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5th Szeged International Workshop on Advances in Nanoscience

24-27 • October • 2012
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BOOK OF ABSTRACTS
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siwan5 5th Szeged International Workshop on Advances in Nanoscience
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PROGRAMME

BOOK OF ABSTRACTS

5th Szeged International Workshop on Advances in Nanoscience

SIWAN5

24–27 October 2012, Szeged, Hungary

Hunguest Hotel Forrás****
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FOREWORD

It is a great pleasure for us to offer you this Book of Abstracts for the 5th Szeged International Workshop on Advances in Nanoscience 2012 (SIWAN5). SIWAN was called to life in 2003 when we realized that the booming nanotechnology field was not represented adequately in the Hungarian conference scene. Our goal was to create a platform that introduces the newest results of internationally recognized experts to local students and colleagues and simultaneously displays relevant Hungarian achievements to the world. The positive feedback of the community encouraged us to proceed and transform a single event into a workshop series.

Now SIWAN5 is honored by the presence of over 180 colleagues from 30 countries spanning from the USA to Japan, South Korea to the UK and Finland to Azerbaijan. Seven keynote lectures, 60 oral presentations and 109 posters are in the program. We stayed true to the original SIWAN concept and accepted contributions from all fields of nanoscience and nanotechnology to promote multidisciplinary discussions. The focal points of the conference emerged spontaneously from the submitted abstracts: energy applications, carbonaceous materials and the interactions of nanoparticles with biological systems. Further fields of interest include e.g. new nanomaterials, nanocomposites as well as spectroscopic and theoretical developments.

This is the first time when SIWAN is organized as a regular conference with a registration cost. However, it is also the first time when we can offer free publishing of all peer-reviewed proceedings in the open access journal *Nanopages* (ISSN: 1788-0718) and provide the participants with all the commodities of a world-class conference. Moreover, SIWAN5 is attended by three times as many researchers as the previous event. Therefore, we hope that getting first-hand access to so many new results, establishing new connections and enjoying the famous Szeged ambience will make you feel that your resources were spent well on SIWAN.

Our warmest thanks go to all plenary and invited speakers, authors and contributors of SIWAN5 for accepting our invitation, visiting Szeged and using SIWAN as a medium for communicating your research results! We hope that you will enjoy the conference and look forward to meeting you again in one of the forthcoming SIWAN events!

Szeged, 9th October 2012

Kukovecz

Dr. Zoltán Kónya
Conference Chair

Dr. Ákos Kukovecz
Conference Vice-Chair

Acknowledgements

SIWAN is the joint effort of many individuals and organizations. First and foremost, we are indebted to our mentor and friend, the late Prof. Imre Kiricsi who initiated the SIWAN series a decade ago. We thank the Hungarian nanoscience community, in particular Profs. Katalin Kamarás, Imre Dékány and László P. Biró for their continuous support of SIWAN. Thanks are also due to our colleagues at the Department of Applied and Environmental Chemistry of the University of Szeged for their assistance in numerous practical issues and to the staff of the Akadémiai Kiadó (Erna Sári and Balázs Réffy) for their faith and dedication to SIWAN.

SIWAN5 is the dedicated dissemination event of the projects in which our research groups are involved today. All of the following projects have provided support to the conference.

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PROGRAMME

24TH OCTOBER 2012, WEDNESDAY

12.00–14.00 *Registration*

14.00–14.20 **Opening Ceremony**

14.20–15.20 **KEYNOTE LECTURE**

Novel nanocarbons: Defective graphenes, nanoribbons with atomically smooth edges and graphene-nanotube hybrid structures (K3)
Mauricio Terrones, The Pennsylvania State University, Pennsylvania, USA; Shinshu University, Japan

SESSION A

15.20–15.40 **On the equilibrium of nano-systems (O40)**
George Kaptay, Bay Zoltán Non-profit Ltd; University of Miskolc, Hungary

15.40–16.00 **Diameter control and one-dimensional N2 gas inside single-walled carbon nanotubes (O11)**
Christian Kramberger, University of Vienna, Austria

16.00–16.20 **Design of semiconductor nanostructured materials using theory (O10)**
Vladan Mlinar, Brown University, USA

16.20–17.00 *Coffee break*

17.00–17.20 **Quasi 2-dimensional actin models: Is the bundling irreversible? (O47)**
Tamás Haraszti, Max-Planck Institute for Intelligent Systems, University of Heidelberg, Germany

17.20–17.40 **Enhanced light harvesting of Si solar cell via luminescent down-shifting using YVO_4 nanophosphors (O17)**
Kien Wen Sun, National Chiao Tung University, Taiwan

17.40–18.00 **Application of nanostructuring techniques for fabrication of getters for mems (O01)**
Anton Boyko, National Research University of Electronic Technology, Russia

18.00–18.20 **Plasmon resonance frequencies and damping rates as a function of size of gold nanospheres (O43)**
Krystyna Kolwas, Institute of Physics, Polish Academy of Sciences, Poland

18.20-18.40 **MP-SPR – A new optical characterization method for ultrathin films (O33)**
Walis Jones, BioNavis Ltd., UK

SESSION B

15.20–15.40 **Luminescent silicon carbide quantum dots prepared by reactive bonding and subsequent wet chemical etching: Characterization and potential applications (O30)**
Dávid Beke, Wigner Research Centre for Physics, Hungary

15.40–16.00 **Surface modification of aerosol nanoparticles for materials applications (O51)**
Jeffrey Thomas Roberts, Purdue University, USA

16.00–16.20 **Universal approach to covalent immobilization of silver nanoparticles on solid substrates (O55)**
Jana Soukupova, Regional Centre of Advanced Technologies and Materials, Czech Republic

16.20–17.00 *Coffee break*

17.00–17.40 **KEYNOTE LECTURE**
Iron, copper and bismuth do not belong to royalty; however, when stabilized and nanostructurated, they become highly prized (K2)
David Díaz, National Autonomous University of Mexico, Mexico

17.40–18.00 **Iron-cobalt nanocrystalline alloy supported on a cubic mesostructured silica matrix (SBA-16): Synthesis and structural characterization (O26)**
Daniela Carta, University of Cagliari, Italy

18.00–18.20 **The study of the inversion degree in zinc ferrite nanocrystals dispersed on a highly porous silica aerogel matrix (O49)**
Anna Corrias, University of Cagliari, Italy

18.20–18.40 **Nitrogen-containing CMK-3 carbon nanorods with different length as efficient cathode for oxygen reduction reaction (O60)**
Jong-Sung Yu, Korea University, Republic of Korea

19.00–21.00 *Welcome Reception*

25TH OCTOBER 2012, THURSDAY

09.00–10.00 **KEYNOTE LECTURE**
Advances in understanding the chemistry of graphene and carbon nanotubes: Fundamentals and applications (K1)
Michael S. Strano, Massachusetts Institute of Technology, USA

SESSION A

10.00–10.40 **KEYNOTE LECTURE**
Toxicology perspectives of nanomedicines (K7)
Marianna Foldvari, University of Waterloo, Canada

10.40–11.20 *Coffee break*

11.20–11.40 **Molecular plasmonics – Biomolecules meets the colourful world of nanoparticles (O32)**
Andrea Csáki, Institute of Photonic Technology, Germany

11.40–12.00 **Functionalization of multi-wall carbon nanotubes with a bio-inspired hydrogenase mimic for hydrogen evolution and uptake (O22)**
Bruno Jousselme, CEA Saclay, France

12.00–12.20 **Laser-based synthesis of multimaterial nanocomposites for medical and optical applications (O29)**
Csaba László Sajti, Laser Zentrum Hannover, Germany

12.20–12.40	**Supramolecular directed assemblies of biotemplated metal/semiconductor nanohybrids (O50)** *Anil Kumar,* Indian Institute of Technology Roorkee, India
12.40–13.00	**Plasmonic nanoparticles for photocatalysis and biomedical applications (O44)** *Imre Dékány,* University of Szeged, Hungary

SESSION B

10.00–10.20	**Unravelling the correlated electronic and optical properties of tailored low dimensional carbon hybrids (O56)** *Thomas Pichler,* University of Vienna, Austria
10.20–10.40	**Photocurrent from planar strips of multi wall carbon nanotubes (O42)** *Valentina Grossi,* University of L'Aquila, Italy
10.40–11.20	*Coffee break*
11.20–11.40	**Grain boundaries and nanoripples in CVD grown graphene (O23)** *László P. Bíró,* Institute of Technical Physics and Materials Science; Korean-Hungarian Joint Laboratory for Nanosciences, Hungary
11.40–12.00	**Infrared signatures of correlation in expanded fullerides (O25)** *Gyöngyi Klupp,* Wigner Research Centre for Physics, Hungary
12.00–12.20	**Optical spectroscopy of 'soluble' nanocarbon: Nanodiamond and graphene oxide (O41)** *Vitaly Korepanov,* National Chiao Tung University, Taiwan
12.20–12.40	**Electronic transport in intermediate sized multiwalled carbon nanotubes (O15)** *Markus Ahlskog,* University of Jyväskylä, Finland
12.40–13.00	**Time resolved optical measurements on different architectures of carbon nanotubes as a basis of new photovoltaic devices (O54)** *Gianluca Galimberti,* Università Cattolica del Sacro Cuore, Italy
13.00–14.40	*Lunch*

14.40–15.40 **KEYNOTE LECTURE**
PCBs detection using Ag nanorods by GLAD (K4)
Zhengjun Zhang, Tsinghua University, China

SESSION A

15.40–16.00 **Langmuir monolayer study of the interaction of biofunctionalised gold nanoparticles with phospholipid membranes (O28)**
Nóra Ábrahám, Supramolecular and Nanostructured Materials Research Group of the Hungarian Academy of Sciences, Hungary

16.00–16.20 **Nanoparticles: Toxicity and penetration across biological barriers (O36)**
Mária Deli, Biological Research Centre, Hungarian Academy of Sciences, Hungary

16.20–17.00 *Coffee break*

17.00–17.20 **Nano-hydroxypatite composites for medical applications (O35)**
Csaba Balázsi, Research Centre for Natural Sciences, Hungarian Academy of Sciences, Hungary

17.20–17.40 **Formation of titanium-dioxide nanostructures on the surface of medical grade implant materials and investigation of their effect on bacteria (O21)**
Miklós Weszl, Budapest University of Technology and Economics, Hungary

SESSION B

15.40–16.00 **Effect of doping via ion-implantation on the crystallization, phase stability and binding energy in TiO_2 nanotubes (O12)**
It-Meng (Jim) Low, Curtin University, Australia

16.00–16.20 **Characteristics of CO and H_2 detection with single nanowire gas sensors (O05)**
Gerhard Tulzer, Austrian Institute of Technology; University of Vienna, Austria

16.20–17.00 *Coffee break*

17.00–17.20 **Nanoporous carbon from unburned carbon in bagasse ash (O37)**
Vidya S. Batra, TERI University, India

17.20–17.40 **Porous nanostructures based on carbon nanotubes and capped platinum electrocatalysts through bottom-up approach: Model and efficient electrodes structures for fuel cells (O46)**
Henri Perez, Laboratoire Francis Perrin, France

17.40–18.00 **Carbon nanotube networks as sensitive layers for gas sensor applications (O03)**
Edgar Muñoz, Instituto de Carboquímica (ICB), Spain

18.00–20.00 POSTER SECTION

P001 **The adsorption and diffusion properties of Li$^+$, Na$^+$ and K$^+$-ions on graphene surface under the effect of external electric field**
B. Peles-Lemli, D. Kánnár, J. C. Nie, H. Li, S. Kunsági-Máté

P002 **Adsorption mechanisms of organic compounds on multiwalled carbon nanotubes**
M. Kragulj, J. Tričković, J. Molnar, B. Dalmacija, G. Kozma, Á. Kukovecz, Z. Kónya, S. Rončević

P003 **Antimicrobial effect of silver functionalized TiO$_2$ coated lamp surface in indoor air sample using LED light sources**
Sz. Tallósy, L. Janovák, E. Nagy, N. Buzás, Á. Juhász, I. Dékány, L. Balázs, I. Deme

P004 **Applicability of MWCNTs and iron modified MWCNTs for removal of selected neonicotinoid insecticides in aqueous solution under natural insolation**
V. Guzsvány, P. Jovanov, S. Ratković, Si. Popov, Sa. Popov, D. Orčić, G. Bošković

P005 **Application of the supercritical fluid technology for the micronization of active pharmaceutical ingredients**
Y.-P. Chen, M. Tang, S.-L. Ho

P006 **Biosensors prepared for detectation of aflatoxins in corn matrix**
A. Majzik, D. Sebők, E. Csapó, T. Bartók, I. Dékány

