2013

Physics & Chemistry Abstracts

First Annual International Conference on **Physics & Chemistry,** 22-25 July 2013, Athens, Greece

Edited by Gregory T. Papanikos

THE ATHENS INSTITUTE FOR EDUCATION AND RESEARCH

1st Annual International Conference on Physics & Chemistry

22-25 July 2013, Athens, Greece

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(In Alphabetical Order by Author's Family name)

Preface

This abstract book includes all the abstracts of the papers presented at the *1st Annual International Conference on Physics & Chemistry, 22-25 July 2013,* organized by the Athens Institute for Education and Research. In total there were 29 papers and 30 presenters, coming from 16 different countries (Algeria, Armenia, Brazil, Canada, China, Germany, India, Israel, Japan, Portugal, South Korea, Spain, Tunisia, Turkey, UAE, USA). The conference was organized into VI sessions that included areas such as Theory, Biomedical Physics, Chemistry/Instrumentation e.t.c. As it is the publication policy of the Institute, the papers presented in this conference will be considered for publication in one of the books of ATINER.

The Institute was established in 1995 as an independent academic organization with the mission to become a forum where academics and researchers from all over the world could meet in Athens and exchange ideas on their research and consider the future developments of their fields of study. Our mission is to make ATHENS a place where academics and researchers from all over the world meet to discuss the developments of their discipline and present their work. To serve this purpose, conferences are organized along the lines of well established and well defined scientific disciplines. In addition, interdisciplinary conferences are also organized because they serve the mission statement of the Institute. Since 1995, ATINER has organized more than 150 international conferences and has published over 100 books. Academically, the Institute is organized into four research divisions and nineteen research units. Each research unit organizes at least one annual conference and undertakes various small and large research projects.

I would like to thank all the participants, the members of the organizing and academic committee and most importantly the administration staff of ATINER for putting this conference together.

Gregory T. Papanikos
President

Athens Institute for Education and Research
Sciences Research Division

1st Annual International Conference on Physics & Chemistry 22-25 July 2013, Athens, Greece

PROGRAM

Conference Venue: St George Lycabettus, 2 Kleomenous Street, 10675 Kolonaki, Athens, Greece.

ORGANIZING AND SCIENTIFIC COMMITTEE

Administration

C O N F E R E N C E P R O G R A M

(The time for each session includes at least 10 minutes coffee break)

Monday 22 July 2013

08:30-09:10 Registration

09:10-09:30 Welcome and Opening Remarks

- Dr. Gregory T. Papanikos, President, ATINER.
- Dr. George Poulos, Vice-President of Research, ATINER & Emeritus Professor, University of South Africa, South Africa.
- Dr. Ethel Petrou, Professor and Chair, Department of Physics, Erie Community College-South, State University of New York, USA & Academic Member, ATINER.

09:30-12:00 Session I: Materials

Chair: George Poulos, Vice-President of Research, ATINER & Emeritus Professor, University of South Africa, South Africa.

1. Dimitris Argyropoulos, Professor, North Carolina State University & University of Helsinki, Finland. Fundamental Polymer Science behind the Creation of High Value Polymers and Copolymers Based on Lignin.
2. Gustavo Zampier dos Santos Lima, Professor, Federal University of Rio Grande do Norte, Brazil. Multifractality in Domain Wall Dynamics of a Ferromagnetic Film.
3. Jerzy A. Szpunar, Professor and Canada Research Chair (T1), University of Saskatchewan, Canada. A Role of Texture and Grain Boundary Structure in Controlling Oxidation, Hydrogen Ingress and Fracture in Materials Used by Nuclear Industry.
4. *Isiah Manuel Warner, Professor, Louisiana State University, USA, Susmita Das, Louisiana State University, USA, Suzana Hamdan, Louisiana State University, USA, Paul Magut, Louisiana State University, USA & Bishnu Regmi, Louisiana State University, USA. Applications of GUMBOS in Chemistry/Materials Science.
5. Nuri Unal, Professor, Akdeniz University, Turkey. Coherent States for Photons in Time Varying Dielectric Media.

12:00-13:30 Session II: Education

Chair: Nicholas Pappas, Vice-President of Academic Affairs, ATINER & Professor, Sam Houston University, USA.

1. Costas Efthimiou, Associate Professor, University of Central Florida, USA, Michael Georgiopoulos, Carla Poindexter, Joo Kim, Wanda Ortiz & Dennis Ahearn, University of Central Florida, USA. Physics and Chemistry ArtWork as Communicator of Research at UCF.
2. Rita Upmacis, Associate Professor, Pace University, USA. Teaching Green Chemistry Principles to Undergraduate Students.
3. Jamal Hassan, Assistant Professor, Khalifa University of Science, UAE & Ahmad Al Nabulsib, Instructor, Khalifa University of Science, UAE. Teaching NMR Product Operator Formalism with MATLAB Software.
4. *Andreas Toupadakis, Lecturer, University of California, Davis, USA & Alyson Wong, Student, University of California, Davis, USA. The Lack of True Understanding in Science Education Today: Reasons, Consequences and Answers.
5. Anmar Khadra, Assistant Professor, McGill University, Canada, Arthur Sherman, Lab Chief and Senior Investigator, Laboratory of Biological Modeling, National Institute of Diabetes and Digestive and Kidney Diseases, National Institutes of Health, USA & Stanko S. Stojilkovic, Lab Chief and Senior Investigator, Section on Cellular Signaling, National Institute of Child Health and Human Development, National Institutes of Health, USA. Deciphering the Kinetic and Gating Properties of P2X7 Receptor Channels.

13:30-14:30 Lunch

14:30-16:30 Session III: Optic Spectroscopy I
Chair: *Isiah Manuel Warner, Professor, Louisiana State University, USA.

