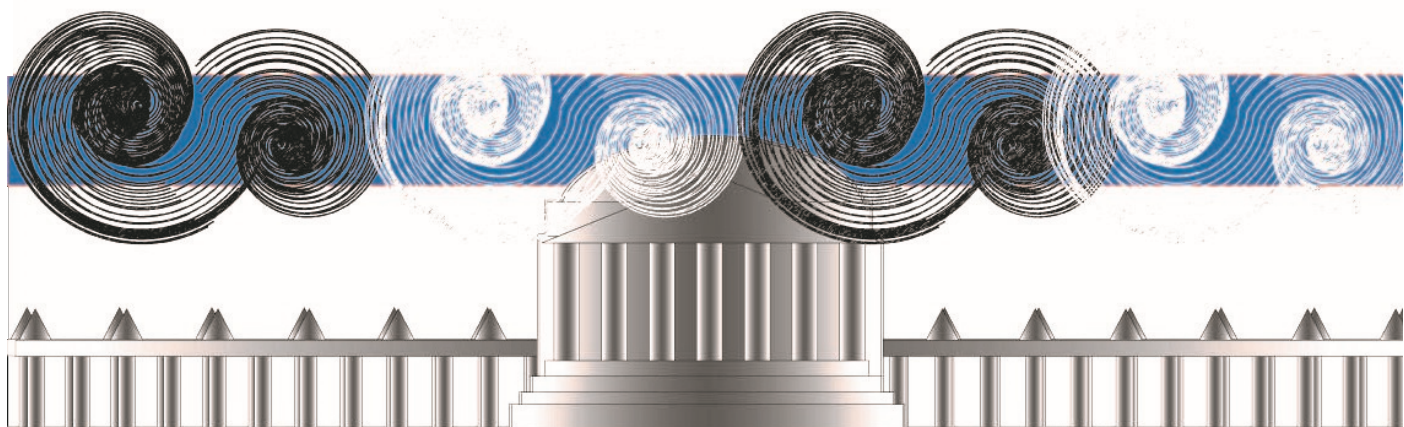
*"From Molecular Modeling to Nano- and Biotechnology", 27-29 June, 2016*

*Tatung University, Taipei, Taiwan*

*Tatung University, Taipei, Taiwan*

## PROGRAMME

### Symposium of Nanotechnology



**ORGANIZED BY:**

**Department of Materials Engineering, Tatung University, Taipei 104, TAIWAN**

**Department of Physical Chemistry and Molecular Modeling, University of  
Opole, Opole, Poland**

**JUNE 27, 2016**



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# Preface

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The conference between Taiwan and Poland has been carried out in the past two years at the beautiful Restauracja Hotel Villa Park, in Opole, Poland. For the greater success of this interdisciplinary research, we continue the symposium in Taiwan. This year, the Third Poland-Taiwan symposium will be held from June 27th to June 29th 2016 at Tatung University in Taipei, Taiwan.

The aim of this interdisciplinary meeting is to bring together specialists of molecular modeling and related fields of research working at the border of nanotechnology and biotechnology from Europe and Taiwan. Topics will cover areas of basic and applied sciences.

The scope of this conference is to bring together experts in the fields of materials development mentioned above. The conference is expected to bring the state-of-the-art work in these fields, show advantages and disadvantages of the relevant techniques and reveal material issues to be solved.

## CONFERENCE ORGANIZERS:

Hong-Ming Lin  
Department of Materials  
Engineering, Tatung University  
40, Chungshan N. Rd., 3rd Sec., Taipei,  
104, Taiwan, R.O.C.  
[hmlin@ttu.edu.tw](mailto:hmlin@ttu.edu.tw)

Teobald Kupka  
Faculty of Chemistry, University of Opole  
48, Oleska Street, 45-052 Opole, Poland  
[teobald@uni.opole.pl](mailto:teobald@uni.opole.pl)



# Symposium Committee



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- Hong Ming Lin (Tatung Technical University, Taipei, Taiwan)
- Małgorzata Broda (University of Opole, Poland)
- Poul Erik Hansen, Department of Science, Systems and Models, Roskilde University(Denmark)
- Chung-Kwei Lin, The School of Dental Technology, Taipei Medical University(Taiwan)
- Michal Straka, Institute of Organic Chemistry and Biochemistry, Academy of Sciences, (Czech Republic)
- Yi Hu, Department of Materials Engineering, Tatung University(Taiwan)
- Małgorzata Broda, Faculty of Chemistry, University of Opole(Poland)
- Yuh-Jing Chiou, Department of Chemical Engineering, Tatung University(Taiwan)
- Karol Jackowski, Faculty of Chemistry, University of Warsaw(Poland)
- Ko-Shao Chen, Department of Materials Engineering, Tatung University(Taiwan)

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- Yuh-Jing Chiou, Department of Chemical Engineering, Tatung University(Taiwan)
- Ko-Shao Chen, Department of Materials Engineering, Tatung University(Taiwan)



# Program at Glance

<b>June 26, 2016</b>	
<b>(Venue : Tatung University, San-Chih Hall Room 106)</b>	
15:00-18:00	Registration
18:00-21:00	Welcome Party, The Riviera Hotel Taipei, Second Floor
<b>June 27, 2016</b>	
09:00-17:00	Visit Industrial Company (Green Energy Technology Co. Ltd.)
<b>June 28, 2016</b>	
08:00-08:30	Registration
08:30-09:00	Opening Ceremony: President of TTU, Professor Kupka, and Dean of TTU R&D
09:00 -10:10	Symposium(I)
10:10-10:40	Tea Break
10:40-11:50	Symposium(II)
11:50-13:30	Lunch and Poster Contest
13:30-15:10	Symposium(III)
15:10-15:30	Tea Break
15:30-17:40	Symposium(IV)
18:30-20:30	Banquet: Hai Pa Wang Restaurant No. 59, Sec. 3, JungShan N. Rd., JungShan Dist., Taipei City 104, Taiwan, Tel : 02-2596-3141
<b>June 29, 2016</b>	
09:00-10:10	Symposium(V)
10:10-10:40	Tea Break
10:40-11:50	Symposium(VI)
11:50-14:00	Poster Awards, Closing Remarks and Lunch
14:00-17:00	Discussion on Future Cooperation
18:30-20:30	Farewell Party, Japanese Buffet-Jhongshan Restaurant



# Symposium & Poster Venue

Venue: Room 106, Shan-Chih Memorial Hall, Tatung University  
No. 22, Sec.3, Jhongshan North Road, Taipei, Taiwan R.O.C.



Shan-Chih Memorial Hall

# Sponsors



- Tatung University, Taiwan



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- Ming Fung Nano-Biotechnology Co., Ltd., Taiwan



# Session Schedule

**June 26, 2016**

(Venue : Tatung University, San-Chih Memorial Hall Room 106)

15:00-18:00	Registration
18:00-21:00	<b>Welcome Party, The Riviera Hotel Taipei, Second Floor, 646 Linsen N. Rd., Taipei, TAIWAN</b>

**June 27, 2016**

09:00-17:00	Visit Industrial Company (Green Energy Technology Co. Ltd. <a href="http://www.getinc.com.tw/">http://www.getinc.com.tw/</a> )
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**June 28, 2016**

(Venue : Tatung University, San-Chih Memorial Hall Room 106)

Time	Activity	Speaker	Chair	Topics
08:00-08:30	Registration			
08:30-09:00	Open	Opening remarks:	Hong-Ming Lin	Director General of Warsaw Trade Office, Maciej Gaca President of TTU, Teobald and TTU Dean of R&D
09:00-09:40	Plenary	Teobald Kupka	Hong-Ming Lin	Molecular modeling of atoms, small molecules and ordered carbon nanosystems: Structure and spectroscopy
09:40-10:10	Invited	Chung-Kwei Lin	Hong-Ming Lin	Synthesis and Characterization of Bioactive glass/carbon nanotubes Composite Powder by Sol-gel Process
10:10-10:40	Tea break Group Picture			
10:40-11:20	Plenary	Wei-Hau Chang	Chung-Kwei Lin	A Fish Virus as a pH-controlled Nano-machinery for Genome Delivery Revealed by Cryo-electron Microscopy at 3.56 Å
11:20-11:50	Invited	Małgorzata Broda	Chung-Kwei Lin	Conformational properties of modified amino acid residues
11:50-13:30	Lunch break/poster contest			
13:30-14:10	Plenary	Yi Hu	Piotr Wieczorek	Studies on the crystal growth mechanism of VO <sub>2</sub> nanoparticles through hydrothermal process
14:10-14:40	Invited	Joachim J. Włodarz	Piotr Wieczorek	Platforms for interactive and data intensive scientific computing
14:40-15:10	Invited	Monika Staś	Piotr Wieczorek	Theoretical modeling of structure, IR, Raman, and NMR spectra of oxazole
15:10-15:30	Tea break			
15:30-16:10	Plenary	Piotr P. Wieczorek	Teobald Kupka	Endocrine Disrupting Compounds As Emerging Environmental Contaminants
16:10-16:40	Invited	Ko-Shao Chen	Teobald Kupka	Effect of Atmospheric Plasma Treatment and Surface Graft Hydrogels on Deposition of Hydroxyapatite-like Films by Alternate Soaking Process
16:40-17:10	Invited	Michal Straka	Teobald Kupka	From Fullerene Spectroscopy to Molecular Memory. Highlights from Our Recent Studies.
17:10-17:40	Invited	Aneta Buczek	Teobald Kupka	Theoretical modeling of structure and Raman spectra related to polyenic pigments in red coral and African snail shell

**Banquet: Hai Pa Wang Restaurant (18:30-20:30)**

Address: No. 59, Sec. 3, JungShan N. Rd., JungShan Dist., Taipei City 104, Taiwan, Tel : 02-2596-3141

**June 29, 2016**

(Venue : Tatung University, San-Chih Memorial Hall Room 106)

Time	Activity	Speaker	Chair	Topics
09:00-09:40	Plenary	Poul Erik Hansen	Ko-Shao Chen	Anions, a new tool in structuring nano- and bio-materials
09:40-10:10	Invited	Yuh-Jing Chiou	Ko-Shao Chen	Synthesis and Characterization of Hybrid MWCNTs Materials for Fuel Cells Application
10:10-10:40	Tea break Group Picture			
10:40-11:20	Plenary	Karol Jackowski	Yuh-Jing Chiou	NMR Spectra of Medium-Sized Molecules in the Gas Phase
11:20-11:50	Invited	Hong-Ming Lin	Yuh-Jing Chiou	Hybrid Multi-Walled Carbon Nanotubes for Electrocatalytic Applications in Fuel Cells
11:50-14:00	Poster Awards, Closing remarks & Lunch break			
14:00-17:30	Discussions on future collaborations			

**Farewell party 18:30-20:30, Japanese Buffet-Jhongshan Restaurant, No. 52, Sec. 2, Zhongshan N. Rd., Zhongshan Dist., Taipei, Telephone No.:02-2542-5858**