P007 **Boron doped single-walled carbon nanotubes from high vacuum CVD and density gradient ultracentrifugation towards doped semiconducting nanotubes**
G. Ruiz-Soria, M. Sauer, K. Yanagi, P. Ayala, T. Pichler

P008 **Bulk Al-Al_2O_3 nanocomposites – Study of their nanosintering with respect to densification and grain growth**
Cs. Balázsi, H. Hargitai, G. Gergely, O. Tapasztó, I. Orbulov, Á. Németh, K. Balázsi, Z. Károly, A. Dhar

P009 **Carbon nanotubes quench singlet oxygen generated by photosynthetic reaction centers**
P. Boldog, É. Hideg, K. Hajdu, M. Magyar, K. Hernádi, E. Horváth, A. Magrez, L. Forró, L. Nagy

P010 **Catalytic activity of molybdenum nanoparticle decorated carbon aerogels**
B. Nagy, D. Ábrahám, Gy. Onyestyák, Gy. Sáfrán, J. Madarász, E. Geissler, K. László

P011 **Cell culture and *in vivo* study of microvesicles for drug delivery across barriers**
Sz. Veszelka, P. Sipos, L. Kiss, A. Bocsik, P. Hülper, P. Szabó-Révész, M. A. Deli

P012 **Characterization of luminescent silicon carbide nanocrystals by photoluminescence and surface infrared spectrocopy**
D. Beke, Zs. Szekrényes, I. Balogh, K. Kamarás, A. Gali

P013 **Characterization of the chemical bonding between Al_2O_3 and nanotube in MWCNT/Al_2O_3 nanocomposite**
T. A. Saleh, V. K. Gupta

P014 **Comparative investigation of photodegradation of oxalic acid and phenol over TiO_2/MWCNT photocataysts**
B. Réti, K. Mogyorósi, A. Dombi, K. Hernádi

P015 **Comparison in physico-chemical properties in In and Ga doped Ge-Te glassy chalcogenides**
V. Ivanova, A. Zaidan, P. Ilchev, Y. Trifonova, P. Petkov

P016 **Conrollable preparation of silver small particles for electronics**
Z.-Y. Zhang, C.-Y. Liu, W.-D. Yang, X.-F. Cui

P017 **Controlling gas sensitivity of spinel ferrites**
A. Sutka, G. Mezinskis

P018 **Crystallization and dielectric properties of barum titanate precipitated in inverse sodium-aluminoborosilicate glasses with high concentration of iron oxide**
R. Harizanova, L. Vladislavova, C. Bocker, G. Avdeev, C. Rüssel, I. Gugov

P019 **Development of low-temperature sol-gel synthesis of TiO_2 to provide self-cleaning effect on the textile materials**
O. Galkina, V. Vinogradov, A. Vinogradov, A. Agafonov

P020 **Development of smart hydrogel fims for treatment of bacterial infections on mucosal surfaces**
L. Janovák, J. Ménesi, N. Buzás, I. Dékány

P021 **Different synthesis approaches improving the photocatalytic performance of titanium dioxide photocatalyst nanoparticles for water purification and hydrogen production**
Zs. Pap, Z. Ambrus, G. Veréb, Á. Kmetykó, A. Dombi, K. Hernádi, K. Mogyorósi

P022 **Control of nano-fibril structure of poly(*p*-phenylene benzobisoxazole) fiber by using multifunctional comonomers**
K. H. Yoon, G. H. Jang, B. G. Min, Y. G. Jeong

P023 **The effect of surface defects and functional groups on the sintering and agglomeration of Pd nanoparticles**
R. Puskás, Á. Kukovecz, Z. Kónya

P024 **Electronic properties of metallicity sorted ferrocene filled carbon nanotube hybrids**
M. Sauer, H. Shiozawa, G. Ruiz-Soria, P. Ayala, X. Liu, A. Chernov, H. Kataura, K. Yanagi, S. Krause, T. Pichler

P025 **Electronic structure of two isomers of C_{82} fullerene polyhydroxylated taking into account Fukui Function**
C. I. Méndez-Barrientos, J. G. Rodriguez-Zavala, F. J. Tenorio, R. Flores-Moreno

P026 **Encapsulation and dynamics of spin-labelled insulin in silica matrix intended for oral administration**
E. Vanea, C. Gruian, H. J. Steinhoff, V. Simon

P027 **Engineering nanostructural coatings using Drosophila genetics**
M. Kryuchkov, G. A. Enin, A. Sergeev, A. A. Timchenko, S. A. Khaustov, V. L. Katanaev

P028 **Enhancing electroremediation by using carbon nanotubes as reactive permeable barrier material – A review**
L. Rajić, B. Dalmacija, S. Rončević, J. Tričković, D. Krčmar, D. Tomašević

P029 **Entropy driven formation of nanographite layers on the nanostructured cerium dioxyde surface**
H. Li, J. C. Nie, S. Kunsági-Máté

P030 **General toxicity, neurotoxicity and the corresponding metal levels in rats treated with nanoparticulated and dissolved manganese**
E. Horváth, Zs. Máté, Sz. Takács, A. Szabó, A. Sápi, P. Pusztai, Z. Kónya, A. Papp

P031 **Germaniun functionalization for the development of organic dielectric thin film**
B. Jousselme, X. Lefèvre, O. Segut, P. Jégou, S. Palacin

P032 **Hexagonal tungsten-trioxide: Preparation, characterization and modification**
M. Szabó, Á. Kukovecz, Z. Kónya

P033 **Highly birefringent photonic crystal fiber by altering patterns and filling media of innermost air-holes**
Y.-F. Chau

P034 **Humidity-sensitive dielectric properties of titanate nanowires (TiONW)**
H. Haspel, V. Bugris, N. Laufer, Á. Kukovecz, Z. Kónya

P035 **Hydrogen peroxide biosensor based on carbon nanotube/horseradish peroxidase bio-nanocomposite**
M. Magyar, L. Ivanov, K. Hajdu, K. Hernádi, T. Szabó, L. Nagy

P036 **Hydrogen production with Au or Pt modified TiO_2 photocatalysts as a function of noble metal nanoparticle size**
Á. Kmetykó, K. Mogyorósi, V. Gerse, K. Hernádi, A. Dombi

P037 **Hydrothermal synthesis and humidity sensing property of ZnO nanostructures, ZnO-In(OH)$_3$ and ZnO-In$_2$O$_3$ nanocomposites**
E. Pál, V. Hornok, R. Kun, A. Oszkó, I. Dékány, M. Busse

P038 **Immobilization of zinc, nickel and copper in sediment using nanoscaled zero-valent iron particles**
D. Tomašević, M. Dalmacija, M. Prica, G. Kozma, Á. Kukovecz, Z. Kónya, B. Dalmacija, S. Rončević, S. Maletić

P039 ***In situ*** **synthesis of Maleic anhydride – Octene 1 – Vinyl Butyl/CdS and Maleic anhydride – Octene 1 – Vinyl Butyl/ZnS nanocomposites and their characterization with several investigation methods**
E. Malikov, O. Akperov, M. Muradov, Á. Kukovecz, R. Puskás, D. Madarász

P040 **The influence of different CO-activators on the photoluminescence properties of SrAl$_2$O$_4$ phosphors**
Z. Győri, V. Havasi, P. Pusztai, D. Madarász, Á. Kukovecz, Z. Kónya

P041 **Influence of preparation pH on the nanostructure of silicate based bioactive glasses**
I. Riti, A. Vulpoi, V. Simon

P042 **Influence of sintering temperature on the microstructure of nanocrystalline Ni-yttria stabilized zirconia cermets**
K. Park, J. Kim, C. M. Kim, D. G. Park, K. H. Cho, S. W. Nam, J. W. Choi

P043 **Influence of the hydrophilic-lipophilic properties of surfactant mixtures on the droplet size and rheological behaviour of nanoemulsions**
É. Bazsó, Á. Juhász, D. Sebők, N. Buzás, I. Dékány, S. Puskás

P044 **Interaction of porphyrin molecules with silver nanoparticles**
R. Patakfalvi, I. Z. Dubé, H. G. Ortega, D. Diaz

P045 **Investigation of sputtered nanocomposite Ti-based biocompatible coatings**
K. Balázsi, M. Vandrovcová, I. E. Lukács, M. Szerencsi, S. Gurbán, M. Menyhárd, L. Bacáková, Cs. Balázsi

P046 **Investigation of structure and thermal denaturation of protein-based drug nanohybrid systems**
M. Benkő, D. Sebők, I. Dékány

P047 **Magic number of standing wave on the surface of a gold-shell nanorod**
Y.-F. Chau

P048 **Magnetic circular dichroism as probe of local magnetic moments in 1D iron-carbon nanotube hybrids**
A. Briones-Leon, P. Ayala, X. Liu, H. Kataura, K. Yanagi, E. Weschke, M. Eisterer, T. Pichler, H. Shiozawa

P049 **Modification of acidic sites on the surface of titanate nanostructures**
D. Madarász, I. Szenti, Á. Kukovecz, Z. Kónya

P050 **Nanomodified PP-fibers for protection against environmental tobacco smoke**
M. Cieślak, H. Schmidt, I. Kamińska, D. Puchowicz

P051 **Nanopore SERS substrate based on silver-coated anodic aluminum oxide**
Y. Bae, K. Lee, D. Choi

P052 **Nanoscale processes in thight reservoir rocks studied by photoacoustic spectroscopy**
N. Tóth, Z. Filus, Z. Bozóki, G. Szabó

P053 **Nanostructured liquid crystals with thiophene unit: Synthesis, properties and applications**
Z. Puterová, J. Romiszewski, J. Mieczkowski, E. Gorecka

P054 **Nasal delivery of meloxicam nanoparticles**
A. Bocsik, L. Kürti, R. Gáspár, E. Kápolna, M. Vastag, Sz. Veszelka, M. A. Deli, P. Szabó-Révész

P055 **Neurotoxicity of combined intratracheal metal nanoparticle exposure in rats**
Zs. Máté, A. Szabó, K. Kovács, E. Tombácz, A. Papp

P056	**Noble metal deposited TiO_2/WO_3 composite photocatalysts for oxalic acid degradation and hydrogen production: the role of the localization of the gold or platinum nanoparticle** *Zs. Pap, É. Karácsonyi, A. Dombi, V. Danciu, L. C. Pop, A. Vulpoi, L. Baia, K. Mogyorósi*
P057	**A novel design of a plasmonic nanoantenna** *Y.-F. Chau, S.-F. Wang, Y. Chu, J.-H. Wei*
P058	**On-line investigation of climate relevant carbonaceous nanoparticles by photoacoustic spectroscopy** *T. Ajtai, Á. Filep, N. Utry, M. Pintér, Z. Bozóki, G. Szabó*
P059	**Optimization of adsorption conditions of thiamethoxam on CNTs by statistical design of experiments (DoE)** *S. Ratković, V. Guzsvány, G. Bosković*
P060	**Photocurrents generated by photosynthetic reaction center protein/bio-nanocomposite systems** *T. Szabó, M. Magyar, K. Hajdu, G. Bencsik, B. Endrődi, Cs. Visy, E. Horváth, A. Magrez, K. Hernádi, L. Forró, L. Nagy*
P061	**Photoluminescence effect in double-walled carbon nanotubes** *P. Rohringer, L. Shi, T. Pichler*
P062	**Photoluminescence of $Ca_{3-3x/2}(VO_4)_2$:xEu ($0.01 \leq x \leq 0.09$) red-phosphors prepared by solution combustion method** *K. Y. Kim, S. J. Yoon, K. Park, D. G. Park, K. H. Cho, S. W. Nam, J. W. Choi, Y. S. Shin*
P063	**Plasmonic coupling of lysozime- and amino acid-gold nanodispersions** *G. Bohus, M. Benkő, Á. Veres, I. Dékány*
P064	**Plasmonic resonances on cysteine-functionalised noble metal nanoparticle aggregates** *A. Szalai, Á. Sipos, E. Csapó, L. Tóth, I. Dékány, M. Csete*
P065	**Polymerizable carbon nanodots hybrid optical functional organic-inorganic gel glasses** *Z. Xie, F. Wang, C.-Y. Liu*

P066 **The potential of organometallic polymeric carriers for paclitaxel delivery to tumor cells**
L. Kiss, E. Csányi, Sz. Veszelka, R. L. Katona, D. Jańczewski, J. Song, X. J. Wei, G. J. Vancso, P. Szabó-Révész, M. A. Deli

P067 **Preparation albumin/polyelectrolite core-shell nanoparticles for controlled drug release**
K. Kristó, M. Szekeres, M. Benkő, B. Roósz, G. Bohus, Zs. Majláth, L. Vécsei, I. Dékány