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2. Yosef Yeshurun, Professor, Bar-Ilan University, Israel, Shaulov A. Levi, A. Frydman, G. B. Koren & Ya. Shapiro. Magnetoresistance Oscillations and Field-induced Enhancement of Superconductivity in Granular $YBa_2Cu_3O_{7-\delta}$ Nano Wires.
3. Canan Karaalioglu, Assistant Professor, Pace University, USA. Detection of Illicit Drugs and Explosives by THz Spectroscopy.
4. Georgios Lefkidis, Lecturer, University of Kaiserslautern, Germany & W. Hubner, Lecturer, University of Kaiserslautern, Germany. Coherent Laser-Induced Manipulation of Magnetism on Molecular Systems.
5. Nasr Sdiri, Teacher, Tunisia. Raman Spectroscopy, and DTA studies B_2O_3 Additions on the Microstructure in P_2O_5-B_20_3-Fe_2O_3 Glasses.
6. Mohand Akli Tafoughalt, Teacher and Researcher, Université A/Mira, Algeria & Madani Samah, Teacher and Researcher, Université A/Mira. Structural, Energetic and Optical Properties of Small Binary Silver-gold Clusters.

21:00–23:00 Greek Night and Dinner (Details during registration)

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1. Christopher Arumainayagam, Professor, Wellesley College, USA. Methanol Radiolysis ofAstrochemical Interest.
2. Haim Taitelbaum, Professor, Bar-Ilan University, Israel. Physical and Chemical Characteristics of Reactive-Wetting at Room Temperature.
3. *Maged Henary, Assistant Professor, Georgia State University, USA. Synthesis of Zwitterionic Fluorescent NIR Dyes for Bioimaging Applications.
4. Emil Wierzbinski, Researcher, University of Pittsburgh, USA, Ravindra Venkatramani, Assistant Professor, Tata Institute of Fundamental Research, India,Kathryn Davis, Assistant Professor, Manchester College, USA, Silvia Bezer, Researcher, University of North Carolina, USA, Catalina Achim, Professor, Carnegie Mellon University, USA, David Beratan, Professor, Duke University, USA & David Waldeck, Professor, University of Pittsburgh, USA. Relationship between Electrochemical Electron Transfer Rate Constant and Single Molecule Conductance.
5. Andrea Micelli, Post-Doctoral, Institut de Fisica d'Altes Energies (IFAE), Spain. 3D Pixel Sensors for Diffractive HEP Experiments.

11:30-13:00 Session V: Biomedical Physics
Chair: *Maged Henary, Assistant Professor, Georgia State University, USA.

1. Yoshio Kobayashi, Professor, Ibaraki University, Japan, Kohsuke Gonda, Associate Professor, Tohoku University, Japan & Noriaki Ohuchi, Professor, Tohoku University, Japan. Imaging Processes Using Core-Shell Particle Colloid Solutions for Medical Diagnosis.
2. *Margarita Matevosyan, Senior Researcher, Institute of Biochemistry and Yerevan State University, Armenia, Andranik Durgaryan, Researcher, H. Buniatian Institute of Biochemistry, NAS RA, Armenia & Armen Galoyan, Head of Department Neurohormones Biochemistry, H. Buniatian Institute of Biochemistry, NAS RA, Armenia. Prophylaxis and Treatment of Generalyzed Infection Induced by Methicillin-Resistant Staphylococcus Aureus (MRSA) in Vivo with Hypothalamic Proline Rich Peptides Galarmin and d-15 Galarmin.
3. Ricardo Dias, Professor, Polytechnic Institute of Braganca, Portugal, Bianca Pires, MSc Student, Luis Pimparel, MSc Students, Diana Pinho, Phd Student and Rui Lima, Professor. Flow of Red Bloods Cells in Highly Branched Microvessels.

13:00-14:00 Lunch

14:00-15:30 Session VI: Theory
Chair: Ethel Petrou, Professor and Chair, Department of Physics, Erie Community College-South, State University of New York, USA & Academic Member, ATINER.

1. *Barbara Szpunar, Senior Research Scientist, University of Saskatchewan, Canada. Multidisciplinary Reactor Safety Studies: Application of First Principles Calculation.
2. Girish Setlur, Associate Professor, Indian Institute of Technology Guwahati, India. Disorder and Correlations in One Dimension using Nonchiral Bosonization.
3. Dukjoon Kim, Professor, Sungkyunkwan University, South Korea. Proton Conducting Electrolyte Membranes based on the Pendant-sulfonated Poly(arylene ether ketone)/polyorganosiloxane Interpenetrating Polymer Networks.
4. Raphael Steinitz, Retired, Ben Gurion University, Israel. Ampere's Law Operating in O, B and A Stars.
5. Qing Zhao, Professor, Beijing Institute of Technology, China. Six-Qubit matrix Calculation from Incomplete Measurement.

17:30-20:30 Urban Walk (Details during registration)
21:00-22:00 Dinner (Details during registration)
Wednesday 24 July 2013
Cruise: (Details during registration)
Thursday 25 July 2013
Delphi Visit: (Details during registration)

Christopher Arumainayagam
Professor, Wellesley College, USA

Methanol Radiolysis of Astrochemical Interest

Our goal is to simulate processes which occur when high-energy cosmic rays interact with interstellar and cometary ices, where methanol, a precursor of several prebiotic species, is relatively abundant. The interactions of high-energy radiation, such as cosmic rays ($E_{max} \sim 10^{20}$ eV), with matter produces large numbers of low-energy (< 15 eV) secondary electrons, which are thought to initiate radiolysis reactions in the condensed phase.

We have investigated the dynamics of low-energy (1–20 eV) electron-induced reactions in condensed thin films of methanol (CH_3OH) through electron stimulated desorption (ESD) and post-irradiation temperature programmed desorption (TPD) experiments conducted under ultrahigh vacuum conditions ($\sim 4 \times 10^{-10}$ torr). ESD experiments indicate that the anions, especially H^-, which desorb from the methanol thin film during electron irradiation are predominantly formed via the dissociation of temporary negative ions formed via electron capture by methanol molecules, a process known as dissociative electron attachment (DEA). However, post-irradiation TPD investigation of radicals, especially $\bullet CH_2OH$ and $CH_3O\bullet$ remaining in the methanol thin film, show evidence for electron impact excitation, not DEA, as the primary mechanism by which methoxymethanol (CH_3OCH_2OH) and ethylene glycol ($HOCH_2CH_2OH$) are formed. The formation of radiolysis products at electron energies as low as 7 eV demonstrates that electron impact ionization cannot be the sole reaction mechanism. The results of surface science experiments such as ours may provide a fundamental understanding of how complex molecules are synthesized in the interstellar medium and comets.