# Poster

10:00-18:00 June 28, 2016

Venue: Central Hall Way of San-Chih Memorial Hall

Time	Poster	Presenter	Topics
11:50-13:30	P1	<b>Teobald Kupka</b>	On a simple way to decrease water imbibition into hardened cement paste and concrete
	P2	<b>Monika Staś</b>	Oxazole In Peptides: Natural Occurrence, Synthesis and Conformation
	P3	<b>Ying-Gui Huang</b>	Nano Hybrid Silver/Iron Nanowires
	P4	<b>Meng-Yuan Chung</b>	Electrocatalytical Property of Hybrid AuPd/Polyaniline/AO-MWCNTs Nanomaterials for Direct Formic Acid Fuel Cells
	P5	<b>Wei-Tse Cheng</b>	Synthesis and Characterization of Magnetic Solid Acid Catalyst for the Application of High temperature Glycerol Reaction
	P6	<b>Tung-Liang Lu</b>	Electrocatalytical Property of Hybrid AuPd/Reduced Graphene Oxide/Multi-Walled Carbon Nanotubes Nanomaterials for Direct Formic Acid Fuel Cells
	P7	<b>Cheng-Hung Yu</b>	Synthesis and Characterization of Nano-hybrid Noble Metals/N doping TiO <sub>2</sub> /SnO <sub>2</sub> /MWCNTs
	P8	<b>Marta Kliber-Jasik</b>	Influence of amino acids on the photostability of water-soluble octacarboxyphthalocyanines of Zn(II), Al(III) and Ga(III)
	P9	<b>Teobald Kupka</b>	On the sensitivity of chemical shift to 5-fluorouracil - C60 complex formation
	P10	<b>Chia-Yi Lin</b>	Immobilization of Biopolymers on e-PTFE film by Cold Plasma and Graft Polymerization Treatment
	P11	<b>Yi-Syuan Wei</b>	Preparation, Structure, Antibacterial Properties of Polyacrylic acid/Silver Nanocomposite Hydrogels
	P12	<b>Yi-Yun Cheng</b>	Surface Modified PET Sheet and TPU nonwoven by Helium Atmospheric Plasma for Improving Graft Polymerization of NIPAAm Hydrogel and Deposit of Hydroxyapatites-like Films
	P13	<b>Ju-Hui. Yeh</b>	Effect of Graft Acrylic acid Reduction Nanosilver on the Bamboo Charcoal
	P14	<b>Bo-Kai Chen</b>	Developed Effect of Stable Treat Plasma Film on Porous UHMWPE Surface by HMDSZ and Oxygen Cold Plasma Treatment
	P15	<b>H.H. Liang</b>	The Applications of Cold Plasma Treatment on the Surface Property of Xuan Paper
	P16	<b>Da-Jhan Chiu</b>	Cold Plasma Treated TPU non-woven for Improving Surface Graft Polymerization of Acrylic Acid, NIPAAm and Their Function Properties
	P17	<b>Chu-Yuan Huang</b>	Surface Modification of Nano Gold by Cold Plasma Treatments for Graft Polymerization of AAC or NIPAAm Hydrogels



# Plenary Talks Abstracts

P1

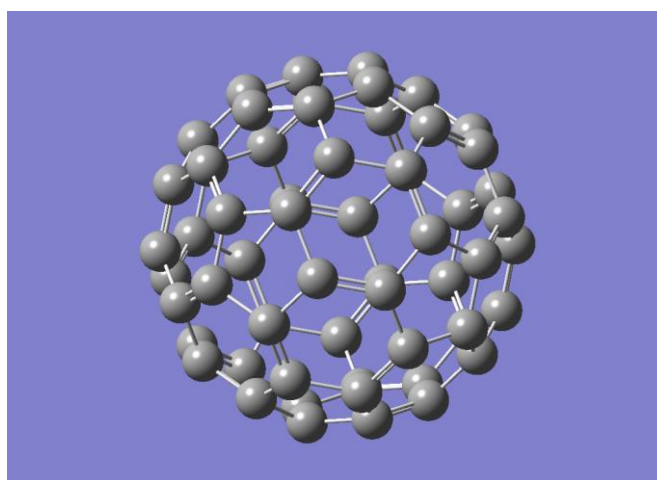
## MOLECULAR MODELING OF ATOMS, SMALL MOLECULES AND ORDERED CARBON NANOSYSTEMS: STRUCTURE AND SPECTROSCOPY

**Teobald Kupka<sup>a</sup>**, Michał Stachów<sup>a</sup>, Marzena Nieradka<sup>a</sup>, Klaudia Radula-Janik<sup>a</sup>, Małgorzata Broda<sup>a</sup>, Aneta Buczek<sup>a</sup>, Leszek Stobiński<sup>b</sup>, Tadeusz Pluta<sup>c</sup>, Karol Pasterny<sup>d</sup>, Elżbieta Chelmecka<sup>e</sup>, Jakub Kaminsky<sup>f</sup>, Stephan P. A. Sauer<sup>g</sup> and Hong-Ming Lin<sup>h</sup>

<sup>a</sup>Faculty of Chemistry, University of Opole, Opole, Poland; <sup>b</sup>Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland; <sup>c</sup>Institute of Chemistry, University of Silesia, Katowice, Poland; <sup>d</sup>Institute of Physics, University of Silesia, Katowice, Poland; <sup>e</sup>Silesian Medical University, Sosnowiec, Poland; <sup>f</sup>Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Prague, Czech Republic; <sup>g</sup>Institute of Chemistry, University of Copenhagen, Denmark; <sup>h</sup>Tatung Technical University, Taipei, Taiwan

In this paper we present a short overview of several approaches leading to accurate modeling of small atomic systems and nanosize objects (single-walled carbon nanotubes, SWCNTs and fullerenes, see **Fig. 1**) using several approximations. Both structural and spectroscopic parameters will be predicted and the results confronted with available experimental data. In particular, IR/Raman and NMR parameters will be studied for pristine and functionalized SWCNTs. The use of noble gas atoms and molecular hydrogen ( $H_2$  and HD) as selective magnetic probes in studies of fullerene size and symmetry will be discussed, too. Besides, we will also show a joint experimental (Raman) and theoretical approach for determination of structure of long polyene chains, confined inside porous, biomineralized matrix.

The aim of this paper is to demonstrate, on selected examples, the role of molecular modeling as efficient tool supporting material science studies.



**Fig. 1.** An example of nanosize carbon system: C60

## References

1. M. Saunders, R. J. Cross, H. A. Jimenez-Vazquez, R. Shimishi, A. Khong, *Science*, 271 (1996) 1693-1697.
2. M. Straka, P. Lantto, J. Vaara, *J. Phys. Chem. A*, 112 (2008) 2658-2668.
3. T. Kupka, M. Stachów, L. Stobiński and J. Kaminsky, *Magn. Reson. Chem*, 51 (2013) 463-468.
4. M. Jankowska, T. Kupka, L. Stobiński, *J. Mol. Graph. Model.*, 62 (2015) 26-37.
5. T. Kupka\*, A. Buczek, M. A. Broda, R. Szostak, H.-M. Lin\*, Lu-Wei Fan, R. Wrzalik and L. Stobiński, *J. Raman Spectrosc.*, (2016), DOI 10.1002/jrs.4922.

## Acknowledgements

M. J., M. S. and K. R.-J. are recipients of Ph. D. scholarships under a project funded by “European Social Fund II” in 2015. WCSS Wrocław and ACK Cyfronet Kraków (including PL-Grid) are thanked for providing computational environment. This work is partly financed from 8/WCH/2016-S (Faculty of Chemistry, UO grant).

## A Fish Virus as a pH-controlled Nano-machinery for Genome Delivery Revealed by Cryo-electron Microscopy at 3.56 Å

Chun-Hsiung Wang<sup>1</sup>, Yi-min Wu<sup>1</sup>, Chan-Shing Lin<sup>5</sup>, Yi-Yun Chen<sup>2</sup>, Yeukuang Hwu<sup>2</sup>, Wei-Hau Chang<sup>1234\*</sup>

<sup>1</sup>Institute of Chemistry, Academia Sinica, Taipei, Taiwan;

<sup>2</sup>Institute of Physics, Academia Sinica, Taipei, Taiwan;

<sup>3</sup>Genomic Research Center, Academia Sinica, Taipei, Taiwan;

<sup>4</sup>Department of Biochemical Science and Technology, National Taiwan University, Taipei, Taiwan;

<sup>5</sup>Department of Marine Biotechnology and Resources, National Sun Yat-Sen University, Kaohsiung, Taiwan

\*Correspondence should be addressed to weihau@gate.sinica.edu.tw; Wei-hau Chang's address: Institute of Chemistry, Academia Sinica: 128 Academia Road, Section 2, Nankang, Taipei, Taiwan 115

Piscine betanodavirus is a major threat to fish aquaculture. We used a 200 kV cryo-EM equipped with a direct detection camera to obtain near-atomic structures of the icosahedral particles from Dragon Grouper Nervous Necrosis Virus (DGNNV) in solution conditions. By restricting dose to  $14 e^{-}/\text{Å}^2$  prior to radiation damage, the shell domain of the capsid protein in weak basic condition mimicking sea water (pH 8) was determined to 3.56 Å, by which an atomic model was built *de novo*, thus allowing identifications of cation- $\pi$  interactions with their roles designated to particle stability, protein stability and gating through mutagenesis analysis. Remarkably, as the solution is switched to acidic condition (pH 5) mimicking that within a late endosome, the protrusion domain changes from an extended form to a compact form and collapses onto the shell with concomitant widening of the 5-fold vertex pores on the shell from 5 Å to 12 Å, which is sufficient for a single-stranded RNA to pass through. Together with a recent crystal structure of a NNV virus that assumes an intermediate conformation between pH 5 and pH 8, we propose a stage-wise conformation model as the structural basis for virus infectious action of “attach-prime-release” and a novel vaccine strategy against it.

P3

## STUDIES ON THE CRYSTAL GROWTH MECHANISM OF VO<sub>2</sub> NANOPARTICLES THROUGH HYDROTHERMAL PROCESS

Yi Hu , C.-F. Wang, C.-C. Lin

Department Materials Engineering, Tatung University

Vanadium dioxide has a metal-insulator phase transition characteristic, which are the significant changes in the optical, electrical properties due to changes in the crystal structure and after the phase transition. Vanadium dioxide thus is a very promising material for development in the use as thermoelectric switches, sensors, storage of materials and wisdom windows applications. In this study, VO<sub>2</sub> nanoparticles were prepared by hydrothermal method under heating in different temperatures with vanadium pentoxide as the raw material and using oxalic acid as a reaction assistant. VO<sub>2</sub> powders of different phases were obtained under different reaction temperature and the microstructure of the powder and the phase transition temperature were investigated using XRD, SEM, TEM, Raman and DSC. The results showed that nanoparticles with predominantly thermally induced phase VO<sub>2</sub> (M) can be obtained by hydrothermally heated at 280°C for 24 hours. The particles size of synthesized VO<sub>2</sub> (M) powder is of about 200 ~ 400nm.

**Keywords:** Vanadium dioxide, Oxalic acid, Hydrothermal, phase transition

## ENDOCRINE DISRUPTING COMPOUNDS AS EMERGING ENVIRONMENTAL CONTAMINANTS

**Piotr P. Wieczorek**

Division of Analytical and Ecological Chemistry  
Faculty of Chemistry, Opole University  
ul. Oleska 48, 45-052 Opole  
e-mail: [Piotr.Wieczorek@uni.opole.pl](mailto:Piotr.Wieczorek@uni.opole.pl); [www.zche.uni.opole.pl](http://www.zche.uni.opole.pl)

In the environment exists many emerging contaminants which effects of both wildlife and humans. Recently, many reports that described the occurrence of chemicals that are responsible for disrupting the endocrine system of living animals (especially water organisms) have been published in recent years. A large number of chemicals have been identified as endocrine disruptors of and humans can be exposed to them either due to their occupations or through dietary and environmental exposure.

An Endocrine Disrupting Compounds (*EDCs*) has been defined by the European Commission and U.S. Environmental Protection Agency (EPA) as an agent that interferes with the synthesis, secretion, transport, binding, or elimination of natural hormones in the body that are responsible for the maintenance of homeostasis, reproduction, some cancer diseases, development and/or behaviour. EDCs are chemicals, or chemical mixtures, that interfere with hormone function and usually acts in very low concentrations.

The presentation gives an extensive overview of the various type of Endocrinologically Active Compounds. This compounds can be classified in two categories, those that occur naturally and those that are synthesized. In the first group we can find natural chemicals from human and animal food, like phytoestrogens (daidzein, genistein, coumestrol, or stilbens), mikoestrogens (e.g. zearalenon) and natural steroid hormones. The second group is much larger and include chloroorganic compounds (polychlorinated biphenyls, dioxins), plastics, plasticizers, pesticides (e.g. dichlorodiphenyltrichloroethane, DDT, atrazine) fungicides, artificial hormones (e.g. contraceptive pills, thyroid medicines), drugs with hormonal side effect (e.g. naproxen, metoprolol, clifobrate) industrial and household chemicals (e.g. phthalates, alkylphenoletoxilate detergents, fire retardants, solvents), cosmetic additives (parabens), some metals (Cr, Cd, Ni) and many other compounds. Additionally, some examples of analytical procedures for EDCs determination is also presented.