P068 **Preparation and characterization of PE/NR-CuS, PbS, CdS, ZnS nanocomposites on the basis of nitrile rubber/ polyethylene polymer composites**
N. Balayeva, R. Alosmanov, G. M. Eyvazova, M. Muradov, A. Azizov

P069 **Preparation and characterization of MWCNT-ionic conducting polymer nanocomposites**
Y. S. Gal, S.-H. Jin, K. T. Lim

P070 **Preparation and characterization of nanoparticles for drug delivery to brain**
P. Sipos, P. Hülper, B. Vajna, Sz. Veszelka, M. A. Deli, P. Szabó-Révész

P071 **Preparation of polarized electrode of an electric double layer capacitor using a spray pyrolysis technique**
T. Momiki, M. Taguti, A. Haruta, D. Tashima

P072 **Preparation of polymeric membranes using functionalised MWCNTs as fillers for desalination processes**
D. Vuono, E. Fontananova, F. Artusa, E. Drioli, J. B. Nagy, M. A. Bahattab, F. M. Alsubaie, M. A. Alowirdy

P073 **Preparation, structures and properties of poly(*p*-phenylene benzobisoxazole) nanocomposites reinforced with graphene**
Y. G. Jeong, J. H. Lee, B. G. Min, K. H. Yoon

P074 **Purification of phenol and *E. coli* contaminated water by visible light activated titanias**
G. Veréb, L. Manczinger, A. Sienkiewicz, L. Forró, A. Dombi, K. Hernádi, K. Mogyorósi

P075 **Raman fingerprint of *stage I–stage VI* graphite intercalation compounds from theory and experiment**
J. C. Chacón-Torres, T. Pichler, L. Wirtz

P076 **Raman mapping in surface analysis of PP-fibers modified with TiO_2**
D. Puchowicz, M. Cieślak

P077 **Reactivity indexes in nitrogen-doped fullerenes**
F. J. Tenorio, J. G. Rodriguez-Zavala, R. Flores-Moreno, G. Guzmán-Ramírez

P078 **Self-assambled nanoplasmonic gold particle on graphene via reduction process**
S. Lee, H.-J. Shin, D. Choi

P079 **SEM-FIB investigation of composition dependent sintering behaviour of $Cu_xNi_{(1-x)}$ printed structures**
R. Kun, E. Pál, V. Zöllmer, D. Lehmhus, M. Busse

P080 **Single Au or Cu atom impurity effect on thermal stabilities of Cu_{55} or Au_{55} clusters with icosahedron geometry**
L. Zhang

P081 **Sorption properties of mechanical modified titanate nanowires and nanotubes**
G. Kozma, A. Sápi, Á. Kukovecz, Z. Kónya

P082 **Spin-dependent interference in lateral superlattices: Conductance properties**
V. Szaszkó-Bogár, P. Földi

P083 **Stability and immune – Modulatory effects of liposomes with various compositions**
A. Szalai-Juhász, Z. Lovrity, É. Kiss-Tóth-Dojcsak, J. Emmer, B. Fodor

P084 **Static and dynamic Jahn–Teller effect in solid fullerides**
P. Matus, Gy. Klupp, K. Kamarás, A. Y. Ganin, A. McLennan, M. J. Rosseinsky, Y. Takabayashi, M. T. McDonald, K. Prassides

P085 **Structural properties and photoluminescence of nanocrystalline gahnite doped with titanium**
M. Vrankic, B. Grzeta, S. Kurajica, V. Mandic, E. Tkalcec, S. Milosevic, M. Ceh, B. Rakvin

P086 **Structure and properties of poly(*p*-phenylene benzobisoxazole) nanocomposites with single-wall carbon nanotubes functionalized under ozone gas flow**
B. G. Min, J. Zhou, Y. G. Jeong, K. H. Yoon

P087 **Structure of nanocomposites on the basis polypropylene and zirconium dioxide nanoparticles**
A. M. Magerramov, M. A. Ramazanov, F. V. Hajiyeva

P088 **Studies on the interaction of mycotoxins and macrocycles by molecular modelling**
B. Roósz, T. Körtvélyesi, I. Dékány

P089 **Study on deterioration factors of cylindrical electric double-layer capacitor cell**
M. Taguchi, T. Momiki, A. Haruta, D. Tashima

P090 **Study on electronic type separated carbon nanotube thin films**
H. M. Tóháti, Á. Pekker, K. Kamarás

P091 **Superconductivity of carbon nanotubes in a longitudinal magnetic field**
P. Eminov, Y. Sezonov, S. Gordeeva

P092 **Synthesis and characterization of SBA16-Fe_xCo_{1-x} magnetic nanocomposites**
S. Bullita, A. Corrias, M. F. Casula, D. Carta, A. Falqui

P093 **Synthesis and investigate of maleic anhydride-oktene-1/CdS nanocomposites**
Z. Q. Mamiyev, O. H. Akbarov

P094 **Synthesis and luminescence of nano-sized $Sr_{2.91}V_2O_8$:$Eu_{0.06}$ phosphors by solution combustion method**
K. Park, S. J. Yoon, K. Y. Kim, D. G. Park, K. H. Cho, S. W. Nam, J. W. Choi, Y. S. Shin

P095 **Synthesis of aerogel nanocomposite catalysts for the production of carbon nanotubes**
C. Marras, S. Bullita, M. F. Casula, D. Loche, Z. Kónya, A. Corrias

P096 **Synthesis of aluminosilicate nanotube from rice husk ash and its characterization**
T. Hongo, J. Sugiyama, A. Yamazaki, A. Yamasaki

P097 **Synthesis, investigation and fields of application of silicon nanocomposites containing rare earth metals**
V. Koval, Y. Yasievich, M. Dusheyko, A. Ivashchuk, O. Bogdan, Y. Yakymenko

P098 **Synthesis, structural characterization and magnetic properties of highly porous $ZnFe_2O_4$-SiO_2 nanocomposite aerogels**
D. Loche, M. F. Casula, C. Marras, A. Casu, A. Falqui, G. Concas, A. Corrias

P099 **Tailoring the functionality of single-walled carbon nanotubes by metallocene filling**
M. V. Kharlamova , H. Shiozawa, M. Sauer, T. Pichler

P100 **A temperature dependent study of the growth yield of linear carbon chains inside double walled carbon nanotubes**
L. Shi, P. Rohringer, P. Ayala, T. Pichler

P101 **Theranostic hyaluronic acid nanoparticles for cancer and Alzheimer's disease**
J. H. Park, K. Kim, I. C. Kwon, D.-G. Jo

P102 **Thermal stability test of one-dimensional $CePO_4$ nanostructures for a potential solid oxide fuel cell application**
P. Pusztai, T. Simon, Á. Kukovecz, Z. Kónya

P103 **Thin films of copper phthalocyanine – 2D conductive polymer**
V. Korepanov, D. M. Sedlovets, M. V. Shuvalov, Y. V. Vishnevskiy, V. T. Volkov, I. I. Khodos, O. V. Trofimov

P104 **Time-resolved GISAXS study of formation of a silver nanoparticle crystal with FCC symmetry**
K. Vegso, P. Siffalovic, M. Jergel, E. Majkova, M. Weis, S. Luby, A. Buffet, S. V. Roth

P105 **TiO_2-Ag/Au/polymer nanohybrid coatings targeting prevention of peri-implant infections of dental implants**
Á. Györgyey, E. Csapó, J. Ménesi, Á. Veres, E. Urbán, C. Gergely, K. Buzás, Z. Rakonczay, K. Nagy, F. Cuisinier, I. Dékány, K. Turzó

P106 **Tuning the optical gap of small diamondoid cages by sulfurization: A time-dependent density functional study**
T. Demjén, M. Vörös, T. Szilvási, A. Gali

P107 **Ultrashort pulse characterization utilizing highly nonlinear ZnO nanostructures**
H. Messaoudi, S. K. Das, M. Bock, E. McGlynn, D. Byrne, F. Güell, R. Grunwald

P108 **Zinc containing bioglass-derived porous scaffolds for tissue engineering**
R. Veres, C. Ciuce, V. Simon

P109 **Hierarchical hollow mesoporous carbon as a highly efficient anode electrode in Li-ion battery**
M.-S. Kim, D. Yang, J. H. Kim, H. Y. Park, M. Y. Song, J.-S. Yu

20.00–22.00 *Optional dinner and wine tasting*

26TH OCTOBER 2012, FRIDAY

09.00–10.00 **KEYNOTE LECTURE**
Preparation of 2D materials and energy storage and optical applications (K5)
Robert Vajtai, Rice University, USA

SESSION A

10.00–10.20 **Isotope engineering in carbon nanostructures (O27)**
Ferenc Simon, Budapest University of Technology and Economics, Hungary

10.20–10.40 **Electronic and optical properties of organic conjugated polymers for optoelectronics (O14)**
Hong Seok Kang, Jeonju University, Republic of Korea

10.40–11.00 **A nanostructure pentacene thin film transistor with good performance using sol-gel derived SiO_2 gate dielectric layer (O38)**
Fahrettin Yakuphanoglu, Firat University, Turkey

11.00–11.40 *Coffee break*

11.40–12.00 **Vibrational spectroscopic methods applied to self-assembled nanostructures (O57)**
Katalin Kamarás, Wigner Research Centre for Physics, Hungary

12.00–12.20 **Bilateral formation of carbon spirals from a high pressure organometallic precursor (O02)**
Hidetsugu Shiozawa, University of Vienna, Austria

12.20–12.40 **Electronic and optical properties of carbon nanotubes on metallic substrates (O13)**
Catalin D. Spataru, Sandia National Labs, USA

12.40–13.00 **Nanocluster Bi-doped CdO thin films for optoelectronic applications (O34)**
Niyazi Ozdemir, Firat University, Turkey

13.00–13.20 **Novel strategy for cancer cell specific oligonucleotide therapeutics with intracellular environmental condition responsible artificial nucleic acid: Peptide Ribonucleic Acids (PRNAs) (O39)**
Takehiko Wada, Tohoku University, Japan

SESSION B

10.00–10.20 **Synthesis and surface modification of nanoparticles for theragnostics (O52)**
Maria F. Casula, University of Cagliari, Italy

10.20–10.40 **Emerging applications of carbon nanomaterials in energy and environment (O16)**
Saikat Talapatra, Southern Illinois University Carbondale, USA

10.40–11.00 **Formation of the copper sulfide nanoparticles by ion exchange from electrolyte solutions (O20)**
Mustafa B. Muradov, Baku State University, Azerbaijan

11.00–11.40 Coffee break

11.40–12.00 **Fabrication and electrical characterization of CdO nanorods CdO/p-Si photosensors (O18)**
Mehmet Cavas, Firat University, Turkey

12.00–12.20 **ZnO nanopowder based on quartz crystal microbalance humidity sensors (O59)**
Cengiz Tatar, Firat University, Turkey

12.20–12.40 **ZnO nanofiber films for UV sensor applications (O58)**
Esat Guzel, Firat University, Turkey

12.40–13.00 **A solid-state photoelectrochemical water splitting cell with a composite Nafion® membrane and gaseous reactants (O48)**
Kingsley O. Iwu, University of Oslo, Norway

13.00–13.20 **Comparison of carbon paste electrodes bulk modified with multiwall carbon nanotubes and gold nanoparticles for determination of hydrogen-peroxide (O07)**
Valéria Guzsvány, University of Novi Sad, Serbia

13.20–15.00 Lunch

15.00–22.00 Optional journey to Ópusztaszer (till 18.00) and dinner

27TH OCTOBER 2012, SATURDAY

09.00–10.00 **KEYNOTE LECTURE**
Spontaneous formation of multiwalled metal oxide nanotubes (K6)
Dmitry V. Bavykin, University of Southampton, UK

SESSION A

10.00–10.20 **Cold-atom scanning probe microscopy (O06)**
József Fortágh, University of Tübingen, Germany

10.20–10.40 **High symmetry rotor-stator cocrystals of fullerenes (O24)**
Éva Kováts, Wigner Research Centre for Physics, Hungary

10.40–11.00 **Complex characterization of magnetic configurations in multiphase nanoparticulate systems (O08)**
Victor Kuncser, National Institute of Materials Physics, Romania

11.00–11.40 *Coffee break*

11.40–12.00 **Textile and antifungal behavior of a cotton woven support to ultrasonically deposited copper oxide nanoparticles by means of two different methods (O53)**
Hortensia Clara Radulescu, National Research and Development Institute for Textile and Leather, Romania

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SESSION B

10.00–10.20 **Carbon nanotubes meet hairy polymers: Superstructures of carbon nanotubes and conjugated polymers having long alkyl tails (O04)**
Maria Cristina dos Santos, University of São Paulo, Brazil

10.20–10.40 **Polymer properties enhancement by hybrid nanofillers (O45)**
Oren Regev, Ben-Gurion University of the Negev, Israel