Dimitris Argyropoulos
Professor, North Carolina State University & University of Helsinki, Finland

Fundamental Polymer Science behind the Creation of High Value Polymers and Copolymers Based on Lignin

Lignin is the second most abundant biopolymer on the plant, next only to cellulose. Most efforts to utilize lignin have been limited by various factors that impart in it characteristics that define it as an unreliable precursor to polymer production. This is because lignin (and more specifically technical lignin) offers relatively unpredictable polymerization characteristics, depending upon its source and the degree of delignification to which the plant materials were subjected. More specifically, the highly functional character of lignin (i.e., rich in phenolic and aliphatic OH groups, as well as reactive benzylic carbons) induces a variety of potential polymerization sites and heat instability in such materials. Both factors promote gelation processes under polymerization conditions or when the temperature increases close to and/or above the glass transition temperature (Tg). In addition, the relatively low molecular weight (a few thousands) for lignin derived from commercial pulping and biorefinery operations makes lignin unsuitable for higher end applications, such, for example, high performance, heat stable engineering thermoplastic applications. During this presentation, the fundamental work of our group will be described aimed at creating reactive lignin materials that are stabilized and rendered better suited for industrial applications. Specifically, our work provides methods for creating lignins of controlled and modulated characteristics exhibiting thermal and polymerization stabilities. Such thermal properties and stable molecular weight distributions of lignins and copolymers produced from commercial lignins provides a means for beneficially modulating the properties of an otherwise intractable bio-polymer. Overall, this effort provides an example of a series of fundamental investigations that when actualized show immediate benefits and solutions for a world less depended on petrochemical resources.

Ricardo Dias
Professor, Polytechnic Institute of Braganca, Portugal
Bianca Pires
MSc Student, Polytechnic Institute of Braganca, Portugal
Luis Pimparel
MSc Students, Polytechnic Institute of Braganca, Portugal
Diana Pinho
Phd Student, Polytechnic Institute of Braganca, Portugal
&
Rui Lima
Professor, Polytechnic Institute of Braganca, Portugal

Flow of Red Bloods Cells in Highly Branched Microvessels

Red blood cells (RBCs) in microvessels and microchannels has tendency to undergo axial migration due to the parabolic velocity profile which results in a high shear stress around wall that forces the RBCs to move towards the centre induced by the tank treading motion of the RBC membrane [1,2]. As a result there is a formation of a cell-free layer (CFL) with extremely low concentration of cells around the walls of the microchannel [1,2].Since the CFL excludes the RBCs from low velocity regions close to the wall of the channels, the average velocity of the RBCs, v_c, is higher than the average blood velocity, v = Q/A, Q being the volume flow rate and A the cross-sectional area of the tube [3]. As a result, the hematocrit (volume fraction of RBCs in the blood) at tube exit, H_d, shows an increased value in comparison with that of the cell suspension before the tube entrance, H_t: the well-known Fahraeus effect [3, 4]. In this work it was studied the velocity of red blood cells in the network of pores present in columns packed with glass spheres (using a chromatographic apparatus), as well as in fabricated transparent microchannels. These latter microdevices were done in polydimethylsiloxane (PDMS) and have characteristics similar to the developed columns packed with glass spheres. The microvisualization system used in this latter study consists of an inverted microscope (IX71; Olympus) combined with a high-speed camera (*i*-SPEED LT). The microchannel was placed on the stage of the inverted microscope and by using a syringe pump (PHD ULTRA) a pressure-driven flow was kept constant. By using this system it was possible to visualize in detail the RBCs flowing in the transparent PDMS microchannels.

Acknowledgments: This work was supported by the projects: PTDC/SAU-BEB/108728/2008, PTDC/SAU-BEB/105650/2008,

PTDC/SAU-ENB/116929/2010, founded by FCT, QREN and COMPETE

1. R. Lima, T. Ishikawa, Y. Imai, M. Takeda, S. Wada, T. Yamaguchi, "Measurement of individual red blood cell motions under high hematocrit conditions using a confocal micro-PTV system", Annals of Biomedical Engineering, Vol.37, 1546-59, 2009.
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Costas Efthimiou
Associate Professor, University of Central Florida, USA
Michael Georgiopoulos
Carla Poindexter
Joo Kim
Wanda Ortiz
&
Dennis Ahearn
University of Central Florida, USA

Physics and Chemistry ArtWork as Communicator of Research at UCF

Israel Felner
Professor, Rac Racah Institute of Physics, The Hebrew University, Israel

Sup Superconducting and Peculiar Magnetic Properties of Amorphous Carbon

The magnetic studies of commercial and synthetic amorphous carbon (a-C) powders and a-C synthesized with sulfur (a-CS) at 400°C exhibit highly magnetically inhomogeneous and irreversible scattered phenomena.

(1) Superconductivity (SC). Magnetization measurements performed on the commercial a-C powder which contains tiny amount of sulfur revealed traces of inhomogeneous SC at various temperatures up to TC= 65 K. These observations motivated us to extend the search of SC on other a-C sources, such as synthetic a-C which was synthesized by melting of pure sucrose ($C_{12}H_{22}O_{11}$). This synthetic a-C and sulfur (a-CS) were mixed and heated at 250- 400°C under protective atmosphere. The products obtained, exhibit scattered results. In one a-CS sample, traces of a SC phase at TC= 17 K was observed. Other samples (from the same a-CS batches) exhibit pronounced peaks around 50-55 K in their zero-field-cooled (ZFC) curves (Fig. 1). The rest did not show any significant magnetic features. Although the superconducting volume fraction in all cases is very low, our results prove the necessity of sulfur for inducing SC in a-CS, and open new pathways to achieve high temperature SC in this unique system of a-C based materials.[1-2]

(2) Magnetism. The procedure exhibited in Fig. 1 is as follows: The first ZFC(i) (in black) and field-cooled via cooling (FCC(i)) (in red) branches were recorded up to 120 K. Immediately after, the second ZFC(ii) (in green) and FCC(ii) (in blue) branches were measured under the same conditions. Unexpectedly, (i) in the first run, around the peak at ~ 50 K, the ZFC(i) branch is much higher than the FCC one, thus at a certain temperature range ZFC(i)>FCC(i). (ii) In the second run, the peak observed in ZFC(i) is totally suppressed (see the ZFC(ii) curve), whereas the two FCC(i+ii) curves coincide which each other. These peculiar observations are unique and to the best of our knowledge were not observed in the past. We eliminate impurities (such as magnetite and/or oxygen) as the origin of the measured properties and believe that they are intrinsic properties of the a-CS materials. We are not aware of any existing theoretical models that would be able to explain these two magnetic phenomena described here.