P5

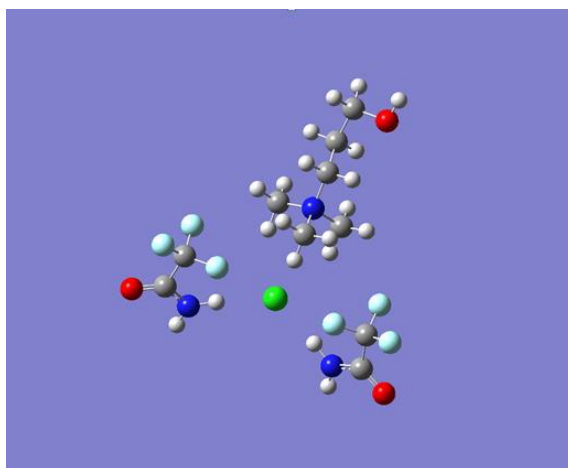
## ANIONS, A NEW TOOL IN STRUCTURING NANO- AND BIO-MATERIALS

**Poul Erik Hansen**

Department of Science and Environment, Roskilde University, Denmark  
[Poulerik@ruc.dk](mailto:Poulerik@ruc.dk)

The talk will concentrate on the role of anions in the creation of structures. The first example will be how they play a vital role in the formation of deep eutectic solvents (DES). Deep eutectic solvents are prepared by mixing two salts such as choline halides and urea, trifluoroacetamide, zinc chloride as well as a series of carbohydrates. The second group is working as proton donors. Various anions are tested. In the halide series fluoride is better (gives a lower melting point) than chloride ions, which again are better than bromide and iodide ions. DES is the new green, bio-type solvent.

DFT calculations are performed to show the importance of the anions and to illustrate the geometries of the interactions as seen in the Figure. The figure shows choline chloride and trifluoroacetamide (1:2). An interesting point is that the OH group of choline chloride is not involved in the interaction.



Water clearly plays an important role for DES and their properties as solvents. NMR is a very strong tool in the study of structures involving hydrogen bonds. Especially for those compounds with fluorine substituents, as a second handle is available. NMR can therefore reveal how water interacts with the DES structure and when it is broken.

Integrated DES solvents based on zinc chloride are used as catalyst in e.g. Friedel-Crafts reactions. This will be illustrated for an acylation reaction also using microwave irradiation. The use of DES based on iodide ions and their possible role in solar cells are also touched upon. Finally, the use of anions in supramolecular structures will be discussed.

## NMR SPECTRA OF MEDIUM-SIZED MOLECULES IN THE GAS PHASE

**Karol Jackowski**

Faculty of Chemistry, University of Warsaw, Pasteura 1, 02-093 Warszawa, Poland

NMR measurements allow the determination of experimental spectral parameters which can be applied for the verification of quantum-chemical calculations of shielding and indirect spin-spin coupling. However, the comparison of experimental and calculated data can be properly performed only if the studied molecular objects are exactly the same, otherwise results of such verification may be not valid, e.g. due to the presence of intermolecular interactions in experimental results. The latter problem can be overcome if all the effects of intermolecular interactions are completely removed from NMR spectra. It is possible when the observation of spectral parameters is performed in the gas phase and the results of measurements are extrapolated to the zero-density limit. At present such experiments can be easily completed also for medium-sized molecules when inert gas is used as a solvent. It is possible due to the high sensitivity of modern NMR spectrometers. In our laboratory we have already performed numerous similar analyses and the NMR spectral parameters were obtained for chemicals which are liquid at room temperature like: water, aliphatic alcohols, amines, benzene, acetone, acetonitrile, DMF and some others. We have also studied the relation between shielding in molecules and the magnitude of observed nuclear magnetic moments. The new values of nuclear magnetic moments were determined for many nuclei using our multinuclear NMR experiments. The multinuclear studies also permitted us to launch a new method for the standardization of NMR spectra which is based on the measurements of shielding and this method has numerous advantages in the analysis of unknown samples [1].

1. K. Jackowski, P. Garbacz, *Nuclear magnetic moments and NMR measurements of shielding*, Chapter 3, pp. 95-125, in *Gas Phase NMR*, Eds. K. Jackowski and M. Jaszuński, Royal Society of Chemistry, Cambridge 2016.





# Invited Talks Abstracts

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11

## **SYNTHESIS AND CHARACTERIZATION OF BIOACTIVE GLASS/CARBON NANOTUBES COMPOSITE POWDER BY SOL-GEL PROCESS**

Fang-Yu Fan, Jhih-Ni Lin, and **Chung-Kwei Lin**

School of Dental Technology, College of Oral Medicine, Taipei Medical University, Taipei, Taiwan

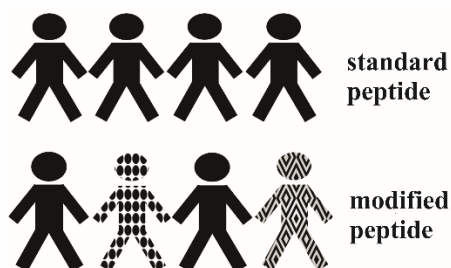
Bioactive glass (BG) is commonly used as bone graft substitutes in biomedical applications due to its excellent bioactivity. In the present study, bioactive glass with a composition of  $60\text{SiO}_2\text{-}36\text{CaO-}4\text{P}_2\text{O}_5$  wt.% were synthesized by sol-gel process where carbon nanotubes were served as templates for nucleation and growth of BG. The pristine BG and BG/CNT composite were followed by heat treatments at 300, 500, 700, and 900 °C, respectively. The synthesized materials were examined by X-ray diffraction, Fourier transform infrared spectroscopy, and scanning electron microscopy to reveal the microstructural and morphological characteristics. The experimental results showed that, after heat treating at 500 and 700 °C, BG/CNT composites were amorphous with numerous silicate nanocrystals. Bioactive glass with different thicknesses can be successfully coated on CNT by changing precursor concentration. By immersing in simulated body fluid solution and MG-63 cell culture assessment, the 500 °C treated BG/CNT composites exhibits excellent bioactivity.

## CONFORMATIONAL PROPERTIES OF MODIFIED AMINO ACID RESIDUES

MALGORZATA A. BRODA, ANETA BUCZEK, ROKSANA WAŁĘSA

Faculty of Chemistry, Opole University, Opole, Poland  
(e-mail: [broda@uni.opole.pl](mailto:broda@uni.opole.pl))

Many of peptides and proteins exhibit high biological activities and could be used as drugs. Unfortunately, there are some obstacles that prevent their direct use in therapy. The main drawbacks are high vulnerability to proteolytic degradation and low permeability through biological membranes. Thus, one way to overcome these difficulties is modification of their structures. The commonly used modifications are *N*-methylation and introduction of non-standard amino acids to a peptide chain. The replacement of a H-atom with a Me group on the N-atom, referred to as *N*-methylation, is a promising way to make the peptide stable in vivo and substantially more hydrophobic. Another promising strategy to improve stability of peptides is incorporation of non-ribosomally coded amino acids to peptide chains, for example  $\alpha,\beta$ -dehydroamino acids (in short: dehydroamino acids,  $\Delta$ Xaa) with the  $C^\alpha=C^\beta$  bond in the side chain.



The aim of this work is to present conformational properties of modified amino acid residues as shown by the example of small model diamides (Fig.1) studied by means of theoretical methods. The structural preferences of the studied peptides were determined by Ramachandran maps showing dependence of potential energy according to torsional angles  $\varphi$  and  $\psi$ , respectively. The research was performed using the Gaussian 09 package, by M06-2X and B3LYP methods both in the gas phase and in the polar environment. Solvent effects are included using the polarisable continuum model (PCM). The  $\varphi$ ,  $\psi$  potential energy surfaces were calculated and all energy minima localized.

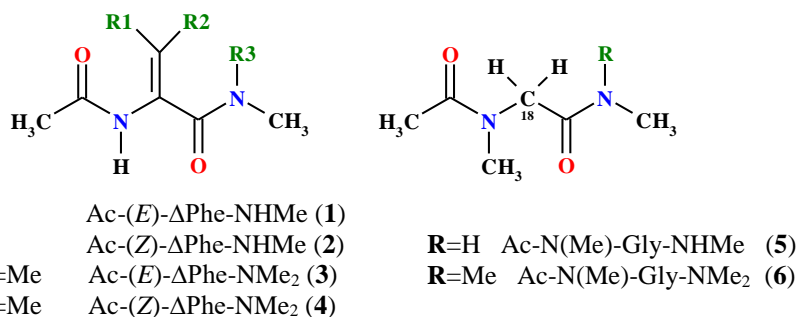


Fig. 1. General formula for the studied compounds.

The obtained results reveals that conformational preferences of the *E* and *Z* isomers of dehydrophenylalanine residue, both with secondary and tertiary C-terminal amide bond, are distinctly different, in particular their tendency to adopt helical conformation and to form intermolecular H-bonds. Combination of  $\Delta$ Phe residue with tertiary C-terminal amide bond completely changes the conformational properties of the model peptides. The isomer *E* of the Ac- $\Delta$ Phe-NMe<sub>2</sub> diamide adopts the helical conformation easier than the isomer *Z*. These studies showed different impact of *N*-methylation on the main chain conformation.

The theoretical calculations show that interactions with solvent are very important for the conformational properties of the studied diamides. The influence of water changes the number of conformers and reduces the energy difference between them. For selected peptoids the higher tendency of adopting *cis* configuration by *N*-methylated amide bond was observed, especially in aqueous environment.

To validate the obtained theoretical results, conformations of the similar structures, gathered in the Cambridge Crystallographic Data Centre (CCDC), were analyzed.

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## Acknowledgements

A. Buczek and M. A. Broda were supported by the Faculty of Chemistry, University of Opole [grant number 8/WCH/2016-S]. Calculations were carried out in Wrocław Centre for Networking and Supercomputing and in the Academic Computer Centre CYFRONET, AGH, Kraków.

## PLATFORMS FOR INTERACTIVE AND DATA INTENSIVE SCIENTIFIC COMPUTING

Joachim J. Włodarz

University of Silesia, Faculty of Mathematics, Physics and Chemistry,  
Department of Theoretical Chemistry, PL 40-007 Katowice, Bankowa 14  
[jjw@us.edu.pl](mailto:jjw@us.edu.pl)

In many areas of research, the processing of large amounts of data in combination with high-performance computations became routine tasks nowadays. The amounts of collected and analyzed data resulting from experiments together with the specific requirements of various research groups makes it very difficult to be performed within remote supercomputing facilities. Another important factor is the increasing demand for interactivity and ease of usage, especially in the areas where computations have been introduced only recently as routine research tools. The increasing demand for computing resources together with dissatisfaction of users of the services available remotely at computing centres gave rise to a project concentrated mainly on alleviation of local needs and problems. According to the *modus vivendi*, the computing platforms and applications were implemented with focus on interactivity. The necessary computing power is provided by a high-performance infrastructure, built around a fast interconnecting network, with computing nodes equipped partially with Intel Xeon Phi and Nvidia Tesla GPU accelerators.

The data acquisition process is supported by specialized laboratory information management system (LIMS) platforms implemented with dedicated environments tailored to the requirements of each particular laboratory and its equipment. Each such environment is a separate virtual machine with dedicated resources and appropriate protection.

The subsequent data processing operations could involve complex or repetitive user tasks and/or system processes, in workflows managed under the control of specialized platforms, such as Galaxy [1]. The implemented SageMathCell [2] and Jupyter [3] platforms are aimed at users of popular computer algebra packages, which are unified within Python-based user interfaces. More time consuming calculations could be run as traditional batch processing queued jobs. The Data Collections Online platform allows an unified, web-browser based access to the archived data collections, convenient for managing and sharing of scientific data.

The installed platforms and applications are updated and enhanced in a systematic way, preferably by free and open-source software. The most important software components like the operating system, batch processing, monitoring and management packages, and also many computing applications came from the open-source world.