10.40–11.00 **Control of relaxation state for nanostructure formation based on glassy alloys (O09)**
Junji Saida, Tohoku University, Japan

11.00–11.40 *Coffee break*

11.40–12.00 **Flexible electrodes prepared by reactive inkjet printing (O19)**
Krisztian Kordas, University of Oulu, Finland

12.00–12.20 **Macroscopic carbon nanotube fibers (O31)**
Geza Toth, University of Oulu, Finland

12.40–13.00 **Closing ceremony**

KEYNOTE LECTURES

Advances in understanding the chemistry of graphene and carbon nanotubes: Fundamentals and applications (K1)

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Our laboratory at MIT has been interested in how the 1D and 2D electronic structure of carbon nanotubes and graphene respectively influences their chemical interactions. We report several new methods for preparing and functionalizing graphene. Bilayer and trilayer graphene with controlled stacking is emerging as among the most promising candidates for post-silicon nanoelectronics. We demonstrate a solution-phase technique for the production of large-area, bilayer or trilayer graphene from graphite, with controlled stacking. The ionic compounds iodine chloride (ICl) or iodine bromide (IBr) intercalate the graphite starting material at every second or third layer, creating 2nd or 3rd stage-controlled graphite intercolation compounds, respectively. The resulting solution dispersions are specifically enriched with bilayer or with trilayer graphene, respectively. Because the process requires only mild sonication, it produces graphene flakes as large as 50 um^2. Moreover, the electronic properties of the flakes are superior to those achieved with other solution-based methods: for example, unannealed samples have resistivities as low as ~1 kOhm and hole mobilities as high as 400 cm^{2}V^{-1}s^{-1}. We show for the first time that solution dispersed bilayer graphene transistor can demonstrate a band gap via dual gate device. In general, chemical functionalization of graphene enables control over electronic properties and sensor recognition sites. However, its study is confounded by an unusually strong influence of the underlying substrate. We show a stark difference in the rate of electron transfer chemistry with aryl diazonium salts on monolayer graphene supported on a broad range of substrates. Reactions proceed rapidly when graphene is on SiO_2 and Al_2O_3 (sapphire), but negligibly on alkyl-terminated and hexagonal boron nitride (hBN) surfaces. The effect is contrary to expectations based on doping levels and can instead be described using a reactivity model accounting for substrate-induced electron-hole puddles in graphene. Raman spectroscopic mapping is used to characterize the effect of the substrates on graphene. Reactivity imprint lithography (RIL) is demonstrated as a technique for spatially patterning chemical groups on graphene by patterning the underlying substrate, and is applied to the covalent tethering of proteins on graphene. Our laboratory has also been interested in how semiconducting single walled carbon nanotubes (SWNT) can be modified such that their fluorescent emission is modulated in response to specific molecules, hence creating a new class of sensor. Advances towards this end will be reviewed, including our work on the label free detection of protein-protein interactions, H_2O_2, NO and glucose, as well interfacing sensor arrays to live cells. Lastly, we fabricate and study SWNT ion channels for the first time (2) and show that the longest, highest aspect ratio, and smallest diameter synthetic nanopore examined to date, a 500 um SWNT, demonstrates oscillations in electro-osmotic current at specific ranges of electric field, that are the signatures of coherence resonance, yielding self-generated rhythmic and frequency locked transport. The observed oscillations in the current occur due to a coupling between stochastic pore blocking and a diffusion limitation that develops at the pore mouth during proton transport. Such pores offer new possibilities in molecular detection, charge transport and separation processes.

Iron, copper and bismuth do not belong to royalty; however, when stabilized and nanostructurated, they become highly prized (K2)

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Keywords: zerovalent metals, strong quantum confinement, stabilized colloidal nanoparticles

In the first part of this oral contribution will discuss a novel, easy, and general synthesis method to prepare zerovalent iron and copper nanoparticles (NPs), from colloids in an environmental friendly organic solvent, ethylene glycol. Conventional metallic salts are used as nanoparticle precursors; sodium borohydride is the reducing agent, and triethylamine is an additional stabilizing nanoparticle species. These reactions take place instantaneously, under normal reaction conditions. Small iron (α-Fe^0 phase) and copper (fcc phase) NPs with average diameters of 10.2 ± 3.3 and 9.5 ± 2.5 nm, respectively, are obtained. The dry ZV-Fe and Cu NP powders that precipitated from the colloids are stable in storage, at room conditions, for more than a year.[1] Once the ZV-Fe NPs were characterized, the interaction between such nanoclusters with the bis-(4-nitrophenyl) phosphate (BNPP) in water was studied. BNPP is a neurotoxic compound, frequently used as agrochemical and remains in the environment for a long time. Our results show that the BNPP degradation takes place at room temperature, during the first 10 minutes.

In the second part of this lecture will show the synthesis of ZV-Bi NPs by a colloidal straightforward one-pot and one-step method. Commercial, conventional, stable, and inexpensive chemical reagents are used. The reactions take place rapidly, under normal reaction conditions, and with high yields. When the reducing agent is in deficit and citrate ions are present in the reaction system, ZV-Bi NPs are produced that are crystalline, well faceted, or quasi-spherical, and stabilized, without any traces of oxide, monodispersed, with an average diameter equal to 3.3 nm (SD 1.0 nm). The dry

ZV-Bi NP powders that precipitated from the colloids are stable in storage, at room conditions, for more than three years.[2] Indirect and direct energy gaps of the ZV-Bi NPs were discovered in the near infrared spectral range indicating the displacement of the conduction and valence bands due to the strong quantum confinement. These bismuth nanoclusters have been tested as inhibitors of *Streptococcus mutans* growth, with results as good as the chlorhexidine.[3]

Acknowledgements: The research leading to these results has received funding from the European Community Seven Framework Programme (FP7-NMP-2010- EU-MEXICO) and CONACYT under Grant Agreement Nos. 263878 and 125141; CONACyT (SEP-CB-132094 and E43662) and DGAPA-UNAM (IN 101009 and IN100907) projects, respectively.

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Novel nanocarbons: Defective graphenes, nanoribbons with atomically smooth edges and graphene-nanotube hybrid structures (K3)

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In this talk, defects within sp^2 hybridized carbon will be discussed: 1) Structural defects, 2) Topological defects, 3) Doping-induced defects, 4) Non-sp^2 carbon defects, and 5) high strain folding.[1] The presentation will emphasize the importance of identifying and quantifying defects in graphene-like materials. Most of the time, the presence of defects and their identification have been overlooked by numerous scientists. However these play a key role in the nanotubes' physico-chemical properties and biocompatibility. There are numerous challenges that will be discussed in this presentation: How do we identify defects efficiently? Could we distinguish among various defects? Would it be possible to establish a protocol able to quantify and control the amount of these defects? How many defects are necessary to fabricate robust polymer composites or 3D architectures? Could one introduce specific defects in order to make materials biocompatible? Is it possible to promote ferromagnetism by introducing specific defects in nanostructures? etc.

We will also describe the synthesis of graphene and graphitic nanoribbons[2,3] via different routes: a) chemical vapor deposition (CVD), and b) by unzipping multi-walled carbon nanotubes using different routes. We have recently developed an innovative route which is able to create graphene and graphitic nanoribbons with atomically smooth edges. These edges exhibited armchair and zigzag edge terminations. The route is environmentally green and involves a mild acid treatment in H_2SO_4 and HNO_3, followed by an abrupt thermal shock using liquid nitrogen and boiling water.[4] We were able to successfully unzip multi-walled carbon nanotubes (MWNTs) and nitrogen-doped multi-walled carbon nanotubes (CNx-MWNTs). More recently, we have been able to synthesize N-doped graphitic nanoribbons via a CVD approach.[5] In particular, the N-doped nanoribbons exhibit semiconducting-like behavior.

Large-area, high-quality monolayer nitrogen-doped graphene sheets were synthesized on copper foils using ambient-pressure CVD.[6] When compared to pristine graphene, nitrogen-doped graphene shows a strong D-band caused by the doping effects or structural defects formed within the lattice. Scanning tunneling microscopy (STM) and spectroscopy (STS) reveal that the defects in the doped graphene samples arrange in different geometrical configurations exhibiting different electronic properties. These experimental results are in agreement with first principles calculations of LDOS of doped graphene. These materials have also been characterized by aberration corrected high-resolution transmission electron microscopy (AC-HRTEM) and X-ray photoelectron spectroscopy (XPS). These doped layers could be used as efficient molecular sensors.

Finally, the synthesis of hybrid carbon materials consisting of sandwich layers of graphene layers and carbon nanotubes have been synthesized by an ionic self assembly route.[7] These films are novel, energetically stable and could well find important applications as catalytic supports, gas adsorption materials[8] and super capacitors.

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PCBs detection using Ag nanorods by GLAD (K4)

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Polychlorinated biphenyls (PCBs) are very harmful to human body and had polluted many places in our environment. Using Ag nanostructures prepared by glancing angle deposition (GLAD) technique, PCBs can be detected rapidly even at trace levels by surface-enhanced Raman scattering (SERS). The Raman signals enhanced by the Ag nanostructures can be enhanced further by specific SERS substrates, e.g., depositing a thin Ag film beneath the Ag nanorods, folding slanted Ag nanorods, pattering the Ag nanorods, etc. Another advantage of this method is that one could recognize isomers of PCBs when knowing fingerprints of these substances, thus offering an alternative method for the trace-level detection and characterization of PCBs in our environment.

Preparation of 2D materials and energy storage and optical applications (K5)

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Atomically thin materials are distinguished by the scientific community because revolutionary electrical applications are visioned. Graphene, hexagonal boron nitride and other atomically thin layers show distinct properties compared to bulk materials.

In this talk we will describe our experimental work to synthetize and characterize intrinsic and structured 2D materials. First, the growth and modification methods designed and optimized for preparation of graphene sheets and several related 2D materials will be briefly summarized. We describe our chemical vapor deposition method, the number of layers produced, and the growth temperature range. Similarly we will describe GO preparation and reduction methods. Second, several characterization techniques and the properties of the materials will be described, focused on electrical conductivity measurements as it is one of the most important parameters in energy storage materials. Third, thin and flexible energy storage device fabrication from graphene, G-h-BN and GO will be described. Single sheet and multiple layer graphene devices fabricated by transfer and layer by layer deposition techniques, respectively, are applied as electrode material in supercapacitors. For GO-based devices we generated the electrode structures by localized thermal reduction on GO papers. These supercapacitors had 100, 400 and 500 microfarad per square cm specific capacity for the single layer graphene, multilayered graphene and RGO devices, respectively. We will introduce briefly our results for preparing flexible electrode materials from hybrids, namely 2D carbon materials and carbon nanotubes. Finally we show several applications of 2D materials in handling and detecting low photon energy electromagnetic radiations.

Acknowledgement: This lecture covers topics explored in collaboration with M. J. Wang, Z. Liu, A. L. M. Reddy, M. Hahm, J. Kono and P. M. Ajayan, their contribution is acknowledged.

Spontaneous formation of multiwalled metal oxide nanotubes (K6)

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Keywords: titanates, TiO_2, silicates, hierarchical nanostructures

Nanotubular metal oxide materials have attracted a great attention last years due to their unusual physico-chemical properties and potential use in many applications. Although the range of materials capable of forming multiwalled nanotubes is constantly growing, a comprehensive mechanism of their formation, which would not only provide an efficient way of controlling nanotube morphology, but would also allow formulation of the synthesis conditions for new nanotubular materials, is still under development.

A general overview of hydrothermal routes for preparation of several metal oxide nanotubes such as $Al_2Si_2O_5(OH)_4$,[1] $Ni_3Si_2O_5(OH)_4$[2] and $H_2Ti_3O_7$[3] is to be discussed. The commonality in the mechanisms of formation of these nanotubes is identified and analysed. The driving forces for spontaneous folding of nanosheets into nanotubes are considered, including intrinsic asymmetry of the nanosheet and the mechanical tensions occurring during their growth.

The bottom-up and top-down methods of preparation of hierarchical nanostructures[4] composed of titanate nanotubes will be presented. The benefit of such nanostructures in several applications including dye sensitized solar cells, fuel cells and lithium batteries will be discussed.