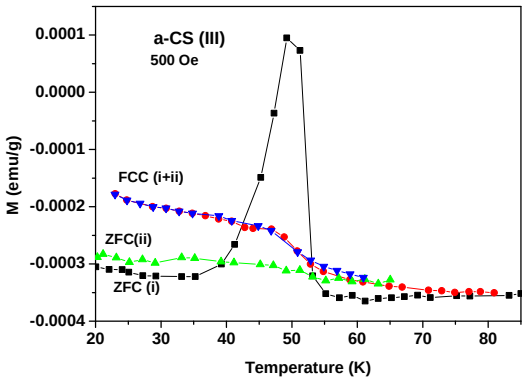

Fig. 1 Two ZFC and FC runs of a-CS measured at 500 Oe.

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Jamal Hassan
Assistant Professor, Khalifa University of Science, UAE
&
Ahmad Al Nabulsib
Instructor, Khalifa University of Science, UAE

Teaching NMR Product Operator Formalism with MATLAB Software

The classical Nuclear Magnetic Resonance (NMR) vector model is known to be very effective and useful in teaching basic NMR 1D experiments such as spin echo. Many instructors still using it effectively to interpret the effect of Radio frequency (RF) magnetic filed and chemical shift on spin ½ nuclei.

On the other hand, for more complicated spin systems that require 2D or higher dimensional NMR experiments density matrix calculation is often used. This method is known to be very complicated and not easy to follow after couple steps. Students usually get lost within calculation and loose the physical meaning of the NMR system under investigation.

As a compromise, another methodology has been developed which depends on the spin angular momentum operators. This is known as Product Operator Formalism in NMR. We have created a Graphical User Interface (GUI) using MATLAB software that is capable of calculating product operator of one, two and three weakly coupled ½ spin systems. The effect of RF pulse, J-coupling, chemical shift between NMR pulses on the spin system is easily calculated using this GUI.

The user need to identify which experiment need to be studied, such as INEPT, DEPT or any other NMR experiment , then to specify the starting magnetization (normally the Z-component) such as I1Z or/and I2Z (I1 and I2 refer to the two spin system under investigation). Then clicking on the appropriate button (such as 90 pulse, J-coupling,…etc) on the GUI, the result is presented on the screen. These can be continued according to the sequence of the NMR pulse sequences under study.

We believe the obtained GUI is an effective teaching tool for new students in NMR and will help them better understand and interpret complicated NMR pulse sequences applied on up to three weakly coupled ½ spin systems.

Maged Henary
Assistant Professor, Georgia State University, USA

Synthesis of Zwitterionic Fluorescent NIR Dyes for Bioimaging Applications

Two fundamental unsolved problems in optical imaging are the nonspecific uptake of near-infrared (NIR) fluorophores by normal tissues and organs, and the incomplete elimination of unbound targeted fluorophores from the body. Novel zwitterionic NIR fluorophores having net charges of -4, -2, 0, +2, and +4 were synthesized and their performance as a function of charge distribution, hydrophilicity/ lipophilicity and receptor-based targeting for image-guided surgery were evaluated in comparison to known compounds.[1] These zwitterionic NIR fluorophores have ideal optical properties, including emission at about 700 nm and 800 nm, elevated extinction coefficients, and high quantum yields in serum. NIR fluorophores were injected intravenously into mice and rats, and their bio-distribution and clearance were measured.[1]

References

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Canan Karaalioglu
Assistant Professor, Pace University, USA

Detection of Illicit Drugs and Explosives by THz Spectroscopy

Terahertz wave is the electromagnetic radiation in a frequency interval from 0.1 – 10 THz. The demand for more secure and robust techniques in safety is pushing demands for security systems into these frequencies since the neighboring regions (microwave and infrared) have already been filled and well developed with many applications. THz research has mainly focused on two fields: sensing and communications. There has been a dramatic increase in interest of implementation of THz spectroscopy and imaging techniques for security applications as well as spectrum analysis over the past 10-15 years. There have been studies to utilize THz radiation to identify concealed weapons, to detect suicide bombers and biological threats, to screen passengers, to detect and identify illicit drugs or other prohibited and/or dangerous chemicals. The three major points which make THz field very attractive for homeland security and social safety are: First of all, THz radiation can detect concealed weapons and illicit drugs since THz radiation can penetrate many non-metallic, non-polar materials, which make them transparent to THz radiation. Secondly, illicit drugs and explosives have very unique spectra in the THz region, which help us to identify them easily. Finally, last but not least, THz radiation poses no health risk for scanning of people since THz radiation has low photon energy in comparison with x-rays, which make them potentially more suitable for people screening.

Real-world street "samples" are contaminated by adding dilutents, adulterants, and impurities, which complicate the spectral analysis. Fortunately, the added impurities are often crystalline organic materials, such as caffeine or lactose, which have their own unique spectral features in THz range. This contamination issue is valid in analyzing of explosives as well. However, since most of nonexplosive components of these impurities are transparent to THz radiation, spectral analysis of plastic explosives are simpler than the drug mixtures.