**Keywords:** scientific computing, data intensive processing, interactive environments

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- [2] SageMathCell, <https://sagecell.sagemath.org>
- [3] Jupyter, <http://jupyter.org>

## THEORETICAL MODELING OF STRUCTURE, IR, RAMAN, AND NMR SPECTRA OF OXAZOLE

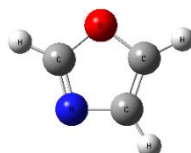
**Monika Staś**, Teobald Kupka, and Małgorzata A. Broda

<sup>1</sup>Faculty of Chemistry, University of Opole, 48, Oleska Street, 45-052 Opole, Poland  
(e-mail: mstas@uni.opole.pl)

It is estimated that approximately 2/3 of all naturally occurring organic compounds contain aromatic heterocyclic rings. The oxazole ring is shown in Fig. 1 and is present in numerous bioactive compounds like thiopeptide antibiotics and alkaloids, which reveal anti-tumor and anti-bacterial activity (Bagley 2005; Siodłak 2015).

The aim of this work is to check the performance of selected theoretical methods and basis sets for prediction of experimental IR, Raman, and NMR spectra of free oxazole in the gas phase. Detailed theoretical studies could support proper assignment of experimental vibrational (IR and Raman) and NMR spectra of oxazoles and their derivatives.

All calculations were performed with Gaussian 09 program. B3LYP and BLYP density functionals and MP2 method combined with 6-311++G\*\*, 6-311++G(3pd,2df), cc-pVTZ, pc-2 and aug-pc-2 basis sets were used for oxazole structure and frequency calculation. In addition, NMR shielding and indirect spin-spin coupling constants were calculated using Jensen-type basis sets dedicated for magnetic properties. The obtained theoretical results were compared with available experimental and literature results (Mille 1975, Kuchitsu 1987).



**Figure 1.** Molecular structure of oxazole ring.

**Keywords:** molecular modeling; DFT, oxazole, spectroscopy

### Acknowledgements

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## EFFECT OF ATMOSPHERIC PLASMA TREATMENT AND SURFACE GRAFT HYDROGELS ON DEPOSITION OF HYDROXYAPATITE-LIKE FILMS BY ALTERNATE SOAKING PROCESS

**Ko-Shao Chen**<sup>1\*</sup> (陳克紹)\*, Yi-Yun Cheng (鄭宜芸), Bo-Kai Chen (陳柏凱), Mu-Rong Yang, (楊木榮), Yao-Chung Liu<sup>2</sup> (劉耀中), Ming-Tse Lin (林銘澤), Wei-Yu Chen<sup>3</sup>, Allan Matthews<sup>3</sup>, and Chi-Kuang Feng<sup>4</sup>

<sup>1</sup>Department of Materials Engineering, Tatung University, Taipei, Taiwan

<sup>2</sup>Department of Bioengineering, Tatung University, Taipei, Taiwan

<sup>3</sup>Sheffield University, Sheffield, UK

<sup>4</sup>Department of Medical Research and Education, Taipei Veterans General Hospital, Taiwan

E-mail: [kschen@ttu.edu.tw](mailto:kschen@ttu.edu.tw)

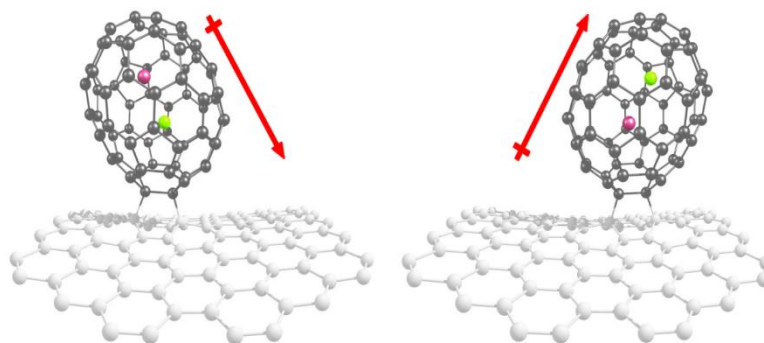
Surface treatment by Helium atmospheric plasma (APT He) on the substrates have many advantages, no vacuum require and form the peroxides groups be reside free radical, it can be used for post surface graft polymerization. In this study atmospheric pressure He plasma (voltage:12,000V, gas flow rate 0.4 l/min, glow distance 10mm) was applied to treat (APT He) polyethylene terephthalate (PET)sheet, bamboo charcoal and thermoplastic polyurethane (TPU) nonwoven in order to activate the surface. UV-induced graft polymerization of the smart hydrogel (Acrylic acid: AAc, or N-isopropylacrylamide: NIPAAm) on the plasma activated material surface was performed subsequently. For deposition of hydroxyapatite-like composites (HA-like), samples were incubated in alternate soaking process in CaCl<sub>2</sub> and Na<sub>2</sub>HPO<sub>4</sub> aqueous solution for different periods of time to investigate the nucleation and growth of HA-like on their surface. Our results shown that the pre-treatment of substrates by APT He process can increase the surface hydrophilicity and also be beneficial to the photo-induced grafting polymerization of NIPAAm or Acrylic acid monomers for immobilized gels on substrates. Characterization of HA-like composites was accomplished by XRD, FTIR, field emission scanning electron microscopy (FESEM), and water contact angle measurement. The results showed that, substrates treated with atmospheric pressure plasma, improved the hydrophilicity. After this treatment could be successfully grafted polys (NIPAAm) or AAc gel on the materials surface. Optical Measurement (OM) and XRD can be confirmed the formation of HA like films on the modified surfaces.

## FROM FULLERENE SPECTROSCOPY TO MOLECULAR MEMORY. HIGHLIGHTS FROM OUR RECENT STUDIES.

Michal Straka

Institute of Organic Chemistry and Biochemistry, Academy of Sciences, Flemingovo nam. 2, CZ-16610, Prague, Czech Republic

Two-state electric field-driven molecular switch based on a dipolar molecule enclosed inside a non-spherical fullerene was studied, see Figure. The operation and functionality of the switch will be shown here on a series of endohedral  $\text{MX}@C_{70}\text{-C}_6\text{H}_{10}$  ( $\text{MX}=\text{LiF}$ ,  $\text{LiCl}$ ,  $\text{NaF}$ ,  $\text{NaCl}$ ) molecules and their response to the electric field by means of density functional calculations. We show, that two possible low-energy minimum orientations of the molecular dipole inside the cavity along the longest axis of the fullerene provide distinguishable molecular states of the system separated by energy barrier connecting these minima. Switching of the molecular states is realized by application of external electric field, which forces reorientation of the enclosed dipole while removing the energy barrier connecting the minimum states.



In the spectroscopic part, we will present the magnetic circular dichroism (MCD) spectroscopy as a useful tool for fullerene distinction. Experimental  $C_{60}$  and  $C_{70}$  spectra were obtained and reproduced with the aid of density functional computations and the complex polarization propagator method. Theoretical spectra of other fullerenes revealed distinctive patterns extremely sensitive to molecular structure as well. Requiring tiny amounts of the sample, the MCD technique thus appears as a useful for detailed fullerene studies.

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### Acknowledgments

Czech Science Foundation, grant 14-03564S.

## THEORETICAL MODELING OF STRUCTURE AND RAMAN SPECTRA RELATED TO POLYENIC PIGMENTS IN RED CORAL AND AFRICAN SNAIL SHELL

**Aneta Buczek**<sup>1\*</sup>, Teobald Kupka<sup>1</sup>, Małgorzata A. Broda<sup>1</sup>, Roman Szostak<sup>2</sup>, Hong-Ming Lin<sup>3</sup>, Lu-Wei Fan<sup>4</sup>, Roman Wrzalik<sup>5</sup> and Leszek Stobiński<sup>6</sup>

<sup>1</sup>Faculty of Chemistry, University of Opole, 48, Oleska Street, 45-052 Opole, Poland <sup>2</sup>Department of Chemistry, University of Wrocław, F. Juliot-Curie 14, 50-383 Wrocław, Poland; <sup>3</sup>Tatung University, 40, Chungshan North Road, 3rd Section, Taipei 104, Taiwan; <sup>4</sup>China University of Geosciences, Wuhan 430074, China; <sup>5</sup>A. Chełkowski Institute of Physics, University of Silesia, Uniwersytecka 4, 40-007 Katowice, Poland; <sup>6</sup>Faculty of Chemical and Process Engineering, Warsaw University of Technology, 1 Waryńskiego Street, 00-645 Warsaw, Poland  
(e-mail: [teobaldk@gmail.com](mailto:teobaldk@gmail.com))

**Keywords:** molecular modeling; DFT, polyenes, corals, *Helixia aspersa* and *maxima*; Raman spectroscopy

### 1. Introduction

Red corals are formed from a hard, porous mineral matrix containing calcium carbonate with confined traces of red pigment of polyenic nature. Less known are black corals containing chitin [1,2]. Unfortunately, there is still an open question about the origin of color in red coral [3]. Recently, it has been postulated that the pigment is formed by polyenes containing 8 – 16 conjugated C=C bonds [4, 5].

A number of ab initio and DFT studies have been reported on structure and C=C stretch mode in all-trans polyenes [5,6]. However, the size of such molecules could be fairly large making calculations with large basis sets and accurate methods including electron correlation impractical [5,6].

Spectroscopic techniques, including infrared (IR) and Raman (R) are widely used to study structure and intermolecular interactions, both in chemical labs and in industry and gemology [7]. The advantage of using Raman spectroscopy is the non-invasive way of investigation, including field studies of mineral and organic objects, as well as jewelery objects, for example amber, coral, mollusk shells and pearl pigments.

### 2. Description of a problem solution

The main question related to the nature of red pigment is the presence of all-trans polyenes formed by a number of C=C double bond units. The structure of such short polymeric structures is directly responsible for the presence of characteristic C=C and C-C stretch bands in experimental Raman spectra. Thus, it should be possible to determine the number of chain subunits by carried out theoretical calculations using density functional theory (DFT). We selected B3LYP and BLYP density functionals combined with 6-311++G\*\* basis set.

### 3. Results

In Figure 1 are shown samples of red coral and African snail shell. Raman spectra of the studied objects contain only two strong peaks due to C=C and C-C stretching modes. The length of the polyenic chains was determined on the basis of theoretical modeling of Raman spectra of a set of polyenes. The best agreement between theory and experiment was observed for



chains containing 14 and 11 12 C=C bonds, respectively. These results were similar to those reported by Hedegaard and coworkers [8].

#### 4. Conclusions

The presence of organic pigments containing 11-12 and 14 carbon-carbon double bond units in case of red coral and African snail was determined from non invasive Raman studies and theoretical modeling.

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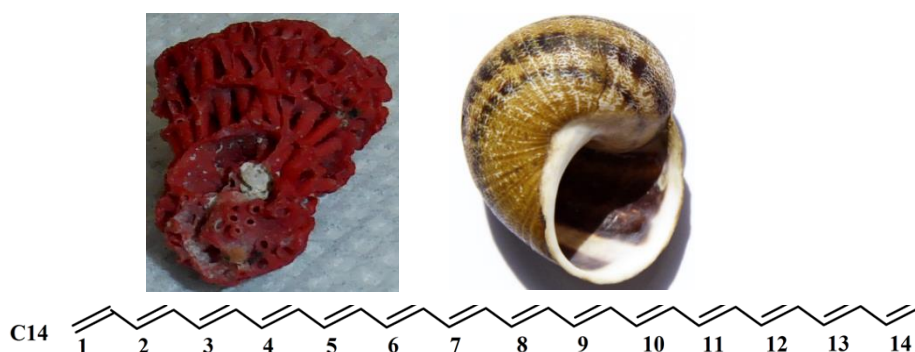


Fig. 1 Samples of raw red coral and African snail shell (top right) and general formula of all-trans polyene containing 14 double bonds.