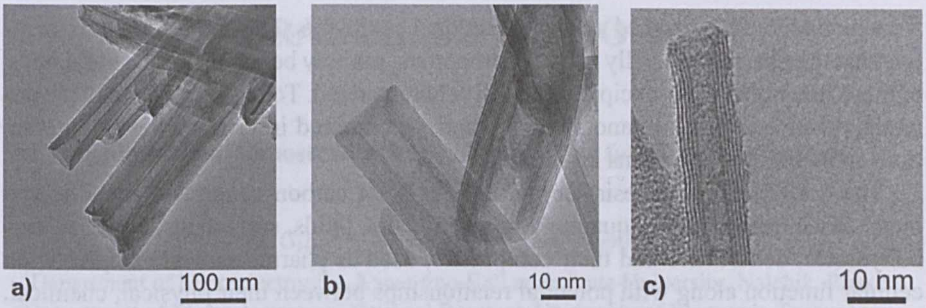

Figure 1. TEM images of (a) $Al_2Si_2O_5(OH)_4$, (b) $Ni_3Si_2O_5(OH)_4$ and (c) $H_2Ti_3O_7$ nanotubes synthesised in our lab via hydrothermal route

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Toxicology perspectives of nanomedicines (K7)

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Nanotechnology could provide a way to address the urgent need for radical improvement of health and disease management. Nanomedicine is a new term, used to define the medical applications of nanotechnology. It encompasses the next era in drug delivery and diagnostics and imaging of health and disease conditions. However, some major issues on their safety versus toxicity remain to be answered and their health risk-benefit ratio remain to be fully determined.

Nanomedicines (drug and delivery system) are made from various nanomaterials with unique and highly tunable physicochemical properties. This makes it possible to engineer specialized and personalized treatments. Drug delivery systems, constructed from nano-sized components that serve as the carrier or targeting ligand for a therapeutic agent have been regarded in the past as inert or non-active components of dosage forms. However, this may not always be true. Exposure to these nanomaterials by dermal, oral, and respiratory routes during manufacturing or after disposal and environmental contamination or after administration into the body as part of a treatment can cause dose-dependent toxicity.

Generally, most nanomaterials are still not well characterized, therefore the specific properties contributing to undesirable effects cannot be ascertained. It is important to develop a framework that will assist in the development of quality requirements for nanomaterials to be used as pharmaceutical excipients. Furthermore, it is imperative that the pharmaceutically relevant properties, toxicity being one of the main ones, of these functional nano-excipients be fully characterized. To better understand the potential adverse effects of nanomaterials, both in vitro and in vivo studies on interactions with biological systems are needed.

The desirable and undesirable ‘nano-effects’ of carbon nanotubes, metallic and metal oxide nanoparticles, quantum dots, polymers, lipids, surfactants, peptides, carbohydrates, dendrimers and their composites, used as pharmaceutical excipients, on cellular function along with potential relationships between their physical, chemical, morphological and intelligent properties and their biological effects will be discussed. The goal of the presentation will be to provide a perspective on risks and their management associated with nanomaterials used in medicine.

ORAL PRESENTATIONS

Application of nanostructuring techniques for fabrication of getters for mems (O01)

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Keywords: getters, nanostructuring, MEMS

Nanostructuring techniques are used to produce various functional materials, including for microelectromechanical systems. We have investigated the use of nanostructuring in formation of getter layers, one of the performance criteria is the presence of highly surface intraphase and interfaces.[1,2]

The way of formation of structures with a high effective surface using magnetron sputtering was explored. The structuring of the matter depends on the peculiarities of implementation of magnetron sputtering.

Technological solutions based on using of porous silicon and allowing to form of effective getters for MEMS are proposed. The first of the proposed options is to shape the nanocomposite getters structure representing as a micro- and mesoporous silicon on the pore walls of which a layer of active metal or alloy based on active metals is deposited. To maximize the effectiveness of the one getter, the metal layer should cover the surface of the pores isomorphically on all thickness of a porous layer. This structure has an effective surface which is almost comparable to the surface of porous silicon and therefore has a high sorption capacity. Such getter can be easily mountable into micro packages by using proven methods of micro-assembly and microfabrication techniques.

Also the method of getters formation based on the use of porous silicon as a sacrificial layer was proposed. In this case the porous silicon is filled with active metal or with active metals alloy. The sacrificial layer is finally removed and we get a structure with an advanced gettering surface. The thickness and the effective surface of gettering structure, as in the first option, are determined by the properties of the porous structure used. In this case the thickness and the effective surface of getter structure are conditioned by the thickness and porosity of the basic sacrificial layer. At the same time the surface morphology is identical to the morphology of the pores of sacrificial layer.

On the basis of proposed technological solution samples getter structures have been produced. The results of experimental investigations of the structures show us the prospects of their use in devices of micro-and nanosystem technology, which requires to maintain the vacuum in small volumes.

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Bilateral formation of carbon spirals from a high pressure organometallic precursor (O02)

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Keywords: Growth symmetry, carbon nanostructure, spirals, electron microscopy, local wave pattern

Our research focuses on understanding and control of nanoscale shape formations via studies of novel synthesis routes to carbon nanostructures.[1,2]

Self-pressured process, in particular, uses a pure organometallic gas to produce novel symmetric nanostructures.[1] The process performed within a sealed vessel at elevated temperatures allows high-pressure molecules to react with each other in a free-standing manner, allowing novel symmetric carbon nanostructures to emerge spontaneously. The growth symmetry is determined at a given temperature and pressure, allowing the phase diagram for a precursor to be produced. In particular, at pressures that exceed 5 MPa mirrored nano-spirals are produced.

Microscopic studies across the symmetry plane show graphene flakes arranged in a collective manner, exhibiting a herringbone arrangement of the graphite layer, normal to which the defects propagate. The local wave patterns are analyzed that unfold the long-range two-fold symmetry of the defect patterns centered around the iron core. All these suggest a stacked-cone structure of the paired graphitic arms, extruded from a growing iron core of the bicone shape with its cone angle increasing over time.

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Carbon nanotube networks as sensitive layers for gas sensor applications (O03)

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Keywords: carbon nanotubes, thin films, gas sensor, resistive sensor, surface acoustic wave sensor, H_2, NO_2

We here report on the use of carbon nanotube films prepared by airbrush spraying as sensitive layers in resistive and surface acoustic wave sensor devices for gas detection. Carbon nanotube sensor films were fabricated by airbrushing nanotube dispersions on alumina or quartz substrates. Networks of different carbon nanotube materials were tested as active sensing element sensors for the detection of pollutant gases (H_2, NO_2, octane, toluene, NH_3). Our results indicate that the nanotube structure and chemical functionalization affect both the CNT entanglement within the airbrushed networks and their gas sensing performance. Thus, highly sensitive NO_2 and H_2 resistive sensors were fabricated out of networks of carboxylic acid functionalized double-walled carbon nanotubes and Pd-functionalized single-walled carbon nanotubes, respectively. Issues related to gas sensing mechanisms of the tested resistive sensors, and device performance dependence upon the sensor operation temperature are also discussed here. All tested resistive sensors provided negligible responses to interfering gases such as NH_3, toluene and octane. On the contrary, our nanotube-based SAW sensors were sensitive only upon exposure to octane and toluene, providing fast responses and recovery times to these volatile organic compounds. Carbon nanotube-based gas sensors made by other carbon nanotube film preparation techniques are reviewed, and their gas sensor performance is compared to those reported here.

Carbon nanotubes meet hairy polymers: Superstructures of carbon nanotubes and conjugated polymers having long alkyl tails (O04)

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Keywords: carbon nanotube suspensions, molecular dynamics, supramolecular structure

Carbon nanotubes suspensions in water or in organic solvents have been successfully used to separate nanotube populations by diameter, electronic type, chirality or chiral angle, among other properties. Solutions containing one or more encapsulating agents, for example surfactants, organic polymers or biopolymers, are used to disperse nanotubes. Polymer wrapping has been shown to be one of the mechanisms by which semiconducting nanotubes can be selectively suspended in organic solutions. Only small diameter nanotubes were observed to be suspended in toluene solutions of poly(9,9-dioctylfluorenyl-2,7-diyl), or PFO, and other polymers. Recently it was demonstrated that larger nanotubes (diameters larger than 1 nm) can be separated by using polymers from the fluorene[1] and the thiophene[2] families of conjugated polymers, provided that the conjugated backbones have large enough alkyl pendant groups.

The present work brings molecular dynamics simulations of nanotubes interacting with poly(9,9-didodecylfluorenyl-2,7-diyl) (PDF) and regioregular poly(3-dodecylthiopnene) (PDT) in toluene. We used impulse dynamics in the microcanonical ensemble, combined with the CVFF950 force field, as implemented in CERIUS2 package. The simulations showed that the larger alkyl tails not only provoke a stronger wrapping of nanotubes but also allow different geometries of wrapping. One of these new geometries is such that a single polymer chain attaches to two distinct nanotubes creating dyads. These structures are stable in toluene and are covered by the polymers in geometries that tend to a helical structure. Evidence of these structures could be found in the luminescence of the nanotube suspensions.

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Characteristics of CO and H_2 detection with single nanowire gas sensors (O05)

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Keywords: nanowire, gas sensor, selectivity, simulation, surface reactions

Numerous applications ranging from personal safety systems to breath analysis for early diagnosis of diseases have a strongly increasing demand for highly sensitive gas detecting equipment. Metal oxide based gas sensors, which rely on changes of electrical conductance due to the interaction with the surrounding gas, are widely used and have been thoroughly investigated in the past decades. In particular, nanowire sensors offer great potential to improve present gas sensor devices due to their high sensitivity that enables the detection of toxic gases with concentrations in the low ppm range.[1] To achieve this goal, computer simulations on the carrier transport in the nanowire including the processes at the nanowire surface are crucial.[2–4]

A lack of selectivity, leading to the problem of cross sensitivity, remains the central issue with gas sensors. In order to overcome this problem, a quantitative understanding of the chemical reactions on the nanowire surface and their dependence on the receptor material is essential. In this work, we compare the reaction of carbon monoxide to the reaction of hydrogen with the sensor surface to gain more insight on the characteristics of the interactions and the actual reaction paths.[5,6] To this end, we perform an estimation of the essential parameters governing these processes, including reaction parameters as well as material parameters, which is done using a simulated annealing algorithm. We use the determined values and the mass action law to simulate the gas-surface interactions and to compute the surface charge, which is done by solving a coupled system of highly nonlinear ordinary differential equations. The results show very good agreement to the given experimental data for both target gases and hence confirm the investigated reaction paths Moreover, they provide physically reasonable results for the numerical values of the estimated parameters. This quantitative information explains the different behavior of the gases, which is an important step towards establishing selectivity for the discussed sensors.

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Cold-atom scanning probe microscopy (O06)

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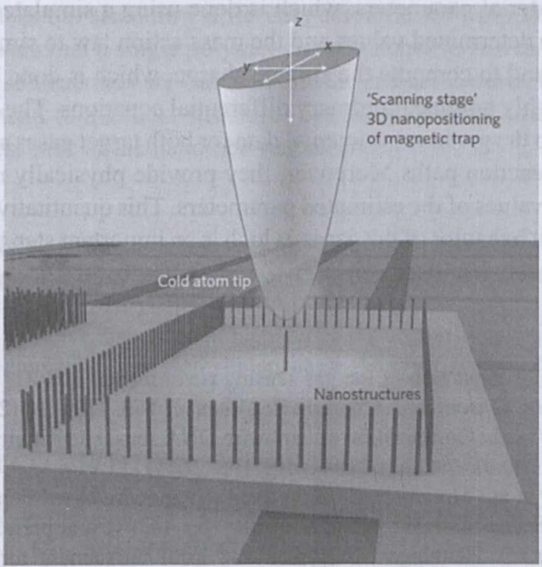
Keywords: cold-atom, Bose-Einstein condensate, scanning probe

Trapping and manipulating atoms by means of microscopic traps has seen enormous advances within the last decade. Today, ultra-cold atom clouds, Bose-Einstein condensates, and Fermi gases are routinely prepared at the surface of microchips. They are trapped in conservative electromagnetic potentials generated by microstructures.[1] Such experiments have delivered important insights into fundamental interactions between atoms and surfaces and offer new perspectives for constructing quantum instruments.



I present the application of ultracold atom clouds as the “tip” of a scanning probe microscope.[2] This tip (typically 10^3–10^5 atoms, density 10^{12}–10^{14} cm^{-3}, temperature 10 nK–1 μK) is scanned in a three-dimensional volume above the surface of interest by means of a magnetic “conveyor belt”. Analog to AFMs, the cold-atom SPM can be operated in contact and dynamical modes for imaging surface topographies and for ultrasensitive force measurements. While AFMs have much sharper tips and reach about four orders of magnitude higher spatial resolution, cold atom tips have up to fifteen orders of magnitude smaller spring constants and reach extremely high force sensitivities in the sub-yN (<10–24N) range.