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&
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Lab Chief and Senior Investigator, Section on Cellular Signaling, National Institute of Child Health and Human Development, National Institutes of Health, USA

Deciphering the Kinetic and Gating Properties of P2X7 Receptor Channels

ATP-gated purinergic P2X7 receptors (P2X7Rs) are trimeric channels with three binding sites for ATP. These receptors are involved in cell differentiation, proliferation and apoptosis. In our previous work, we showed, using biophysical and computational approaches, that the same receptor can mediate such opposing effects. In fact, we demonstrated that they are capable of exhibiting both pore dilation (leading to the formation of biphasic currents) and desensitization (manifested as a decline in current amplitude) during agonist activation, particularly at high ATP concentrations. This was done in part by developing a 12-state Markov model consisting of naïve, sensitized and desensitized states that reproduced all the whole-cell current recordings generated experimentally. In this model, we assumed that the occupancy of one or two ATP-binding sites of naïve receptors favored a slow transition to desensitized states which was calcium-independent, whereas the occupancy of the third binding site favored a transition to sensitized/dilated states. Our goal here is to extend this modeling study to show how these two gating patters interact when cells expressing P2X7Rs are bathed in mediums containing large cations, e.g. N-methyl-D-glucamine (NMDG+). We illustrate the various current recordings produced under such ionic conditions and determine why the shift in reversal potential and the dilation of the channels are accompanied paradoxically by a decrease in the total conductance during voltage ramp protocols. The model adds more evidence to our previous hypothesis suggesting that dilation is masking desensitization These results are expected to eventually elucidate the role of P2X7Rs as cytolytic and apoptotic receptors, as well as decipher their function in controlling sustained cellular responses, including cell growth and proliferation.

Dukjoon Kim
Professor, Sungkyunkwan University, South Korea

Proton Conducting Electrolyte Membranes based on the Pendant-sulfonated Poly(arylene ether ketone)/polyorganosiloxane Interpenetrating Polymer Networks

An organosiloxane polymer network (OSPN) was pre-synthesized from 3-glycidyloxypropyltrimethoxysilane and 1-hydroxyethane-1,1-diphosphonicacid, and a pendant-sulfonated poly(arylene ether ketone) (PSPAEK) from the intermediate containing carboxylic acid. Proton-conducting polymer electrolyte membranes were prepared in semi-interpenetrating polymer network (semi-IPN) form from PSPAEK and OSPN. The prepared membranes exhibited superior proton conductivity but similar methanol permeability to the pristine PSPAEK. The water uptake increased only to 64 % as the OSPN content was increased to 50%, even at 80^{o}C. The single direct methanol fuel cell (DMFC) performance based on the semi-IPN membrane possessing 50 wt% OSPN showed an excellent power density of 70 mW cm^{-2}. The chemical and morphological structures of the synthesized membranes were characterized using Fourier transform infrared (FTIR) spectroscopy and small angle X-ray scattering (SAXS) and their results were correlated with the essential membrane properties such as water uptake, proton conductivity, and methanol permeability. The thermal and mechanical stabilities were also investigated using thermogravimetric analysis (TGA) and a universal tensile machine (UTM).

Yoshio Kobayashi
Professor, Ibaraki University, Japan
Kohsuke Gonda
Associate Professor, Tohoku University, Japan
&
Noriaki Ohuchi
Professor, Tohoku University, Japan

Imaging Processes Using Core-Shell Particle Colloid Solutions for Medical Diagnosis

Contrast agents improve performance of imaging processes using X-ray, magnetic resonance and fluorescence in medical diagnosis. Various contrast agents are commercially available, and typical commercial contrast agents are solutions containing iodine compounds for X-ray imaging, Gd complexes for magnetic resonance imaging (MRI) and Cd compound nanoparticles (QD) for fluorescence imaging at molecular or nanometer levels. Metallic Au nanoparticles can also reveal X-ray imaging ability. These contrast agents are not strongly dragged in fluid because of their small sizes. Consequently, they cannot stay in living bodies for a long period, which provides difficulty taking steady images. Formation of particles of the contrast agents and an increase in apparent particle size are promising solutions to the problem, because of their projected area larger than molecules or nanoparticles, and consequently their residence time will increase. In addition, the contrast agents may cause adverse reactions derived from iodine, metallic Au, Gd ions, and Cd. Coating of the particles with shell inert to living bodies is a candidate for controlling the adverse reactions, since the particles cannot contact with living bodies. Our research group has recently studied on development of methods for preparing colloid solutions of core-shell particles composed of core of materials with imaging ability and shell of silica that is inert to living bodies, and on their imaging properties. The methods used are based on hydrolysis and condensation of silicone alkoxide in the presence of particles such as iodine compound nanoparticless prepared by mixing $AgClO_4$ aqueous solution with KI aqueous solution, metallic Au nanoparticles prepared by reducing $HAuCl_4$ with citrate, Gd compound nanoprticles prepared with a homogeneous precipitation method and commercially-available QD. The particle colloid solutions prepared revealed imaging abilities worthy of note. In the present contribution, we introduce our recent studies on them.

Georgios Lefkidis
Lecturer, University of Kaiserslautern, Germany
&
W. Hubner
Lecturer, University of Kaiserslautern, Germany

Coherent Laser-Induced Manipulation of Magnetism on Molecular Systems

After the discovery of laser-induced demagnetization [1] the optical manipulation of the magnetic state of materials has become an increasing field of research. In this talk first a brief report of some advances will be given in which the concept of the lambda process as a mechanism for coherent light-induced magnetization dynamics [2,3] and its logic functionalization [4] will be explained. A discussion pertinent to the design of magnetic structures (including some experimental aspects) that can actively serve this purpose will follow [5]. Finally some emphasis will be given on the structural aspects of the most successful nanostructures as well as their electronic-level scheme [6]. The role of intrinsic properties (e.g. correlations) and degrees of freedom (e.g. phonons), along with externally tunable parameters (e.g. temperature and laser chirp) will also be addressed. It will be thus shown that theoretical calculations have the power to not only reveal microscopic mechanisms behind the interaction between light and magnetic nanostructures but also to actively accompany the design of magnetic logic applications and pave the way to new concepts of modern IT and spintronics technology.