#### Acknowledgements

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## SYNTHESIS AND CHARACTERIZATION OF HYBRID WO<sub>3</sub>/MWCNTS FOR FORMIC ACID FUEL CELLS APPLICATIONS

Yuh-Jing Chiou<sup>1\*</sup>, Yueh-Lin Lee<sup>1</sup>, Hong-Ming Lin<sup>2</sup>, Andrzej Borodzinski<sup>3</sup>, Leszek Stobinski<sup>4</sup>, Piotr Kedzierzawskim<sup>3</sup>

<sup>1</sup> Department of Chemical Engineering, Tatung University, Taipei, Taiwan

<sup>2</sup> Department of Materials Engineering, Tatung University, Taipei, Taiwan

<sup>3</sup> Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland

<sup>4</sup> Faculty of Chemical and Process Engineering, Warsaw University of Technology, Woloska 141, 02-507 Warszawa, Poland

\* chiou@ttu.edu.tw

Direct methanol fuel cells (DMFCs) and direct formic acid fuel cells (DFAFCs) emerge as very promising devices for providing energy with high efficiency because of convenient fuel feeding and easy operation at low temperature. To increase catalyst activity and tolerance in fuel cells, Pt or Pd nanoparticles are usually supported on modified support materials to avoid poison and enhance the performance. MWCNTs can be modified by appropriate oxides, for example, cerium oxide, zirconium oxide and N-doped titanium dioxide, to enhance the electrocatalytic performance.

In this study, WO<sub>3</sub>/MWCNTs of cubic or orthorhombic structures were prepared in argon and air respectively. Then metal nanocatalysts were synthesized on the supports in polyol process or reduction by NaBH<sub>4</sub>. The structures, morphologies, compositions and electrochemical characteristics were measured and discussed. In Pd series, the addition of WO<sub>3</sub> decreases the activity of the electrocatalysts. In the contrary, the addition of WO<sub>3</sub> may have hydrogen spillover effect in Pt series catalysts, and it caused better electrochemical performance.

**Keywords:** electrocatalysis, Fuel cells, Pt, Pd, CNT.

## HYBRID MULTI-WALLED CARBON NANOTUBES FOR ELECTROCATALYTIC APPLICATIONS IN FUEL CELLS

Hong-Ming Lin<sup>1\*</sup>, Yuh-Jing Chiou<sup>2</sup>, Andrzej Borodzinski<sup>3</sup>, Leszek Stobinski<sup>4</sup>

<sup>1</sup>Department of Materials Engineering, Tatung University, 40, Chungshan N. Rd., 3<sup>rd</sup> Sec, 104 Taipei, Taiwan

<sup>2</sup>Department of Chemical Engineering, Tatung University, 40, Chungshan N. Rd., 3<sup>rd</sup> Sec, 104 Taipei, Taiwan

<sup>3</sup>Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warsaw, Poland.

<sup>4</sup>Faculty of Chemical and Process Engineering, Warsaw University of Technology, Woloska 141, 02-507 Warszawa, Poland

Nanomaterials have large surface areas and high surface energy intrinsically. For hybrid nanomaterials, interaction driven by surface activities is a common phenomenon, where each component has strong enhancement for hybrid property, resulting in different interfacial properties from the traditional composition. The structure and property of hybrid nanomaterials are affected significantly by interface bonding and their surface composition. The size and thermal effect also affects surface composition and materials properties. Therefore, characterization of interfacial bonding and surface composition for hybrid nanomaterials, especially for nano-scale materials, is the demanding and important task for applications. In the present research, the size effect, interfacial properties, and surface compositions of nano hybrid electrocatalyst are studied for fuel cell applications.

Hydrogen energy will be an important power source in the near future. The studies of hydrogen production, hydrogen purification, hydrogen application and hydrogen storage have attracted much attention and been studied widely in academic and technologic fields. Electrocatalyst plays a transformation role in this renewable energy system. The synthesis and characterization of nano-hybrid electrocatalyst will be provided an effective method to enhance the catalysis for energy application. The exploration includes Pt/Metal oxide/MWCNTs and bimetallic Pd-Au/MWCNTs hybrid electrocatalysts for anode materials of direct methanol and formic acid fuel cell. Nano hybrid electrocatalysts have been synthesized by chemical reduction method with various annealing treatments. The particle size distribution, hybrid structure, and interfacial properties of each component can be controlled by changing the process parameters, such as precursor concentrations, temperatures, pH values, and heat treatments conditions. The structure of the hybrid catalyst is characterized by XRD, SEM, and HRTEM. The weight contents of each component in hybrid materials are determined by TGA analysis. The properties of surface catalysis behavior, redox reaction, and electrochemistry reaction of the hybrid electrocatalysts will be examined by TPR, CO oxidation conversion, and cyclic voltammetry measurement. The results indicate the rich oxygen promoting effect of metal oxide and solid solution structure of bimetallic metal in the hybrid electrocatalysts can enhance surface activity and electrocatalysis in direct methanol and formic acid fuel cell applications, respectively.

\* Corresponding author: e-mail: [hmlin@ttu.edu.tw](mailto:hmlin@ttu.edu.tw), Tel.: 886-2-2586-6030; Fax: 886-2-2593-6897;



# Poster Abstracts

PO1

## ON A SIMPLE WAY TO DECREASE WATER IMBIBITION INTO HARDENED CEMENT PASTE AND CONCRETE

Andrzej Kałamarz<sup>1</sup> and Teobald Kupka<sup>2\*</sup>

<sup>1</sup> Alvana Company, Opole, Poland

<sup>2</sup> University of Opole, Faculty of Chemistry, Opole, Poland  
([teobald@uni.opole.pl](mailto:teobald@uni.opole.pl); [teobaldk@gmail.com](mailto:teobaldk@gmail.com))

Among indoor and outdoor construction materials are cement and concrete. These materials have been used for years due to their availability and excellent physico-chemical and mechanical properties. They are formed in the process of hardening and the final product is a porous system with different pore distribution, ranging from very small to medium and large interconnected and also isolated “holes”. The obtained solid materials are often exposed to water (and salts in the roads, bridges or harbor constructions). Therefore, the extent of water imbibition (soaking) and salt diffusion is of primary concern for durability of products formed from cement and concrete. For example, it could be related to general corrosion of mineral content, as well as metal bars forcing the constructions. Additionally, water imbibition and salt diffusion promotes harmful degradation of constructions in winter conditions.

Among several ways of improving cement and concrete resistance to water, and therefore decreasing its harmful action is the decrease of pore size or changing the hydrophilic character of pore surface to hydrophobic. Obviously, it is possible to combine both procedures.

**Hydrozol K** is a solid formulation designed to decrease the porosity of hardened cement paste and concrete and its resistance against water and dissolved electrolytes (various salts). Its application as a small amount of powder (1.5% of cement used) in water, mixed with freshly prepared cement pasta is simple and fast.

As result of a number of earlier laboratory tests in Opole (a town known as a capital of limestone and cement production in Poland) and in Germany, **Hydrozol K** received the certificate as an waterproof admixture to concrete for building and construction applications (No. 461/83, PN90/6729-04, PN-EN 480-14 2008 and DIN 1048).

**The aim of the current study is to show the mechanism and applicability of Hydrozol K in industrial works.**

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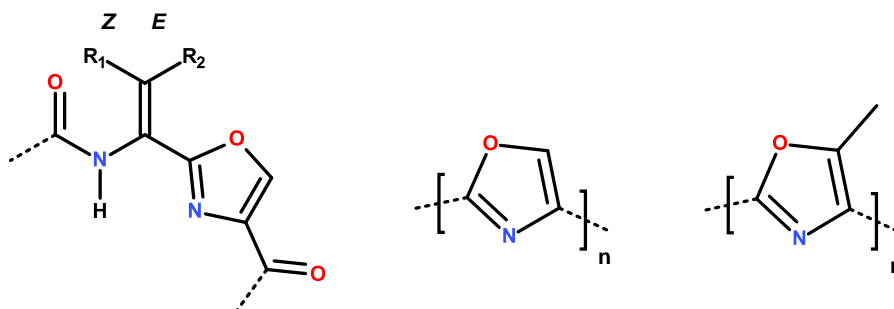
This work was supported partly by the Faculty of Chemistry, University of Opole (Grant 8/WCH/2016-S) and by Alvana, Opole.

## OXAZOLE IN PEPTIDES: NATURAL OCCURENCE, SYNTHESIS AND CONFORMATION

**Monika Staś**, Monika Porada, Dawid Siodłak

Faculty of Chemistry, University of Opole, Oleska 48, 45-052 Opole, Poland  
(e-mail: mstas@uni.opole.pl)

Oxazole structural motif occurs in bacteria's origin peptides, which reveal primarily antibiotic activity [1]. Our studies indicate that incorporation of oxazole to peptide main chain results in atypical conformation, which potentially can influence bioactivities of natural or designed peptides [2,3]. Based on dehydrophenylalanine, new synthetic procedure has been developed, which enables conversion of oxazoline/oxazole ring as well as *Z/E* position of the side chain within single amino acid residue [4]. The present studies are focused on conjugated polyoxazoles, which also occur in nature, and have potential application in optoelectronic and as ligands in metalorganic catalysts.



**Keywords:** Molecular modeling; DFT, oxazole, oxazoline, spectroscopy, Hantsch synthesis, polyoxazoles,

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## NANO HYBRID SILVER/IRON NANOWIRES

**Ying-Gui Huang**<sup>1</sup>, Mihita Ajmera<sup>2</sup>, Yu-Chung Lin<sup>3</sup>, Yuh-Jing Chiou<sup>4</sup>, Wei-Syuan Lin<sup>1</sup>, Hong-Ming Lin<sup>1\*</sup>, Yeu-Kuang Hwu<sup>3</sup>

<sup>1</sup> Department of Materials Engineering, Tatung University, Taipei 104, Taiwan

<sup>2</sup> Mechanical and Manufacturing Engineering Department, Manipal Institute of Technology, Manipal 576 104, Kamataka, India

<sup>3</sup> Institute of Physics, Academia Sinica, Nankang, Taipei 115, Taiwan

<sup>4</sup> Department of Chemical Engineering, Tatung University, Taipei 104, Taiwan

\*Corresponding author: [hmlin@ttu.edu.tw](mailto:hmlin@ttu.edu.tw)

Silver/Iron nanowires (Ag/Fe NWs) hybrid materials towards high magnetization performance are described in this research. Fe NWs used as support to deposit Ag nanolayers by chemical reduction method (NaBH<sub>4</sub>) using the precursors of iron salts and silver nitrate in an external magnetic field. After formation of iron NWs, the silver precursors are added and reduced by sodium borohydride that is coating a thin nanolayer of silver on the surface of iron NWs. Silver nanolayers provide a passive layer to prevent oxidation of Fe NWs. The structures of Ag/Fe NWs are measured by X-ray diffraction patterns (XRD) that ensures the nature structure of Fe and Ag. Field emission scanning electron microscope (FESEM) are used to observe surface morphologies of Ag/Fe NWs. ICP is used to determine the composition of silver and iron. VSM (Vibrating Sample Magnetometer) analysis is used to examine the magnetic properties of Ag/Fe and pure Fe NWs. The results indicate the saturation magnetization of Ag/Fe NWs is greater than 2000 emu/g that is almost ten times of pure iron (217 emu/g).

**Keywords:** hybrid materials, Ag/Fe nanowires, passive layer.

## Electrocatalytical Property of Hybrid AuPd/Polyaniline/AO-MWCNTs Nanomaterials for Direct Formic Acid Fuel Cells

Meng-Yuan Chung<sup>1</sup>, Yuh-Jing Chiou<sup>1</sup>, Hong-Ming Lin<sup>2</sup>

<sup>1</sup> Department of Chemical Engineering, Tatung University, 104 Taipei, Taiwan

<sup>2</sup> Department of Materials Engineering, Tatung University, 104 Taipei, Taiwan

DFAFCs (direct formic acid fuel cells) can be a promising green energy which will not increase the carbon dioxide concentration. In order to promote the application of DFAFCs, nano palladium catalyst should be prepared with good electrocatalytic performance and stability to be applied as anodic catalyst for formic acid oxidation. This study is to develop a novel Pd based electrocatalyst which is supported on an electrical conductive polymer, Polyaniline (PANI), modified MWCNTs. Two PANI to AO-MWCNTs proportions of 20:80 and 80:20 are prepared as PANI/AO-MWCNTs-20/80 and PANI/AO-MWCNTs-80/20 as the catalyst supporters. This PANI modification is expected to suppress electron trapping by defect on the surface of AO-MWCNTs and enhance the conductivity of the electrocatalyst. Three kinds of methods, x-ray photosynthesis, NaBH<sub>4</sub> reduction and polyol method, are applied to deposit Pd or AuPd nanoparticles on PANI modified AO-MWCNTs.