We non-destructively measure the position and height of free standing carbon nanotubes and measure dispersion forces between atoms and nanotubes.[3]

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Comparison of carbon paste electrodes bulk modified with multiwall carbon nanotubes and gold nanoparticles for determination of hydrogen-peroxide (O07)

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Keywords: carbon paste electrodes, gold nanoparticles, MWCNT, H_2O_2 analysis

Nanotechnology has become one of the most interesting disciplines in science and technology today which serves new materials with very specific performances (high mechanical strength, and high conductivity, electronic transport properties etc.) for different applications. In electroanalytical sensing the modification of electrode substrates with carbon nanotubes and/or gold nanoparticles has been documented to result in low detection limits, high sensitivities, reduction of over-potentials, and resistance to surface fouling.[1] In our work optimization experiments were performed to prepare carbon paste electrodes (based on graphite powder and paraffin oil) bulk doped with unmodified (MWCNT-CPE), chemically oxidized multiwall carbon nanotubes (C-MWCNT-CPE), and with gold nanoparticles. The influence of the dopant nature, and content were investigated. Electrochemical characterization of prepared electrodes by cyclic voltammetry for test system ferro/ferri cyanide showed that the rate determination step was diffusion controlled, and quasi-reversible. The electrodes were tested for determination of hydrogen-peroxide by hydrodynamic amperometric measurements. Based on the results obtained with optimized analytical method 5% w/w of MWCNT in carbon paste electrode showed better analytical performances in terms of hydrogen-peroxide determination than the unmodified CPE, and the 5% w/w C-MWCNT-CPE, because of lower noise level and higher reproducibility of the developed method. The CPE modified with gold nanoparticles showed better analytical performances in alkaline supporting electrolyte than the MWCNT-CPE and C-MWCNT-CPE.

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Complex characterization of magnetic configurations in multiphase nanoparticulate systems (O08)

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Keywords: magnetic nanoparticulate systems, complex characterization, bio-medical applications

The development of advanced magnetic nanomaterials, of deep technological impact in our days, was related to both the refinement of the processing methods as well as to the improvement of the investigations tools. In addition, many efforts have been devoted to the comprehension of new physical phenomena specific to such nanosized magnetic systems. The remarkable new phenomena observed in magnetic nanostructures derive from the interplay between the intrinsic properties of the components, finite size effects and interphase interactions.

There is always an unavoidable difficulty to stabilize a definite crystalline structure or phase along the diameter of a few nanometer-sized particle, with direct influence on spin configuration and related magnetic relaxation phenomena. The work reports on various possibilities for a detailed characterization of magnetic configurations and relaxation mechanisms in multiphase nanoparticulate systems obtained by laser pyrolysis. Temperature/field/frequency dependent magnetometry techniques, combined with the powerful Mossbauer spectroscopy method provide relevant information in this respect. Iron oxide and iron carbide multiphase nanoparticulate systems with an average size of particles ranging from 3 to 10 nm, depending on processing conditions, are analyzed. Suitable methodologies for answering to delicate issues regarding the case of multiphase nanoparticles versus the case of nanoparticles of different phases, specific spin structures in case of multiphase nanoparticles, magnetic coupling of interfaced phases inside the same nanoparticle versus interparticle interactions, etc., are described and exemplified. The importance of such efficient characterization related to bio-medical applications is revealed.

Control of relaxation state for nanostructure formation based on glassy alloys (O09)

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Keywords: metallic glass, relaxation state, crystallization, nanostructure

Glassy alloys have attracted extensive interest in the field of materials science owing to the unique mechanical properties such as high strength, elastic modulus, hardness and so on. Recently, a number of glassy alloy compositions with high glass-forming ability have been developed, which results in the success of the production of *"Bulk metallic glasses (BMGs)"*. Glassy alloys are also evaluated as appropriate materials for the synthesis of nanocomposite by annealing due to their homogeneous structure in nano- or atomic-scale level.

It is well known that the relaxation state of glassy structure correlates to the structure, transformation behavior, mechanical and magnetic properties of glassy alloys. The authors have succeeded in controlling the relaxation state in Zr-based glassy alloys by changing cooling rates.[1] In the current study, the effect of relaxation state on the transformation kinetics of nucleation and grain growth is investigated.[2] The grain growth rate of the primary phase increases with relaxation. In contrast, the homogeneous nucleation rate decreases in the relaxed glassy alloys. The compressive plasticity is also lost with the relaxation. We conclude that the relaxation state has a marked effect on properties of glassy alloys. The results also provide useful information on the application of BMGs as well as the structural control of themselves, especially for the synthesis of nanostructured materials starting from the glassy phase.

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Design of semiconductor nanostructured materials using theory (O10)

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Keywords: semiconductor nanostructures, inverse design, machine-learning methods, third-generation photovoltaics

Understanding the structure-property relationship in semiconducting nanostructures is key to tailoring technologically important physical properties and can lead to the design of new nanostructured materials.[1] Examples include nanostructures in optoelectronic devices ranging from solar cells and novel lasers, to physical representations of a quantum bit, or single polarized photon sources emitting quantum bits.

However, a "complete" understanding of the relationship in nanostructures between the structural properties at atomic or molecular scales and their macroscopic properties is still pending. In the case of macromolecules or small alloy systems, it has been possible to relate a physical property, e.g., spectra, to the underlying structure, using predictive theory. However, for semiconductor nanostructures, typically containing $>10^4$ atoms, it is unclear what structural motifs, e.g., group of atoms, interface, or possibly mesoscopic quantities such as size, shape, or chemical profile, are responsible for a given physical property.[1]

The sizes of these nano-systems limit experimental methods and theoretical predictions. For example, the position of each and every atom within the nanostructure cannot be probed or controlled during the fabrication processes. Thus, the relevant structural information for the understanding of underlying physics and for technological applications is often limited to structural motifs such as constituent materials, geometry, and chemical composition profile (see e.g., Mlinar et al.[2]). From a theoretical viewpoint, the size of the system limits the usage of the atomistic first principle calculations. The empirical nature of the methods and various levels of approximations, introduce uncertainties in theoretical predictions. This suggests that theory and experiment can get only partial information about such large systems.[1]

In this talk, I will (i) show how to establish the relationship between the structure and properties in nanostructures; (ii) discuss the role of theory in the design of nanostructures with target physical properties; (iii) discuss the possibility of using theory to "guide" fabrication of nanostructures;[1] and (iv) address application of the nanostructures for renewable energy issues, in particular solar cells for third generation photovoltaics.

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Diameter control and one-dimensional N_2 gas inside single-walled carbon nanotubes (O11)

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Keywords: aligned SWNT, Nitrogen doped SWNT, Nitrogen gas filling, X-ray photoemission and absorption

Diameter controlled single-walled carbon nanotubes (SWNT) were synthesized from pure and mixed ethanol/acetonitrile feedstocks.[1] Vertically aligned films are grown from dip coated Co/Mo binary catalyst via no-flow chemical vapor deposition. With increasing acetonitrile concentrations the nitrogen incorporation of the sp^2 carbon network saturates at ~1 at.%. The incorporation of nitrogen correlates with a significant diameter reduction from 2.1 nm down to 0.9 nm. Heteroatom mediated diameter control on flat substrates is found to be independent of catalyst preparation and represents a versatile tool for the direct synthesis of tailored nanotubes.

The unexpected presence of a linear arrangement of co-axially oriented N_2 molecules inside sub-nm narrow aligned SWNT is revealed by high resolution near-edge X-ray absorption spectroscopy.[2] The encapsulated N_2 molecules exhibit free stretching vibrations with a long electronic lifetime of the X-ray-excited anti-bonding π^* states. Molecular dynamics simulations confirm that narrow-diameter nanotubes ($d < 1$ nm) are crucial for stabilizing this one-dimensional arrangement of aligned N_2 molecules.

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Effect of doping via ion-implantation on the crystallization, phase stability and binding energy in TiO_2 nanotubes (O12)

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Production of limitless hydrogen fuel by visible light splitting of water using the photo-electrochemical technology is cost-effective and sustainable. To make this an attractive viable technology will require the design of TiO_2 photocatalyst capable of harnessing the energy of visible light. One possible solution is the doping of TiO_2 to reduce its band gap. In this paper, the effect of Cr- and In-doping by ion-implantation on the crystallisation and phase stability of TiO_2 nanotubes at elevated temperature is described. The influence of Cr- and In-doping on the resultant microstructures, phase changes, binding energy and composition depth profiles are discussed in terms of synchrotron radiation diffraction, scanning electron microscopy, X-ray photoelectron spectroscopy ion-beam analysis and Rutherford backscattering spectrometry.

Electronic and optical properties of carbon nanotubes on metallic substrates (O13)

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Keywords: carbon nanotubes, ab initio, quasiparticles, excitons

We address theoretically the influence of a metallic substrate on the electronic and optical properties of carbon nanotubes. Recent STM experiments[1] have measured the bandgaps of single carbon nanotubes either directly in contact with a metallic substrate or at different heights from it. The image charge effect has been shown to lead to significant renormalization of the quasiparticle bandgaps, even for apparent heights larger than 1 nm. We study this long-range polarization effect on the electronic and optical properties of carbon nanotubes using state-of-the-art many-body *ab initio* approaches such as the GW approximation[2] for the electron self-energy and solving the Bethe-Salpeter equation[3] for excitonic effects. In particular, we will answer the question: do excitons in carbon nanotubes get quenched near a metallic substrate due to the image charge effect?

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Electronic and optical properties of organic conjugated polymers for optoelectronics (O14)

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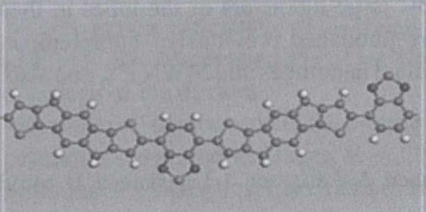
Keywords: semiconducting polymers, band structure, frequency-dependent dielectric response, HS06 hybrid DFT calculation

In this talk, I will describe my recent quantum mechanical calculations on the electronic and optical properties of conjugated semiconducting polymers for optoelectroincs. Specifically, we will focus on the fused ladder indacenpdithiphene alternating copolymers with both thieno-[3,2-b]thiophene (TT) and benzothiadiazole(BT), which are known to exhibit excellent charge carrier mobilities up to 1 $cm^2/(V\ sec)$. First, I will show that their UV-VIS absorption spectra are well described by the frequency-dependent dielectric response obtained from the calculation using the HSE06 hybrid DFT functional, when those polymers are described by one-dimensional (1D) systems in which a primitive cell contains two units of monomers in trans-confirmations. Major transitions responsible for the absorption maxima are also analysed in terms of band structures of those 1D systems.



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Electronic transport in intermediate sized multiwalled carbon nanotubes (O15)

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Keywords: carbon nanotube, electronic transport

We have measured the low temperature transport properties of single multiwalled carbon nanotubes (MWNT) of diameters (D) in the range 2–10 nm. Almost all previous work on MWNT's has been on tubes with diameters above 10 nm. In nearly all samples in this work, with $D < 10$ nm, the gate dependent conductance exhibits a gap whose size increases with the inverse tube diameter and increasing electrode separation. This so called transport gap is attributed, based on the experimental findings, on a combination of localization effects and narrow diameter induced gaps in the electronic band structure.

These results have significant similarities to the current research on graphene nanoribbons (GRN). As graphene does not intrinsically possess a bandgap, GNR's are fabricated, where a gap is created via quantum confinement due to the narrow width of the channel/nanoribbon. The size of the gap is then roughly in a similar inverse relation with the width of the constriction as in the case of the diameter dependence of the MWNT's in our work.

The transport gap has not generally been observed in the previous works on MWNT's because of the large diameters of the tubes in these. Our work, of which some early results were published previously,[1] complements and bridges previous works on both single walled nanotubes and MWNT's, and also to the field of GNR's.

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Emerging applications of carbon nanomaterials in energy and environment (O16)

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Over the past several decades there has been an explosive growth in research and development related to nano materials. Among these, carbon based nano-materials, have led the way in terms of their fascinating structure as well as their ability to provide function-specific applications ranging from electronics, to energy and biotechnology. In this talk we will present some of our recent investigations highlighting the use of carbon based nano materials (mainly carbon nanotubes and graphene) in energy storage applications (electrochemical double layer capacitors) as well as in energy conversion application (production of liquid fuels using carbon catalysts). Further, we will discuss the use of carbon nanotubes in the removal of toxics from contaminated water as well as in the control of the bioavailability of contaminated sediments.

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Enhanced light harvesting of Si solar cell via luminescent down-shifting using YVO_4 nanophosphors (O17)

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YVO_4:Bi^{3+}, Eu^{3+} phosphors are promising UV-absorbing spectral converters for solar cells because they possess broadband absorption in the whole UV region of 250 nm to 400 nm and they allow to the emission of intense visible lights. The current study demonstrates the increase in conversion efficiency of Si solar cells by incorporating rare-earth element-doped YVO_4 luminescent nanoparticles directly (without host materials) onto the textured surface of the devices.