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Prophylaxis and Treatment of Generalyzed Infection Induced by Methicillin-Resistant Staphylococcus Aureus (MRSA) in Vivo with Hypothalamic Proline Rich Peptides Galarmin and d-15 Galarmin

Epidemiological data indicate that Staphylococcus aureus and particularly methicillin-resistant strains of S.aureus (MRSA) are responsible for the majority of complicated cases of Staphylococcus infections and are increasingly implicated as a cause of nosocomial and community associated infections worldwide. Proline-rich peptides (Galarmin and analogues) are new brain cytokines isolated from neurosecretory granules of hypothalamus by Prof. A. Galoyan and coworkers with a broad-spectrum of biological activities including antibacterial, antitumor, and immunomodulatory properties. This allowed us to conclude that Galarmin and its analogues can be efficient against generalyzed infection induced by MRSA on mice model in vivo.

Received data indicate that Galarmin and its analogue d-15 Galarmin are strong remedies for the prophylaxis and treatment of MRSA infection in vivo. Galarmin at the concentration of 1 μg/mice express its highest protective effect for the prophylaxis (administration 24h before infection) and treatment (1h post-infection) by increasing the survival of experimental animals up to 100% over the control (non-treated) group. For the parallel administration more efficient are higher concentrations of Galarmin: 5 and 10 μg, which increase the survival of animals by 50-60%. In that case the absence of bacterial growth from the blood of treated animals was observed. The most efficient protective concentration of d-15 Galarmin is 16 μg administrated 8h before the infection which increase the survival of infected animals by 80%.

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3D Pixel Sensors for Diffractive HEP Experiments

Pixel detectors with cylindrical electrodes that penetrate the silicon substrate (so called 3D detectors) offer advantages over standard planar sensors in terms of radiation hardness, since the electrode distance is decoupled from the bulk thickness. In the framework of the ATLAS Forward Physics (AFP) program, work has been carried out to study the suitability of 3D pixel devices for forward proton tracking. Minimal dead area and high efficiency after inhomogeneous irradiation are critical requirements the AFP. Recent results of the characterization and beam test studies of in-homogeneously irradiated 3D pixel devices will be presented together with electrical measurements of slim edged sensors.

Two 3D CNM devices were irradiated non-uniformly at CERN PS up to fluencies of 9×1015 neq./cm2 in 2012. The devices were characterized in the IFAE laboratory before being subjected to beam tests at CERN SPS H6 line. The electrical characterization and the hit reconstruction efficiency studies will be presented.

At the same time a project to reduce the dead area of the 3D sensors was carried out using the SCP (Scribe Cleave Passivate) technique. The electrical characterization of these non-irradiated devices with slim edges for AFP will also be presented.

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Roman Spectroscopy, and DTA studies B2O3 Additions on the Microstructure in P2O5-B203-Fe2O3 Glasses

The glass samples have been prepared by melting at 1100°C and rapidly cooling at room temperature.

Glasses in the system (90-x) P_2O_5+xB_2O_3+10Fe_2O_3 (x = 0 mol. %, 10 mol. %, 20 mol. %, 30 mol. %, 40 mol.%) were prepared and characterized by measuring their density (ρ).

All of these values were found to vary with the B_2O_3 content of the glasses. The glass transition temperature (Tg) system have been determined from the change of the line in the DTA chart. The Raman confirmed these structural changes. The investigation led to the conclusions that boron was mainly present in BO_4 environments and that B-O-P bonds were present in the ternary glasses. Absorption peaks occur due to the vibrational mode of the borate network in these glasses. The vibrational modes of the borate network are seen to be mainly due to the asymmetric stretching relaxation of the B–O bond of trigonal BO_3 units.

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Disorder and Correlations in One Dimension using Nonchiral Bosonization

An alternative to the conventional bosonization in 1D that uses chiral right and left movers is presented which is ideally suited to study problems involving correlated fermions where translational symmetry is lacking. Examples include the Kane-Fisher problem (Luttinger liquid with an impurity), resonant tunneling in Luttinger liquids (LL), mobile impurities in LL, ladder systems and so on. An earlier work provided a closed formula for the full Green function of the Kane-Fisher problem (to be published in Annals of Physics). Here we address the next question of two impurities and the consequent exponents related to resonant tunneling. The formalism is developed in sufficient generality to enable a straightforward application to the other problems mentioned.

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Ampere's Law Operating in O, B and A Stars

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Multidisciplinary Reactor Safety Studies: Application of First Principles Calculation

Traditionally nuclear reactor safety course includes predominantly reactor physics component. However real nuclear accidents (like for example the recent in Fukushima) demonstrate that a nuclear accident should be viewed using interdisciplinary tools.

The fuel melting for example occurs not only because of enhanced neutron flux but also because of the degradation of thermal conductivity of fuel when fuel oxidation takes place [1]. In another studies [2] it was shown that in order to account for the observed fission product releases after completion of clad oxidation, it was necessary to assume a greater atmospheric exchange due to possible cracking of the brittle oxide layer. The detailed calculations that were presented before [1,2] will be reviewed and a summary suitable for a multidisciplinary audience will be provided.

Next we will present application of first principles calculations to evaluate structural, mechanical and thermal properties of traditional nuclear fuel like urania and new, inherently safer thoria fuel. The application of density functional theory (DFT) to assess changes in the properties of urania (UO_2) when it is oxidized to U_3O_8 during a severe nuclear accident scenario will be presented. Knowledge of the lattice constants for higher oxidation state oxides of uranium is important in nuclear safety analysis, since the formation of U_3O_8 in a defective fuel element can cause cracking or split the fuel sheath after disposal, because there is a net 32-36% volume increase when UO_2 is transformed into U_3O_8. This is in contrast to thoria fuel where such oxidation does not take place during accident. Additionally we will demonstrate from first principles calculations that the thermal expansion of thoria is lower than urania even for very high temperatures for which there are no experimental data. The comparison between these two fuels will be provided with respect to reactors safety.

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A Role of Texture and Grain Boundary Structure in Controlling Oxidation, Hydrogen Ingress and Fracture in Materials Used by Nuclear Industry

Rate of deterioration of properties of nuclear materials in service can be lowered if we better understand a role of microstructure in control of the processes of corrosion, oxidation and fracture.