The structures and morphologies of these hybrid nanomaterials are characterized by X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM) and transmission electron microscopy (TEM). The contents of PANI and precious metals are analyzed by thermogravimetric analyzer (TGA), Raman spectroscopy and inductively coupled plasma-optical emission spectrometer (ICP-OES). Cyclic voltammetry (CV) are used to evaluate the catalytic activities for formic acid electro oxidation. By the results, PANI modification can be a promising method which improves the electrocatalytical property of Pd based nanomaterials.

**Keywords:** Electrocatalyst, Pd, Polyaniline, DFAFCs, MWCNTs



## Synthesis and Characterization of Magnetic Solid Acid Catalyst for the Application of High temperature Glycerol Reaction

Wei-Tse Cheng<sup>1</sup>, Yuh-Jing Chiou<sup>1</sup>, Hong-Ming Lin<sup>2</sup>

<sup>1</sup> Department of Chemical Engineering, Tatung University, 104 Taipei, Taiwan

<sup>2</sup> Department of Materials Engineering, Tatung University, 104 Taipei, Taiwan

This study is to develop a novel solid acid catalyst supported on magnetic materials. The magnetic solid acid catalyst can be applied for the conversion of surplus and getting cheaper glycerol into high valued diesel additives. The magnetic property can benefit the catalyst recycling process after glycerol reaction.

In this study, the one-dimensional iron rod can be obtained by NaBH<sub>4</sub> reduction of iron chloride under a high magnetic field to form rod-shape iron with thin film iron oxide coated outside. A heteropoly acid Sn-Ti-O with Keggin structure, which has good thermal stability, high acidity and high oxidizing ability as widely used acid catalyst, will be deposited on the magnetic supporter.

After calcination under proper temperature, the obtained magnetic acid catalysts can be applied for the high temperature glycerol reaction with tert-butyl alcohol. The organic and aqueous products will be analyzed by GC and TGA. The solid catalysts can be magnetically recycled and conducted the reaction repeatedly. All the prepared or recycled magnetic catalysts will be characterized by XRD, NH<sub>3</sub>-TPD, Pyridine-FTIR, VSM, ICP-OES, and SEM.

**Keywords:** Solid acid catalysts, Magnetic Material, Glycerol

PO6

## Electrocatalytical Property of Hybrid AuPd/Reduced Graphene Oxide/Multi-Walled Carbon Nanotubes Nanomaterials for Direct Formic Acid Fuel Cells

Tung-Liang Lu<sup>1</sup>, Yuh-Jing Chiou<sup>1</sup>, Hong-Ming Lin<sup>2</sup>

<sup>1</sup> Department of Chemical Engineering, Tatung University, 104 Taipei, Taiwan

<sup>2</sup> Department of Materials Engineering, Tatung University, 104 Taipei, Taiwan

In recent years, because of the energy crisis and environmental awareness, scientists are actively finding the solutions of possible energy alternatives. Multi-walled carbon nanotubes (MWCNTs) and reduced graphene oxide (rGO), which have exceptional mechanical properties, electromagnetic properties, good electrical conductivity, thermal stability, mechanical strength and large specific surface area and other properties, are considered to be good catalyst substrate. This study will develop a novel MWCNTs or rGO supported Pd based electrocatalysts for the application of direct formic acid fuel cells (DFAFCs).

X-ray photosynthesis method is used for the reduction of Pd or AuPd on the hybrid carbon nanomaterials. The prepared nanoparticles are characterized by XRD, SEM, HRTEM and ICP-OES to confirm the structure, surface morphology and composition of the metal catalyst content. FTIR and Raman qualitative analysis are for the carbon substrate identification. Cyclic voltammetry test, I-t experiment and ECSA measurement are conducted in a formic acid environment to analyze the performance of Pd or AuPd nanoparticles as anodic electrocatalysts in DFAFCs.

**Keywords:** Pd, AuPd, reduced graphene oxide, MWCNTs, DFAFCs

## Synthesis and Characterization of Nano-hybrid Noble Metals/N doping TiO<sub>2</sub>/SnO<sub>2</sub>/MWCNTs

Cheng-Hung Yu<sup>1</sup>, Yuh-Jing Chiou<sup>2</sup>, Hong-Ming Lin<sup>1</sup>, Chung-Kwei Lin<sup>3</sup>

<sup>1</sup> Department of Materials Engineering, Tatung University, Taipei 104, Taiwan

<sup>2</sup> Department of Chemical Engineering, Tatung University, Taipei 104, Taiwan

<sup>3</sup> School of Dental Technology, College of Oral Medicine, Taipei Medical University, Taipei, Taiwan

\*Corresponding author: [hmlin@ttu.edu.tw](mailto:hmlin@ttu.edu.tw)

Recently, energy and environment are two problems of the world biggest concerns, it is imperative to search and develop new and clean sources of energy. The fuel cell is considered to be one of the most useful renewable energy. The fuel cell is an electrochemical device, as long as continue to provide fuel which is capable of continuously convert chemical energy into electrical energy. Its advantages are low pollution, high efficiency, and without charge. Therefore, the fuel cell can be regarded as an important green energy. Direct formic acid fuel cells (DFAFCs) demonstrate a potential use in future fuel cell devices, although further research is needed in improving formic acid electro-oxidation catalysts.

Novel metal catalysts are easily poisoned by CO adsorption or leaching in oxidation of formic acid that leads to decrease the performances of catalyst. In order to increase the catalyst activity and poison tolerance in fuel cells, novel metal nanoparticles are usually supported on modified materials to enhance its performance. In this study, TiO<sub>2</sub>/MWCNTs and TiO<sub>2</sub>/SnO<sub>2</sub>/MWCNTs are synthesized by sol-gel method. Also, ammonium is used to dope nitrogen into TiO<sub>2</sub> to modify its electrical and chemical property. MWCNTs, TiO<sub>2</sub>/MWCNTs, N-doping TiO<sub>2</sub>/MWCNTs, TiO<sub>2</sub>/SnO<sub>2</sub>/MWCNTs and N-doping TiO<sub>2</sub>/SnO<sub>2</sub>/MWCNTs are used as supporters in this study to examine the effects of supporters on the electrocatalytic performance of Pd and AuPd catalysts. Pd, Au-Pd are photo-synthesized by exposure supporters at 1A-Hard X-ray in National Synchrotron Radiation Research Center (NSRRC), Taiwan for eight to 16 minutes. The results indicate the synthesized metal nanoparticles are uniformly dispersed on the surfaces of MWCNTs, TiO<sub>2</sub>, N-doping TiO<sub>2</sub>, TiO<sub>2</sub> /SnO<sub>2</sub>, and N-doping TiO<sub>2</sub>/SnO<sub>2</sub> modified MWCNTs.

## Influence of Amino Acids on the Photostability of Water-soluble Octacarboxyphthalocyanines of Zn(II), Al(III) and Ga(III)

**Marta Kliber-Jasik**, Małgorzata A. Broda, Joanna Nackiewicz

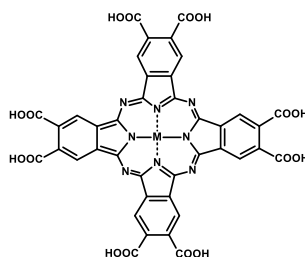
Faculty of Chemistry, University of Opole, 48, Oleska Street, 45-052 Opole, Poland  
(e-mail: [broda@uni.opole.pl](mailto:broda@uni.opole.pl))

**Keywords:** Phthalocyanines, Metallo-octacarboxyphthalocyanines, Amino acids, Photodynamic therapy, Photostability, UV-Vis spectra, DFT calculations

### 1. Introduction

Phthalocyanines (Pcs) are well known synthetic porphyrin analogs that have been the subject of study due to their specific physicochemical properties. Pcs have been used in a wide range of different applications: catalysts, liquid crystals, chemical sensors, solar cells, organic light-emitting diodes, photovoltaic cells, organic semiconductors, electrocatalytic systems, photoactive element in photocopiers, electrochromic display and in liquid crystalline materials, nonlinear optical materials [1, 2]. In recent years, much attention has been paid to the possibility of using these compounds as second generation photosensitizers in photodynamic therapy (PDT) [3, 4]. The properties of Pcs can be tuned by introduction of appropriate functional groups (e.g., carboxyl groups) on the peripheral position of the ligand.

The subjects of our research are zinc, aluminium and gallium phthalocyanines that have eight carboxylic groups attached to the benzene rings (Fig.1). These polar groups markedly improve their water solubility in comparison to unsubstituted phthalocyanines. This is advantageous from the viewpoint of PDT. In addition, so far conducted studies have shown that the complexes of phthalocyanines that have in the center of the ring such metals as aluminum, zinc or gallium are particularly promising in terms of their use in PDT [5].



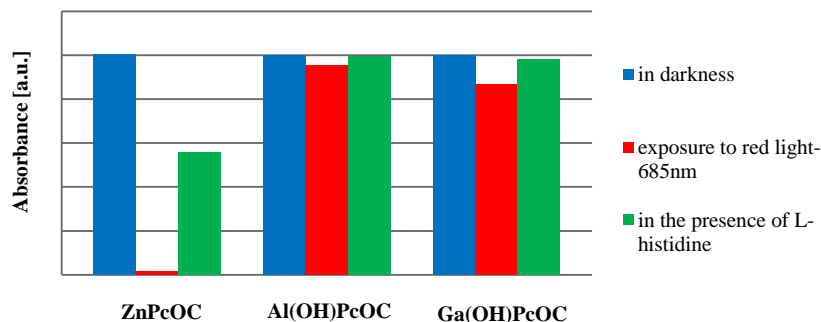
**Fig. 1.** Structure of metallo-octacarboxyphthalocyanine (MPcOC), M – Zn, Al(OH), Ga(OH).

### 2. Description of a problem solution

Photostability of MPcOC has fundamental importance for their applications as photosensitizers in photodynamic therapy and therefore the resistance of dyes to photodegradation is desirable. The aim of our research was to investigate the phenomenon of photostability of octacarboxyphthalocyanines of Zn(II), Al(III), Ga(III) and the influence of selected amino acids (glycine, *L*-histidine, *L*-cysteine, *L*-serine, *L*-tryptophan) on this phenomenon in the phosphate buffer at pH = 8.0. Additionally, theoretical calculations were conducted to investigate the problem of interaction of amino acids with MPcOC. The geometric structures of the axial and equatorial complexes of MPcOC - amino acids both in the gas phase and in aqueous solution were optimized at the B3LYP/6-31G\* level of theory.

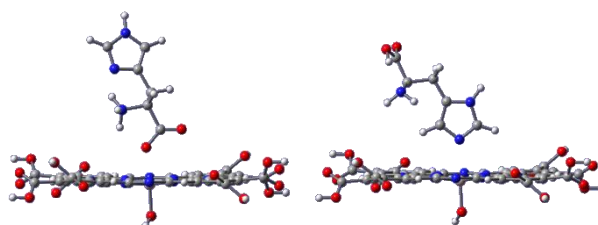
### 3. Results

Octacarboxyphthalocyanines of Zn(II), Al(III), Ga(III) are very stable in the absence of light, while the absorbance of the main Q band gradually decreases for the samples with exposure to visible light and exposure to daylight. Additionally, the presence of amino acids in aqueous solution increases the octacarboxyphthalocyanines photostability (Fig. 2).