The crystalline Si (c-Si) solar cell device used in the current experiment was manufactured following the procedures reported in Huang et al.[1] The SEM image of the YVO_4 nanophosphors shows that the nanophosphors had a nearly spherical shape with an average diameter of approximately 20 nm. The PLE spectrum shows the broad resonance expansion from 250 nm to 410 nm with a peak centered at around 352 nm, indicating that the YVO_4 nanophosphors exhibit the photon down-shifting property by absorbing of ultraviolet photons and converting them into visible with a high luminescent quantum efficiency of approximately 15%.

Spin-coating technique was used for nanophosphor deposition. Uniform and perfect light scattering YVO_4 nanophosphor thin films with a thickness of about 100 nm were obtained under properly controlled spin-coating rates. The c-Si cells with and without the nanophosphors were evaluated at room temperature based on the illuminated current density versus voltage (J-V) characteristics, external quantum efficiency (EQE), and reflectance. The highest efficiency increase of 0.7% was achieved when the solar cell surface was covered with YVO_4 nanophosphors using a concentration of 5 mg/ml. The presence of the YVO_4 nanophosphors provides a clearly visible EQE enhancement in the UV, indicating that the increase in photocurrent is mostly due to the enhanced absorption of UV by the YVO_4 nanophosphors. The EQE measurements are in agreement with the reflectance results, where the cell response improved in the wavelength ranges of UV and NIR because of the luminescent down-shifting and scattering of the YVO_4 nanophosphors. In the best case, the EQE enhancement ratio of the c-Si solar cells with YVO_4 nanophosphors was over 28% in the UV regions. V_{oc} and FF remained almost unaffected as J_{sc} increased from 35.3 mA/cm^2 to 36.8 mA/cm^2 with the integrated YVO_4 nanophosphors. Therefore, the enhancement in cell efficiency can indeed be attributed to the increase in photocurrent and light absorption.

The proposed hybrid system was shown to significantly enhance power conversion efficiency using the AM 1.5 illumination. The underlying mechanisms of the observed enhancement are attributed to luminescent down-shifting, as well as to index matching and light trapping.

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Fabrication and electrical characterization of CdO nanorods CdO/p-Si photosensors (O18)

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CdO nanorods were grown by sol gel technique and the structural properties were analysed by X-ray diffraction and AFM measurements. CdO films were grown onto p-type silicon substrates. Optical band gap was determined by optical absorption. The optical band gap of the CdO film was changed by Al dopant. Heterojunction diodes based on undoped and aluminum doped CdO/p-Si were fabricated using sol-gel spin-coating technique.The effect of light intensity on junction properties of the diodes was studied. The ideality factor of the diodes were obtained to be 2.30, 2.95, and 2.80, for undoped, 0.1%, and 1.0% for Al doped CdO diodes, respectively. The transient photocurrent results indicate that photocurrent under illumination is higher than the dark current. The on/off ratio values of the diodes were observed to be 5.84, 7.50, and

3.96 for undoped, 0.1%, and 1.0% Al doped CdO respectively. The observed decrease in the capacitance and increase in the conductance with increase in frequency was explained on the basis of interface states. The obtained results indicate that the photoresponse properties of the CdO/p-Si are controlled by Al doping.

Flexible electrodes prepared by reactive inkjet printing (O19)

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Keywords: flexible electrodes, inkjet printing, reactive ink

Conductive oxide materials such as indium tin oxide (ITO) and aluminum-doped zinc oxide (AZO) are widely used in advanced electronics and optoelectronic devices to meet the demands of having optically transparent coatings (T ~ 90%) with low sheet resistance (10–50 Ω/sq).[1] A gradually emerging disadvantage of these oxides is the shortcomings of indium and zinc resources, which are soon expected to result in increased market price and – in the worst case scenario – depletion of supplies. Therefore in the last decade tremendous efforts have been made to find alternatives for substituting ITO and AZO in transparent and conductive applications.[2] Here, we describe a novel technique to prepare flexible conductive films by inkjet printing reactive inks yielding deposits of metal films patterns on surfaces. Sheet resistance and optical transparency of grid- and ring networks with different spacing and line thickness have been assessed and compared to the performance of other types of coatings.

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Formation of the copper sulfide nanoparticles by ion exchange from electrolyte solutions (O20)

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Keywords: nanoparticles, copper sulphide, cadmium sulphide, ion exchange, band gap

One of the interesting materials for optoelectronics, solar cell, photo detectors and photovoltaic devices is copper sulfide semiconductor. This is due to the fact that this material can be formed in various stoichiometric forms . These materials possess very different physical properties and physic-chemical properties of these compounds strongly depend on stoichiometric composition. There are various methods of formation nanomaterials on the basis of copper sulfide: chemical bath deposition from electrolyte solutions, pyrolysis, vacuum evaporation, sonochemical syntheses and oth. Among them there is an attractive one – successive ion layered adsorption and reaction (SILAR). In the given work there was studied the possibility of transformation cadmium sulfide nanoparticles into copper sulfide nanoparticles by an ion exchange from electrolyte solutions. The technology of obtaining copper sulfide nanoparticles in a polymer matrix was carried out in two stages. First with help of successive ionic layer adsorption and reaction (SILAR) cadmium sulfide nanoparticles were formed in a polymer matrix(gelatin, polyvinyl alcohol or polybutadien). The second stage of this method consisted transformation of the cadmium sulfide nanoparticles into copper sulfide by an ion exchange from aqueous solution. At immersing a samples CdS/polymer nanocomposites in the water solution $CuSO_4{\cdot}H_2O$ of there is taken place an ion exchange process. The copper ions displace cadmium ions from the sample to solution. As a result of ion-exchange, cadmium ions move into the electrolyte solution. In the polymer matrix, cadmium sulfide nanoparticles are transformed to copper sulfide nanoparticles. The morphology of the obtained samples was investigated by the use of AFM. The average size of particles for 3 cycles of growth (initial stage of growth) are about 3 nm. The sizes of particles were growing with increasing of quantity of cycles. At 5 growth cycles the average size of particles are 14 nm. The results of XRD and EDAX investigation showed that when exchange time reaches ~29 hours cadmium sulfide nanoparticles are completely transformed into copper sulfide nanoparticles. In such kind of samples there are not observed reflexes from cadmium atoms. It should be noted that speed of the process of transformation defined by concentration, temperature and other environmental factors. It was investigated the transmission spectra for initial samples CdS and for samples after ion exchange with two concentrations of $CuSO_4$ solutions, 0.01 M and 0.03 M. Ion-exchange time was 130 minutes in both cases. Experiments showed, that, the concentration of the ion exchange solution affects the spectra and it begins to look more and more like copper sulfide nanoparticles spectra.

Using the transmission data, the dependence of $(\alpha h\nu)^2$ against $h\nu$ is calculated band gap of nanocomposites before and after an ion exchange were calculated. The band gap of samples decreases by increasing the concentration of ion exchange solutions. The initial CdS/PVA samples yielded a band gap is 2.48 eV whereas after ion exchange the bandgap reduces to 2.37 eV (for concentration of solutions 0.01 M), and to 2.30 eV (for concentration 0.03 M).

Increasing the ion-exchange time of the samples in the $CuSO_4$ solutions did not significantly affect the transmission spectra.

There were investigated FTIR spectra of nanocomposite samples on the basis of cadmium sulfide and polyvinyl alcohol in the far infrared region. A range of wavelengths is 70 sm^{-1}–500 sm^{-1}. After an ion exchange an absorption maximum of vibration spectres is displaced into the high energy area. This picture is characteristic at replacement of heavy atoms by light ones.

With help of the combination of successive ionic layer adsorption and reaction (SILAR) and ion exchange methods from aqueous solutions in a polymer matrix was formed CuS nanoparticles. The process of transformation of cadmium sulfide nanoparticles into copper sulfide nanoparticles has been studied. There have been investigated morphology, stoichiometric composition and optical properties of these structures depending on ion exchange time of CdS/polymer samples in $CuS0_4$ solution.

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Formation of titanium-dioxide nanostructures on the surface of medical grade implant materials and investigation of their effect on bacteria (O21)

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Keywords: nano-titanium, bacteria, implant

During the last couple decades many biomaterials have been developed as potential implant materials empowered by high biocompatibility. A lot of distinguished scientific achievements have been translated to implant products, however, the improved biocompatibility of implant materials with somatic cells entails their increased susceptibility for bacterial infections, as well.[1] Like in case of any implant material biofilm formation poses severe threat to the survival of titanium implants once they have been contaminated with pathogenic bacteria.[2] Most of the current titanium implants have micro pits and furrows on their titanium-dioxide surface because these structures are believed to support the attachment of osteogenic cells that play pivotal role in bone tissue formation around the implant.[3] Our hypothesis is that the increase of surface roughness of titan-dioxide in the nano range may bestow antibacterial attributes to titanium implant materials through contact interaction with bacteria, while it does not affect the attachment and survival of osteogenic cells on the surface. In our ongoing study we are preparing nanostructures on the surface of Grade 2, Grade 5 and nanocrystalline titanium discs by anodic oxidation and test their mechanical properties, resistance against bacterial infections, the attachment and differentiation of mesenchymal stem cells *in vitro*. As a result, we expect for definite answer to the question whether medical grade titanium materials with titanium-dioxide nanostructures on their surface are subjected to the same risk of infection than microporous titan-dioxide surfaces. Further expected result might be the exact determination of that value of surface roughness titanium implant materials that supports the adequate bone tissue formation but destroys the attaching bacteria.

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Functionalization of multi-wall carbon nanotubes with a bio-inspired hydrogenase mimic for hydrogen evolution and uptake (O22)

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Keywords: functionalization, material electrode, hydrogen

Among the new energy technologies, the use of hydrogen is an attractive solution. However, the hydrogen energetic chain must produce hydrogen in large quantities from water in devices called electrolyzers, and secondly use hydrogen in fuel cells to provide electricity through its oxidation. Currently these processes require using platinum as a catalyst. However, this metal is extremely rare and therefore very expensive. Getting rid of platinum and developing efficient materials that contain only abundant and cheap elements is a major challenge for the future of the hydrogen energetic chain.

To substitute platinum by abundant and low cost metals, researchers look at the chemical processes at work in living organisms which know how to use hydrogen as an energy source, or to produce it from water from abundant metals like iron and nickel.

That bio-inspired approach which tries to reproduce those natural processes involves the synthesis of compounds based on nickel and iron mimicing the active site of hydrogenase enzymes present in biosystems.

We present the catalytic activity for both the production and the uptake of hydrogen of nickel-based bio-inspired catalysts covalently bound on carbon nanotubes. This extremely stable material operates in highly acidic environment and is compatible with the Nafion® membranes. The development of this new material represents a new stage in the race for the improvement of the hydrogen solution for energy.

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Grain boundaries and nanoripples in CVD grown graphene (O23)

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Keywords: graphene, CVD growth, grain boundaries, STM, amorphous, polarized light microscopy, wave packet dynamic simulation

Chemical vapor deposition (CVD) of graphene is the most promising route towards the large scale production of the one single atom thick graphene films.[1] The material produced in this way is polycrystalline.[2] The grain boundaries (GBs) will have a significant impact on the electron transport in the CVD graphene.[3,4] The detailed characterization of the GBs is of utmost importance for the production of good quality CVD graphene. Another source of "built in" defects in the CVD graphene are the nanoripples originating from the steps formed on the surface of the Cu, they influence the electron transport even after the transfer of graphene onto an insulator substrate.[5]

Scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) are particularly useful tools in the investigation of graphene GBs on the Cu substrate used for growth. In this way all possible alterations of the GBs by the transfer process, or by e-beam irradiation can be excluded. STM and STS clearly indicate that the structure and the electronic structure of the GBs is different from that of graphene crystallites.[6]

We developed recently a polarized light microscopy (PM) based method that makes visible the graphene on the Cu substrate and also visualize the orientation of the Cu steps which are responsible for the formation of the nanoripples.[7]

Computer simulations based on numerically solving the time dependent Schrödinger equation shows that the GBs have a major impact on charge spreading in graphene.[8]

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High symmetry rotor-stator cocrystals of fullerenes (O24)

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Keywords: fullerene, cocrystal

Fullerenes have an unusually large number of solid state derivatives, like alkali metal salts, polymers and coctystals formed with a variety of inorganic and organic molecules. Most of the cocrystrals of fullerenes are host-guest or donor-acceptor materials.