Examples are discussed to illustrate and simulate a development of oxide structure and texture in nickel and Zr-Nb alloys. Models of oxygen transport were proposed to explain the oxidation kinetics. These models incorporate a role of the substrate orientation, state of stress in oxide, nucleation condition and differences in surface free energy and allow predicting the microstructure, texture and grain boundary character distribution. Simulated microstructure was used to predict the oxidation kinetics that agrees with the experimental data. Hydrogen permeation through different oxide structure was evaluated and a correlation between strength of monoclinic Zr oxide texture and rate of hydrogen ingress was established. TEM investigations allow identifying and describing structure of monoclinic oxide that may be considered as an effective barrier against hydrogen ingress.

Research on oxidation of nickel and nickel based alloys allow developing methods that will allow improving the oxidation resistance at high temperature by order of magnitudes. The method proposed is based on surface texturing and application of reactive element coatings. Oxidation of steels, oxide removal and descaling processes were described based on detailed investigations of the phase composition, microstructure, texture and the state of stress in wustite, magnetite and hematite. Finite element simulation of oxide under stress allows us to develop a model of rescaling in low carbon steel.

Corrosion and oxidation process is initiated predominantly at interfaces and grain boundaries having high energy. In materials like nickel based intermetallics and nickel and its alloys the intergranular fracture predominates. Concepts of grain boundary engineering can be used to increase the percentage of certain CSL boundaries and arrest the crack that nucleated and starts to propagate through the structure. Computer model of crack propagation and crack arrest in polycrystalline materials was developed based on Markow statistical model and calculated energy and stress strain curves of various type of

boundaries in metals. Molecular Dynamics EAM method was used to calculate properties of grain boundaries under stress.

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Structural, Energetic and Optical Properties of Small Binary Silver-gold Clusters

The structural, energetic and optical properties of small binary silver-gold clusters Ag_nAu_m (with n+m=8) have been systematically investigated using *ab. initio* method. The structural and energetic properties of the ground-state are calculated within the framework of DFT using SIESTA code and the optical properties within the framework of TD-DFT using OCTOPUS code.

By substitution of Ag and Au atoms, in the optimized lowest energy structures of pure gold and silver clusters, we determine the ground state conformations of the bimetallic silver–gold ones. The results show that the ground state optimal structures are planar when the number of silver atoms is less than three. Their properties are intermediate between those of pure silver and pure gold clusters. The binding energy and the ionization potential increase with the number of Au atoms.

The analysis of the calculated absorption spectra shows that the incorporation of Au atoms induces a widening of the transitions and a reduction of the absorption spectrum intensity. In the 1.5-6 eV energy range, the number of transitions in clusters with an odd number of gold atoms is greater than in clusters with an even number. Furthermore, the intensity of transitions is more important in clusters having an even number of Au atoms.

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Physical and Chemical Characteristics of Reactive-Wetting at Room Temperature

We report on physical and chemical characteristics of reactive-wetting at room temperature. Specifically, we present non-trivial spatio-temporal patterns observed in reactive-wetting of mercury droplets spreading on thin metal (silver or gold) films at room temperature. This is the only known study of reactive-wetting at room temperature. We show that there exist two main regimes, the bulk propagation regime and the interface kinetic roughening regime. In both regimes, rich spatio-temporal patterns are observed. We study and characterize these patterns using statistical physics tools, such as the growth, roughness and persistence exponents, as well as DLA where observed, and analyze the chemical composition of these patterns.

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The Lack of True Understanding in Science Education Today: Reasons, Consequences and Answers

The purpose of this investigative study was to examine the different reasons contributing to the lack of true understanding in science education and in general education. The reasons have been categorized into three types:

1. Those due to parents
2. Those due to educators
3. Those due to students

Ultimately,parents and educators are primarily responsible for students that feel lazy about learning. Laziness arises from a culture that teaches students instant gratification from an early age. Thus, the effect of culture and more recently,globalization,on the lack of true understanding in science education cannot be ignored, and this is apparent when examining the results of international test competitions in recent decades.

Which countries score high and which score low? Why? The modern dream of life does not help the world to become truly educated. Last year, according to Joy Resmovits, a Huffington Post education reporter,"Across the board, East Asian countries occupied the upper ranks in the comparison of more than 60 world education systems, far outperforming the United States….U.S. SecretaryofEducation Arne Duncancalled theU.S.scores encouraging, butdescribed older students' performance *as* 'unacceptable'."The trend holds true across several exams.

There is an urgent need in our challenging times to rediscover Pythagorean thought. As educators, parents and students,we all need to become members of the Pythagorean School. Science needs to be taught by truly embracing logic andethics. Introspection and silence need to be honored, abundantly exercised, and given much more attention in our schools again if we want to see a safer world tomorrow.

In this study, students from different cultures and backgrounds are allowed to express their opinions in essays about today's educational system.Specific examples from chemistry teaching will be presented that demonstrate how desire for instant gratification leads authors of science textbooks tomake inaccurate simplifications and generalizations.

Most importantly, this presentation not only states problems and suggests solutions to the present challenges in educational reform, but it also shows many different approaches that we have already practiced on our campus and in our teaching. It shows the results that have been achieved so far as examples to be followed by other educators and students. The approaches for educational reform can be followed with almost no financial support; only a strong desire for true educational reform is needed.

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Teaching Green Chemistry Principles to Undergraduate Students

The environment is affected by the actions of mankind in multitudinous ways, many of which are detrimental, giving rise to pollution and toxic waste, ultimately making our planet less inhabitable. While we can remediate, regulate, phase out or ban, substitute and incorporate plans that prevent pollution and toxic waste, there is also a need to change the behavior of future generations of consumers and producers of new products. Future chemists and innovators are charged with the responsibility of developing new chemical processes and products that not only meet the needs of energy, clean water and food to sustain our growing population, but also protect human health and the environment. Green Chemistry is a revolution in the design of molecules that provides new opportunities for economic development while considering the impact on health and the environment. Green Chemistry utilizes a set of guiding principles, originally provided by Paul Anastas and John Warner (Green Chemistry: Theory and Practice, 1998), aimed at decreasing/removing the use/generation of hazardous substances in the design, manufacture and application of products. Key differences from traditional approaches are that Green Chemistry considers: (i) function along with the impact on health and environment, (ii) safety and hence hazard reduction, (iii) the whole life cycle of the product (*i.e.* from cradle to grave and then back to cradle again) and (iv) *chemistry as providing the solution* and not the problem.