**Fig. 2.** The absorbance of the main Q band of MPcOC after 60 min (intensity of the LED lamp used was 6.4 mW/cm<sup>2</sup>).

To explain the increased photostability of phthalocyanine in the presence of amino acids we performed DFT calculations of 1: 1 phthalocyanine - amino acid complexes. We assumed that these complexes may be formed in two ways: axially or equatorially. In the axial complexes the amino acid electrostatically interacts with the metal in the centre of phthalocyanine. On the other hand, the equatorial complexes are formed due to hydrogen bond between the carboxyl group of the MPcOC and a carboxyl or amino group of amino acid. Geometry optimization of such complexes allows estimating the interaction energies and structural parameters of the complexes.



**Fig. 3.** Structure of two types of Al(OH)PcOC – L-histidine axial complexes calculated at B3LYP/6-31G(d) level of theory

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## On the Sensitivity of Chemical Shift to 5-fluorouracil - C60 Complex Formation

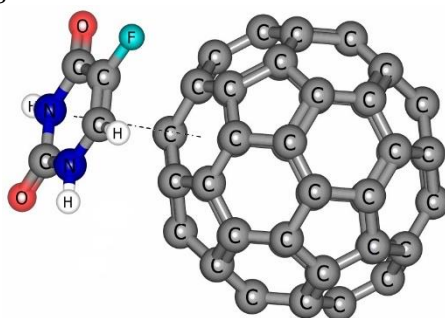
Mehrnoosh Kh. Hazrati<sup>1</sup>, N. L. Hadipour<sup>1</sup> and Teobald Kupka<sup>2\*</sup>

<sup>1</sup>Department of Chemistry, Torbiat Modares University, P. O. Box 14115-175, Teheran, Iran

<sup>2</sup>University of Opole, Faculty of Chemistry, 48, Oleska Street, 45-052 Opole, Poland

([teobald@uni.opole.pl](mailto:teobald@uni.opole.pl); [teobaldk@gmail.com](mailto:teobaldk@gmail.com))

Despite its severe side effects and general toxicity, 5-fluorouracil (5FU) has been used in cancer therapy for years. With the recent advances in nanotechnology, including medicine, the idea of controlled and “safe” drug delivery is very tempting. Among the drug carriers are  $\beta$ -cyclodextrin “baskets”, fullerenes and single-walled carbon nanotubes (SWCNTs). The main idea of drug transport is related to reversible chemical bonding or weak physical interactions between the carrier molecule and drug. The latter idea is easily imagined using fullerene [1] capable of  $\pi$ -bond formation with selected drug molecules, for example forming a kind of a stacked sandwich. Obviously, the energy of drug-C60 complex formation should be favorable at room temperature (say 2 to 6 kcal/mol). The DFT optimized structure of the titled complex is shown schematically in **Figure 1**.



**Figure 1.** M06-2X/6-31G\* optimized structure of 5FU-C60 complex in the gas phase [2]

**The aim of the current theoretical study is to show the potential applicability of C60 as carrier of 5FU drug in nanomedicine and therapy with the help of detailed GIAO NMR calculations.**

Gauge including atomic orbital (GIAO) approach was employed to calculate isotropic nuclear magnetic shieldings and chemical shifts (relative to benzene and TMS) on previously M06-2X/6-31G\* optimized geometries of 5FU-C60 complex in the gas phase [2] and the individual components. Significant differences between the predicted chemical shifts of the formed complex and free 5FU [3] were noticed (about 6 ppm for F, 2 ppm for C and 0.5 ppm for H).

#### 4. Acknowledgements

This work was supported partly by the Faculty of Chemistry, University of Opole (Grant 8/WCH/2016-S). The use of hardware and software of Wroclaw (WCSS) and Krakow (ACK Cyfronet and PL-grid) is also acknowledged.

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## **Immobilization of Biopolymers on e-PTFE film by Cold Plasma and Graft Polymerization Treatment**

Ko-Shao Chen<sup>1</sup>, **Chia-Yi Lin**<sup>1</sup>, Hsin-Ming Wu<sup>1</sup>, Chung-Yih Wang<sup>2</sup>

<sup>1</sup> Department of Materials Engineering, Tatung University, Taiwan

<sup>2</sup> Department of Bioengineering, Tatung University, Taiwan

kschen@ttu.edu.tw

Expanded polytetrafluoroethylene (e-PTFE) thin film is a hydrophobic material with stability. In order to improve the surface hydrophilicity and enhance cell affinity, this study used argon gas low temperature plasma to activate the surface of e-PTFE film to create activated free radical on the surface. Then, UV light induced grafting was used to graft acrylic acid (AAc) to create hydrophilic functional groups on the surface of e-PTFE film. Finally, EDC/NHS were used as cross-linking agents to immobilize biopolymers on the surface by the chemical cross-linking method in order to increase the cell affinity of e-PTFE material. By elemental analysis and chemical bonding analysis of immobilization of biopolymers by chemical cross-linking, the results indicated the occurrence of N atoms and the O=C-N and N-H bonding, which evidently supports the immobilization of biopolymers on the film surface. Further, fibroblast cells (3T3) were used to conduct cell adhesion experiment for culturing cells on the e-PTFE-modified surface film. It was found that the cell growth of the samples subjected to ePTFE-gAAc-Gelatin/Chitosan (1:1) treatment was significantly better than that of the untreated sample. In this study, the originally hydrophobic e-PTFE, after surface modification, has been illustrated to improve its hydrophilicity and biocompatibility, and can be applied in biological engineering such as drug release, artificial dressing, cell or enzyme immobilization.

**Keywords:** Polytetrafluoroethylene, Plasma polymerization, Hydrophilic, AAc, Chitosan, Gelatin

**PO11**

## **Preparation, Structure, Antibacterial Properties of Polyacrylic acid/Silver Nanocomposite Hydrogels**

**Yi-Syuan Wei (魏翊軒)<sup>1</sup>, Ko-Shao Chen (陳克紹)<sup>1\*</sup>, Lii-Tzu Wu (吳禮字)<sup>2</sup>, Chih-Wei Chou (周志調)<sup>3</sup>**

<sup>1</sup>Department of Materials Engineering, Tatung University, Taipei, Taiwan

<sup>2</sup>School of Medicine, China Medical University, Taichung, Taiwan

<sup>3</sup>Department of Cosmeceutics, China Medical University, Taichung, Taiwan

Silver nanocomposites embedded within a polymer matrix have attracted attention in recent years, it can be obtained relatively uniform particle size of silver, and there is good chemistry, physical properties and antibacterial properties. Polyacrylic acid having carboxylic acid functional group, it can stable compound with a metal ion. In this study, we used acrylic acid and silver nitrate to prepare nanocomposite hydrogels through ultraviolet (UV)-light irradiation. The formation of hydrogels and reduction of silver nanoparticles were affected by the preparation parameters, that is, the monomer content and silver nitrate concentration. The morphology, structure, and size of the silver nanocomposite hydrogels were evaluated through field emission scanning electron microscopy (FESEM) and transmission electron microscope (TEM). The biocompatibility of the samples was tested by A549 cells. The antimicrobial activity of the samples was tested against *Escherichia coli* and *Staphylococcus aureus*. The silver nanocomposite hydrogels contained interior porous structures and open networks structures, and could absorb 400 to 550 grams of deionized water per gram of dried hydrogel. The silver nanoparticles size was about 5 to 23 nm. Moreover, these hydrogels had a good biocompatibility and strong antibacterial effect, which can be useful in developing new superabsorbent antimicrobial pharmaceutical products.



## PO12

### Surface Modified PET Sheet and TPU nonwoven by Helium Atmospheric Plasma for Improving Graft Polymerization of NIPAAm Hydrogel and Deposit of Hydroxyapatites-like Films

Yi-Yun Cheng (鄭宜芸), Yao-Chung Liu (劉耀中), Ko-Shao Chen (陳克紹)\*, Bo-Kai Chen (陳柏凱), Mu-Rong Yang (楊木榮), Ming-Tse Lin (林銘澤)

<sup>1</sup> Department of Materials Engineering, Tatung University, Taiwan

<sup>2</sup> Department of Bioengineering, Tatung University, Taiwan

E-mail: [kschen@ttu.edu.tw](mailto:kschen@ttu.edu.tw)

Surface graft polymerization can induce pure functional groups on surfaces which has a wide range of applications. In this study helium atmospheric plasma treat (APT He) polyethylene terephthalate (PET) and thermoplastic polyurethane (TPU) nonwoven in order to activate the surface. Subsequently UV-induced graft polymerization of the temperature sensitive hydrogel N-isopropylacrylamide (NIPAAm) on the plasma activated material surface was performed. For deposition of hydroxyapatite (HA:  $\text{Ca}_5(\text{OH})(\text{PO}_4)_3$ ), treated samples were immersed in two separate solutions ( $\text{Ca}^{2+}$ - and  $\text{PO}_4^{3-}$ - source) for 30 min in each solution per cycle. The results showed that, APT He treated (voltage:12,000V, gas flow rate 0.4 l/min, glow distance 10mm), improved the hydrophilicity. After this treatment could be successfully grafted polys (NIPAAm) gel on the materials surface. By optical Measurement (OM) we can confirmed the formed HA on the surfaces.

## PO13

### Effect of Graft Acrylic Acid Reduction Nanosilver on the Bamboo Charcoal

Ju-Hui. Yeh<sup>1</sup>(葉茹蕙), Ko-Shao. Chen<sup>1\*</sup>(陳克紹), Ming-Tse. Lin<sup>2</sup>(林銘澤), Chi-Yuan. Huang<sup>1</sup>(黃繼遠)

<sup>1</sup>Department of Materials Engineering, Tatung University, Taiwan

<sup>2</sup>Department of Bioengineering, Tatung University, Taiwan

Email: kschen@ttu.edu.tw

Bamboo charcoal is widely used in life, but the Bamboo charcoal used in biomedical research Antibacterial it does not have much. In this study, the reduction nano-silver particles on the Bamboo charcoal composite surface. Use Hexamethyldisilazane (HMDSZ) deposited on Bamboo charcoal layer having a hydrophobic functional group, or oxygen plasma surface activated and made the Bamboo charcoal surface hydrophilic. Graft polymerization of acrylic acid can be adsorbed silver nitrate and NaBH<sub>4</sub> that reduction nano silver particles. The use of graft / fixed density measurement, measuring surface wettability, sem, icp, antibacterial tests analysis are discussed. The results illustrate that the water contact angle of bamboo charcoal increases from 71.6° to 127.6° after the HMDSZ plasma processing, and it decreases under 10° after the O<sub>2</sub> plasma treatment. The particle size of nano silver for pAAc reduce about 40-80 nm by SEM. By *Escherichia coli*, *Staphylococcus aureus*, *Pseudomonas aeruginosa*, antibacterial experiments 1mM and 10mM concentration of nano silver can significantly reduce the number of bacteria

**Keywords :** Bamboo charcoal, HMDSZ, Plasma, hydrophilic, Antibacterial

**PO14**

## **Developed Effect of Stable Treat Plasma Film on Porous UHMWPE Surface by HMDSZ and Oxygen Cold Plasma Treatment**

**Bo-Kai Chen** (陳柏凱), Ko-Shao Chen(陳克紹)\*, Li-dung Hung(洪力東)

Department of Materials Engineering, Tatung University, Taipei, Taiwan  
e-mail:kschen@ttu.edu.tw

Porous Ultra High Molecular Weight Polyethylene (UHMWPE) has excellent biocompatibility. It is widely applied in the field of medicine as a biomaterial. It can be used in medical polymer devices, such as heart valves, artificial joints and surgical correction, etc. In this study, Hexamethyldisilazane (HMDSZ) monomer was deposited on UHMWPE surface by cold plasma deposition and the change of surface hydrophobicity were investigated after modification. It could be found that the water contact angle (WCA) was 90° very stable after HMDSZ plasma treatment on UHMWPE. The WCA of oxygen plasma treatment was also stable after sixty days. Using scanning electron microscopy (SEM) the dendritic structures on the surface of 1 minute oxygen plasma treatment could be observed. Over 5 minutes HMDSZ plasma treatment, the surface of substrate became smooth and it would be found the creaks on the film because the hole is disappear. Higher power of Oxygen plasma treatment, the deposited film on the surface would be decomposed causing clogging pores. In this study, the effect of the plasma treatment times on the holding holes.