To help improve the creative and innovative thinking behind Green Chemistry, it is important to expose chemistry students to these principles at the undergraduate level. While suitable Green Chemistry experiments are known, successful implementation requires running test trials and performing additional basic research. We have embarked upon the testing and further design of experiments for implementation into an undergraduate laboratory course and will report our experiences in this endeavor.

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Coherent States for Photons in Time Varying Dielectric Media

In this atudy we discussed the coherent states of photons in a time varying media. First, the quantum fluctations of photon is reduced to harmonic oscillator with time varying mass and frequency. Second, the coherent states are discussed and uncertainties of electric and magnetic field are evaluated for the system.

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Applications of GUMBOS in Chemistry/Materials Science

My research group has been exploring the analytical applications of room-temperature ionic liquids (RTILs) for several years. Recently, we haveextended the range of these materials to include analytical applications of similar solid phase materials, i.e. organic salts with melting points ofsolid ionic liquids (25 °C to 100 °C) and up to melting points of 250 °C. To contrastthese new solid phase materials with RTILs, we have created the acronym, GUMBOS(*G*roup of *U*niform *M*aterials *B*ased on *O*rganic *S*alts). These GUMBOShave the tunable properties frequently associated with RTILs, including tunablesolubility, melting point, viscosity, thermal stability, and functionality. Thus, when taken in aggregate, these properties allow the production of solid phase materials which have a wide range of applications in chemistry and materials science. In this talk, I will highlight the applications of GUMBOS which we have recently explored forchemistry and materials science, including GUMBOS as sensors, imaging agents, stimuli-responsive materials, and for production of nanoGUMBOS. In regard to nanoGUMBOS, we believe that our methodology represents an extremely useful approach to production ofnanomaterials since our materials are designed and assembled for specific uses, rather than adapted for use as is often done for manynanomaterials. Selectedapplications, including sensor applications,will be highlighted in this talk. Particular emphasis will be placed on biomedical applications of nanoGUMBOS.

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Relationship between Electrochemical Electron Transfer Rate Constant and Single Molecule Conductance

The ability of molecules to transmit charge can be probed experimentally by measuring unimolecular charge-transfer rate constants, standard electrochemical rate constants, and molecular conductances. In unimolecular charge-transfer, charge moves between discrete electronic states of the molecular donor and acceptor. In electrochemical charge-transfer, charge flows between discrete electronic state(s) of a molecular donor/acceptor and a high density of electrode states. In molecular conductance measurements the molecular bridge links two electrodes, each with a large density of electronic states, and one must account for transfer over a range of energies. If the applied bias potential is not large enough to alter the electronic structure of the molecular bridge, one expects that the (near zero-bias) molecular conductance, the electrochemical rate constant, and the unimolecular charge-transfer rates of a molecule will be closely related.

Here we report our conclusions on the correlation between the molecular conductance, as measured in scanning tunneling microscope-controlled break junction (STM-BJ) experiments, and the standard electrochemical rate constant, across the same molecules in electroactive self-assembled monolayer films, for several types of molecules: alkanes and DNA oligomers, which were previously characterized by others, and peptide nucleic acids (PNA) oligomers. The correlation is examined as a function of (i) the molecular length, (ii) the molecular sequence in

nucleic acid oligomers, and (iii) the charge transport mechanism (superexchange and hopping).

Although simple models predict a linear correlation between the molecular conductance and the charge-transfer rates, the experimental data show a power-law relationship within a specific class of structures. Furthermore, we show that the rate-conductance correlation can break down entirely when comparing data for different chemical species. The experimental observations are rationalized by accounting for differences in the energy barrier heights for charge transport and the differing amounts of bath-induced electronic decoherence for the molecules that arise in the STM-BJ and electrochemistry experiments.

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Magnetoresistance Oscillations and Field-induced Enhancement of Superconductivity in Granular YBa2Cu3O7-δ Nano Wires

Magneto-transport measurements in $YBa_2Cu_3O_{7-\delta}$ nano-wires, comprising a single layer of small number of grains, reveal periodic magnetoresistance oscillations in a wide temperature range below the transition. The rich structure of these oscillations manifests a negative magnetoresistance in the initial part of each cycle beginning at zero magnetic field. The salient features of these unique oscillations indicate the presence of π Josephson junctions in the granular wires, arising from the d-wave pairing symmetry in $YBa_2Cu_3O_{7-\delta}$.

Gustavo Zampier dos Santos Lima
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Multifractality in Domain Wall Dynamics of a Ferromagnetic Film

We investigate the multifractal properties in the dynamics of domain walls of a ferromagnetic film. We apply the Multifractal Detrended Fluctuation Analysis method in experimental Barkhausen noise time series measured in a 1000-nm -thick Permalloy film under different driving magnetic field frequencies , and calculate the fluctuation function Fq(s), generalized Hurst exponent h(q), multifractal scaling exponent τ(q), and the multifractal spectrum f(α). Based on this procedure, we provide experimental evidence of multifractality in the dynamics of domain walls in ferromagnetic films and identify a rich and strong multifractal behavior, revealed by the changes of the scaling properties of over the entire Barkhausen noise signal, independently of the driving magnetic field rate employed in the experiment.

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Six-Qubit matrix Calculation from Incomplete Measurement

Since Candes, Donoho, and Tao proposed compressive sensing (CS) in 2005, it has been applied in many fields for classical signals, such as medical CT imagining, radar imaging and recently to quantum state tomography, and so on. In this paper, we apply the CS theory to the experiment of 6 photon system. The 6 photon density matrix is recovered through a few measurements using a priori knowledge. The fidelity of the system calculated from the recovered density matrix in terms of CS is in agreement very well with the result by the usual calculation. Furthermore, the results show that much fewer measurements are enough to obtain high fidelity comparable with the standard quantum tomography. Furthermore the expectation values of entanglement witness for the 6-system are also calculated through the density matrix. This result turns out that the compressive sensing theory can be applied to multi-photon entangling system to reduce the measurements in great deal. Therefore, even usually the CS theory works for classically incoherent signals, but as the same as in other works, in this example it has a great potential to predict some new entries based on a small number of real measurements.