**Keywords :** HMDSZ, stable, (WCA), Plasma, hydrophilic

**PO15**

## **The Applications of Cold Plasma Treatment on the Surface Property of Xuan Paper**

**H.H. Liang, K.S. Chen\***

Department of Materials Engineering, Tatung University  
Email:kschen@ttu.edu.tw

Xuan paper (XP) is a kind of paper which made of natural cellulose, originating in ancient China used for writing and painting. Most of ancient Chinese calligraphic artwork or books used it. Because the Xuan paper is soft, hydrophilic and easy to mildew, it is hard to preserve that valuable Chinese calligraphy, books or painting. In this work, we try to make an organosilicon compound thin film for Xuan paper protecting by Hexamethyldisilazane (HMDSZ) plasma treatment. Though RF-Cold Plasma Treatment deposit a homogenous and hydrophobic thin film, which is without organic solvent and pollution. It is a clean process and thickness controllably by treatment time and not influences optical properties and tensile strength. The result of Preliminary experiments show the HMDSZ plasma treated XP has water contact angel increasing from  $0^{\circ}$  to  $130^{\circ}$  and maintaining long time. This treatment is also using for adhesion of XP protecting, the result show that the pasted XP can maintain adhesive over one day in the water after HMDSZ plasma treatment. Preparation of a hydrophilic protective film is also available by O<sub>2</sub>-plasma after HMDSZ plasma treated

**PO16**

## **Cold Plasma Treated TPU non-woven for Improving Surface Graft Polymerization of Acrylic Acid, NIPAAm and Their Function Properties**

**Da-Jhan Chiu<sup>1</sup>** , Ko-Shao Chen <sup>\*1</sup> , B. K. Chen<sup>1</sup>

<sup>1</sup>Department of Material Science and Engineering, Tatung University

\*Corresponding author's e-mail: kschen@ttu.edu.tw

In this study, we used thermoplastic polyurethane (TPU) non-woven fabric substrates to graft with acrylic acid (AAc) and N-isopropylacrylamide (NIPAAm) polymer on the surface, however the TPU surface was hydrophobic and non-activated chemical groups that couldn't be reactive. It's difficult to apply to the people's livelihood and biological aspects of research. Therefore, we use Hexamethyldisilazan (HMDSZ) plasma treatment, and then, using oxygen plasma treatment to activated surface. After this process, it could be grafted with different percentage of AAc and NIPAAm by UV graft polymerization system. Prepare pAAc/NIPAAm thin film, using water contact angle. graft amount and swelling ratio to realize the influence between different percentage of AAc and NIPAAm. Except the surface have Acid and Base sensitive and thermal sensitive.

**Keywords:** Plasma, Polymerization, AAc, NIPAAm, UV graft

**PO17**

## **Surface Modification of Nano Gold by Cold Plasma Treatments for Graft Polymerization of AAC or NIPAAM Hydrogels**

**Chu-Yuan Huang** (黃楚淵)<sup>1</sup>, Yi-Hsuan Yang (楊宜璇)<sup>1</sup>, Ko-Shao Chen, (陳克紹)\*<sup>1</sup>, Ju-Hui Yeh(葉茹蕙)<sup>1</sup>, Yi-Syuan wei(魏翊軒)<sup>1</sup>

Department of Materials Engineering, Tatung University  
大同大學材料工程學系  
[kschen@ttu.edu.tw](mailto:kschen@ttu.edu.tw)

The study is use the method of Oxygen plasma processing to generate free radicals on 11-Mercaptoundecanoic acid nano gold particles (MUA). Oxygen plasma can rapid oxidation of the material surface and formation of free radicals on surface. Than the use of UV-induce surface graft polymerization of N-isopropyl acrylamide(NIPAAM), acrylic acid(AAc) grafted onto nano-Au particles, the aim is to preparation of temperature or pH sensitive gels of the (poly N-isopropyl acrylamide) nanoparticles. The use of hexamethyldisilazane (HMDSZ) plasma treated MUA-Nano Au to be hydrophobic, and then use O<sub>2</sub> plasma treatment change to hydrophilic. The research will discuss the impact of hydrophobic and hydrophilic on the concentration of gold nanoparticle. The results show we can success prepare the pH or Temperature sensitive hydrogels on Nano-Au particles.

# Advertisement of Contributed companies

## ● Eclat Textile Co. Ltd., Taiwan



### About Us

- Company Profile** >
- History
- Our Vision
- Vertical Intergrate

### Company Profile

Home > About Us > Company Profile

#### *Setting the pace for excellence - your All-In-One supplier*

ECLAT utilizing the most professional manpower, swiftest response and most competitive cost to obtain maximum yield for protecting shareholder's equity and satisfying customer demands.

We provide the employees a fine working environment, aspiring the employee's creativity and wisdom to grow alongside with the company.

Enlisting strategic worldwide marketing hubs helping to close in on the market, satisfy customer needs, together with streamlining the flexible functional knit fabric manufacturers in vertical integration. Becoming a global professional functional apparel maker that would help to achieve a vertical integration to streamline production and to satisfy the customer with volume and competitiveness is one stop shopping.



We Upholding a maximum merchandising pursuit to the core concept of our business, producing the flexible functional fabric varieties and professional functional apparels that would enhance the consumer's living quality, together with ongoing technical refinement, aiming to excel industry competitiveness and securing maximum profit in creating a sustainable management.

Company Name	ECLAT TEXTILE CORPORATION LTD.
Year of Establishment	1977
CEO	C.H. Hung
Employees	1,100 ( Taiwan ); 8,000 ( Worldwide )
Headquarters	No.28 ,Wu Chuan Rd., Wuku Dist., New Taipei City , Taiwan
Status	IPD listed in Taiwan Stock Market in 2001.
Annual Turnover ( 2010 )	Taiwan : USD 300,000,000 ( Fabric 46% , Garment 54% )
	ECLAT Group : USD 450,000,000 ( Fabric 50% , Garment 50% )

## ● Eclat Foundation, Taiwan



財團法人儒鴻教育基金會  
ECLAT EDUCATION FOUNDATION



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### 《 創設緣起 》

### 《 業務宗旨 》

### 《 董事會成員 》

本會發起人洪鎮海先生，本著取之於社會，用之於社會的信念，發起成立本基金會。

台灣為島國，經濟成長動能以出口貿易為主，長期以來，紡織產業一直扮演創匯的重要角色。

外語能力是能與世界各國發展經貿往來的重要能力，也是企業及個人在國際競賽中，必須具備的競爭力。

人才的培育與加入，則是產業可以永續的根本。

因此，洪鎮海先生希望藉由本基金會設置獎助學金，以鼓勵青年學子向學，提升外語能力，強化個人競爭力。

於2013/11/25本會核准成立(法人登記證號：102年證財字第6號)，設立基金共新臺幣參仟壹佰萬元整，

由儒鴻企業股份有限公司、洪鎮海先生、蔡賢欽先生等11人共同捐助。

儒鴻企業股份有限公司 | 智慧財產權與法律聲明  
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- Joinsoon Electronics Mfg. Co., Ltd, Taiwan

# Your Reliable Green Partner Timely Capacity Provider

*In this year, JEM will announce a whole new USB type C product series,  
but also present you the Wi-Fi DAS & HUB.*



## Joinsoon Electronics Manufacturing CO., LTD.

JEM is one of the world's leading providers of interconnection products and electronics manufacturing service. We design and manufacture a broad range of signal cables, medical leadwires, connectors, and computer peripheral antennas.



Head Quarter: Taipei, Taiwan



Factory I: Dong-Guan, China



Factory II: Su-Zhou, China

<http://www.jem.com.tw>

| 2016/6/27

● Ming Fung Nano-Biotechnology Co., Ltd., Taiwan



**攜帶式**  
**MT-P6**  
**濾水器**  
Portable Water Filter

# 奈米生化科技

Nano Bio-technology  
A Miracle of Water

## 濾出奇蹟之水

可殺菌及抑制細菌滋生、濾除農藥殘毒、化學元素、  
重金屬...等多重淨化水質功能





### 過濾方式

Filtration method

**注意事項**  
Cautions

第一次使用將注滿水的寶特瓶口與濾芯接頭旋緊，用手擠壓出約1公升的水後，即可飲用。  
For the first time use, to connect pet bottle(with water) and water filter jointer and screw it tight, then compress the bottle to let water out about 1 liters and Start drinking it.

### 擠壓式

Compress type

- 將注滿水的寶特瓶口與濾芯接頭旋緊  
To fix pet bottle with water and connect it with water filter jointer and screw it tight
- 再將寶特瓶倒立瓶口朝下，用手緩緩擠壓寶特瓶身即可過濾。  
Let the bottle outlet upside down the gently compress the bottle to let the water out.

### 吸管式

Straw type

- 先將吸管套入濾芯的矽膠套管內  
Insert the straw into silicon tube at water filter
- 接著將濾芯接頭與寶特瓶口結合，注意不可旋緊，能讓空氣對流  
fix filter with Pet bottle, beware not to screw tighten it closely to let air in.
- 即可吸飲

**使用期限** Lifetime of water filter

本濾芯可過濾600公升的自來水，等於1000瓶600C.C.寶特瓶礦泉水，方便又省錢。  
It capable for 600 liters water filtration, equal to 1000 bottles of 600 c.c. bottle Mineral water, so convenience and money saving







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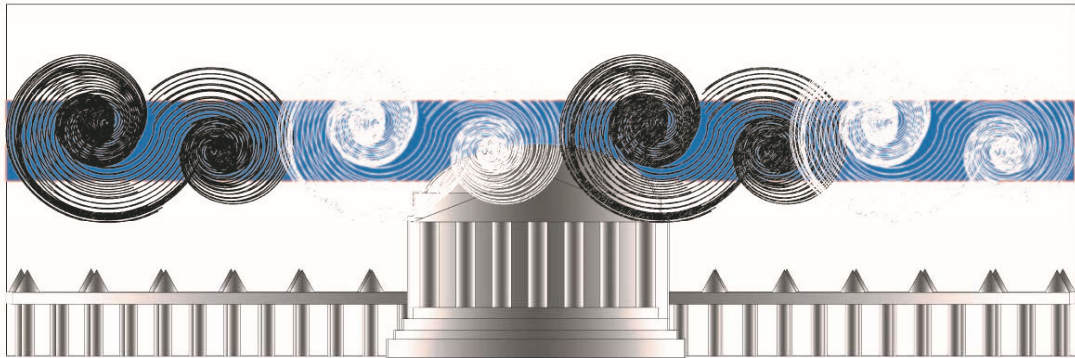
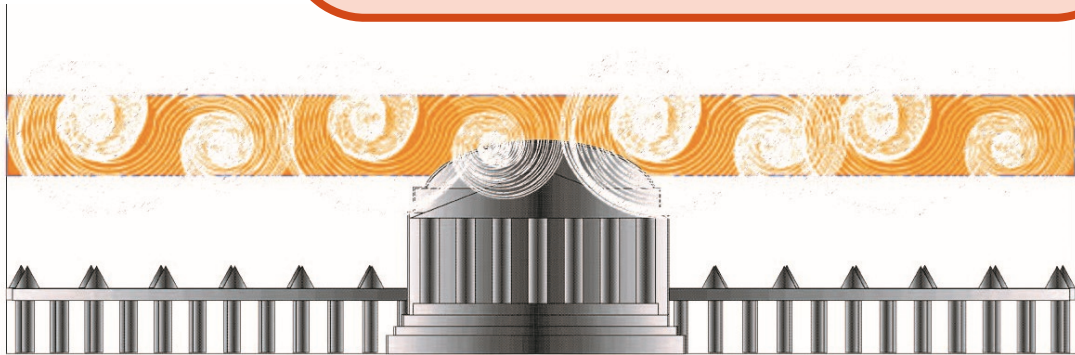
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