However, fullerene-cubane cocrystals belong to a special family: they are built from separate sublattices, no host lattice can be defined in the structure.[1]

In the prototype of this family C_{60} molecules form an expanded face center cubic lattice in which cubane molecules occupy the octahedral voids. The topological recognition of the slightly concave faces of cubane (C_8H_8) and the convex surface of spherical C_{60} stabilizes the structure without preventing the rotation of fullerenes. Thus, the static cubanes behave like molecular bearings between the rotating fullerene molecules. As a result of this effect, the orientational ordering phase transition of fullerene-cubane takes place at the lowest temperature in all fullerene-based materials.[2]

A series of related cocrystals made of higher fullerenes and 1,4-disubstituted cubane components have similar structural characteristics but the influence of the lower symmetry gives rise to somewhat modified properties. Recently we extended the family of the rotor-stator materials to new high-symmetry derivatives: the cubane and mesitylene cocrystals of the endohedral trimetallonitride compound of C_{80}. $Sc_3N@C_{80}{\cdot}C_8H_8$ has a rocksalt structure with static cubane and rotating fullerene molecules. Interestingly, at ambient temperature the endohedral Sc_3N unit also rotates inside the fullerene cage.

Here we present the synthesis and crystal structure of the recently discovered members of the fullerene-based rotor-stator cocrystals and discuss the effect of the molecular geometry on the crystal structure and the rotor-stator dynamics. We compare the most important characteristics of these cocrystals with those of the host-guest type derivatives of fullerenes.

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Infrared signatures of correlation in expanded fullerides (O25)

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Keywords: fullerene, infrared, superconductivity

Cubic expanded fullerides are correlated superconductors; they show a phase diagram similar to that of cuprates. From the Mott insulating state lattice contraction leads to a metallic phase, with superconducting transition temperatures as high as 38 K in A15 structured Cs_3C_{60}. The metal-insulator transition leads to a drop in the electronic background absorption of the mid-infrared spectra and a lineshape transition of the vibrational peaks. In the insulating phase and in the case of high-symmetry crystal fields, Jahn-Teller distortion will appear in the vibrational spectrum. The presence of dynamic Jahn-Teller effect could be proven in both polymorphs of Cs_3C_{60}.

Iron-cobalt nanocrystalline alloy supported on a cubic mesostructured silica matrix (SBA-16): Synthesis and structural characterization (O26)

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Catalysts formed by active nanoparticles dispersed in an ordered mesoporous templated support have attracted much attention in recent years for their high potential in the fields of catalysis, sensors, separation membranes, electronic and magnetic devices, biology and nanotechnology. Until now, the research has been mainly focussed on the preparation of catalysts based on the ordered hexagonal mesoporous silica support (SBA-15), characterized by a two-dimensional array of ordered mesopores. However, the corresponding cubic mesoporous silica phase, SBA-16, appears to be more promising as a catalysts support since it is characterized by a three-dimensional ordered network of interconnected pores which provides better accessibility for reactants.

A series of nanocomposites consisting of FeCo alloy nanoparticles supported on a three-dimensional cubic mesoporous silica matrix (SBA-16) were prepared by wet impregnation of the matrix with a solution of Fe and Co nitrates. FeCo alloy nanoparticles were obtained by heat treatment at 800°C in reducing atmosphere of the impregnated SBA-16 previously calcined at 500°C. Three different SBA-16 types were used as a support of the nanophase. The influence of the matrix on the absorption of Fe and Co ions was investigated using X-Ray diffraction and X-ray absorption spectroscopy. In particular, extended X-Ray absorption fine structure (EXAFS) and X-Ray absorption near-edge structure (XANES) techniques at the Fe and Co K-edges were used in order to identify the intermediate products before reduction and to study the formation of the bcc FeCo alloy, which cannot be assessed unambiguously using X-Ray diffraction. Results have shown that most of the samples after calcination in air contain two separate phases: one phase containing cobalt, where Co has an oxidation state either +2 or intermediate between +2 and +3 and one phase containing iron, always with oxidation state +3. After the reduction treatment, FeCo alloy nanoparticles are formed in all samples; however, they show a certain degree of oxidation that varies with the matrix, and also with the concentration of the nitrate solution used for the impregnation and with the Fe:Co ratio. An important influence of the matrix has also been observed in the phases formed before reduction and in the size of nanoparticles.

Isotope engineering in carbon nanostructures (O27)

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Isotope engineering is the control over the ^{13}C enrichment of this otherwise weakly abundant nuclei. We achieved isotope engineering in single-wall carbon nanotubes (SWCNTs) with two avenues: one was direct growth from ^{13}C graphite the other was the growth of inner tubes inside SWCNTs from ^{13}C enriched fullerenes[1] (see Figure). These unique materials i) enabled identification of otherwise hidden vibrational modes, ii) provided clues about the mechanism of tube growth, iii) and enabled NMR experiments with an unprecedented sensitivity and specificity to the tubes.[2] The NMR studies provided evidence for the existence Tomonaga– Luttinger liquid ground state in the SWCNTs and for the occurrence of the so-called Luther–Emery liquid as a ground state.[3] The magnitude of the hyperfine coupling is the matter of intensive debate in the SWCNTs with transport studies contradicting to the common wisdom about the magnitude of the HFI in ^{13}C. NMR studies completed with the TLL theory resolve this issue.[4]

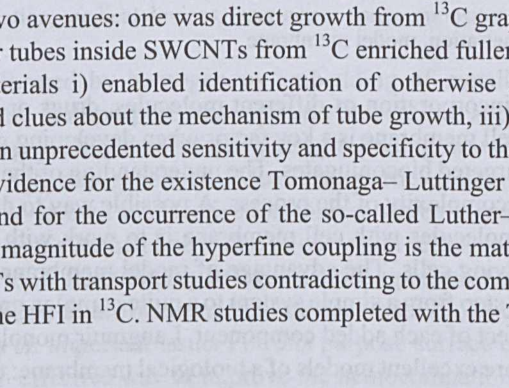

Figure 1. Schematics of the isotope engineered double-wall carbon nanotubes. The outer wall is of natural carbon, while the inner shell is highly ^{13}C enriched

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Langmuir monolayer study of the interaction of biofunctionalised gold nanoparticles with phospholipid membranes (O28)

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Keywords: gold, penetration, model membrane

The transport and incorporation of different molecules, drugs or bioconjugated systems in the living cell membrane is a key factor when developing new drugs, drug delivery systems or targeted bioconjugates. The understanding of the mechanism is very difficult due to the complexity of the process. A possible way to discover the interactions of different molecules with cell membrane is to work with model membranes which mimic the living cells. The advantage of model membranes is to build up the membranes step by step from a simple system to a quite complex one so it is possible to characterize the effect of each added component. Langmuir monolayers formed at the air water interface are excellent models of a biological membrane: there are a lot of parameters which can be varied easily such as the lipid composition, additional constituents (e.g. peptides), the subphase (composition, ionic strength, pH, etc.) and temperature to mimic the biologial membranes.

In this work we have prepared model membranes at the air/water interface: Langmuir monolayers of phospholipids. We have synthesized spherical gold nanoparticles and biofunctionalisation with cysteine and gluthation were carried out. The gold nanoparticles were characterized with TEM and DLS methods. The penetration of the biofunctionalized gold nanoparticles into the model membrane was studied by measuring the surface pressure of a preformed model membrane. The effect of membrane composition and the initial surface pressure were investigated. Monolayer films were transferred with Langmuir-Blodgett technique onto solid substrates and supported films were characterized with AFM technique.

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Laser-based synthesis of multimaterial nanocomposites for medical and optical applications (O29)

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Keywords: laser ablation, medical devices, laser-active nanocomposites

Nanocomposites, formed by homogenous embedding of metallic nanoparticles in polymer matrices, are multipurpose materials and find various applications in medical and optical devices providing anti-infective, drug-releasing, wavelength-sensitive linear and non-linear light absorption, etc. Metal nanoparticles such as silver, copper or zinc are already well- known as bioactive ion sources which in oxidative e.g. aqueous surrounding (such as the human body) due to corrosion release metal ions and therefore render antibacterial functionality to these nanocomposites. On the other hand, for an efficient application in artificial medical devices with blood-contacting surfaces, biocompatibility is an important issue. For this purpose surface endothelialization is considered to be an effective way to improve the hemocompatibility of artificial surfaces. Thus, we investigated the improvement of endothelization of polymers by integration of gold and platinum nanoparticles. It is however almost completely unknown that identical 'medical–purpose' nanocomposites provide great potential in a vast majority of optoeletronic applications.

In this study, we utilized a laser-based fabrication technique for the synthesis and direct embedding of ultrapure nanoparticles into various types of polymer matrices and analyzed their anti-infectivity, optical limiting behaviour and their effect on late outgrowth endothelial colony forming cells (ECFCs). Beside antibacterial potential, we also examined the effect of a broad concentration range of noble metallic nanoparticles (0.01–1 wt%) on the adhesion, proliferation as well as the inflammatory and antithrombogenic status of ECFCs cultivated on metal nanocomposites. Optical limiting effect of the same nancocomposites was analyzed in a femtosecond Z-scan study.

We observed that integration of nanoparticles significantly enhance cellular adhesion of polymer surfaces as a function of nanoparticle load and material. The highest amount of adhered cells were measured for the nanocomposite with 0.1 wt% Platinum nanoparticles resulting in a 4.5 ± 0.3 fold higher adherence of cells combined with significantly higher proliferation rates. Analysis of activation marker expression (ICAM-1, VCAM-1, E-Selectin, Thrombomodulin and Tissue Factor) and adhesion tests of leukocytes and platelets showed that the cultivated cells are in a non-activated but fully functional state. On the other hand for silver nanoparticle-embedded polymers perfect anti-infective property was found for 1 wt% Ag content. Finally non-linear light absorption started to occur for 10^{-6} J/cm^2 and higher laser fluences and provides total ultrafast laser-shielding for 0.1 wt% gold or silver nanoparticle content.

To sum up, embedding of various types of laser-generated metallic nanoparticles significantly improves the bio- and hemocompatibility, long-term stability and antibacterial property of used polymeric materials and provide also countless applications in optical devices and are considered as promising novel materials.

Luminescent silicon carbide quantum dots prepared by reactive bonding and subsequent wet chemical etching: Characterization and potential applications (O30)

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Visual analysis of biomolecules is an integral avenue of basic and applied biological research. Quantum dots (QDs) are semiconductor inorganic nanoparticles that are emerging as alternative or complementary tools to the organic fluorescent dyes currently used in bioimaging. In comparison with traditional organic fluorophores, QDs have a number of advantages including broad excitation and narrow emission spectra. QDs are more resistant to photobleaching than their organic counterparts, making QDs as a superior alternative of bio-imaging and further its applications in basic and applied biology. QDs are often made from of group II and VI elements (e.g. CdSe and CdTe) or group III and V elements (e.g. InP and InAs). Although these QDs have great potential as probes for bioimaging, certain limitations may restrict their applications. These QDs were found to be cytotoxic through the release of free metallic ions. Therefore, a protective shell must be systematically added. However, no protective shell can guarantee an efficient chemical isolation of the extremely toxic elements from the living cell environment. Cytotoxicity strongly influencing is one of the major limiting factors for the application of II–VI QDs in efficient *in vivo* imaging. We propose silicon carbide (SiC) QDs for bioimaging in order to eliminate numerous disadvantages of traditional QDs. SiC is a stable, chemically inert wide band gap indirect semiconductor. SiC QDs, with about 3 eV excitation energy, were successfully fabricated in many ways. The typical diameter is often less than 5 nm. Small size is also of importance in living cell applications for clearance. In addition, biocompatibility of bulk SiC and SiC QDs has been proven by several research teams. We developed a two-step experimental routine of producing SiC QDs. First, microcrystalline SiC (SiC MCs) is formed by reactive bonding method which, principally, allows us to produce highly doped SiC MCs in order to modulate the optical properties of the prepared SiC QDs made from them. SiC QDs form by electroless wet chemical etching of the SiC MCs. Under the etching, highly porous layer is created on the SiC MCs by using an acid mixture of HNO_3 and HF. SiC QDs are obtained by sonication of the porous SiC MCs in a specific solvent. These SiC QDs are less than 3 nm in diameter and make stable suspension in water without any surfactant added or any surface modification thanks to the surface termination that was studied by attenuated total internal reflection infrared spectroscopy (ATR IR). We found clear evidence of surface related IR bands characteristic of Si-O-Si, C-O-C, CH as well as COOH and OH. These polar groups on the surface give hydrophilic characteristic of the SiC QDs and give a chance to functionalize these QDs for sensing selected biomolecules and for therapy.

Toxicity of SiC QDs were determined through the Alamar blue assay using HeLa cells and we found that that there is no toxic effect if we attend the cells SiC QDs solution under 200 μg/ml SiC QDs concentration. The fluorescence of cell cultures with SiC QDs were successfully observed by means of fluorescence microscope and two photon microscope as well.

Macroscopic carbon nanotube fibers (O31)

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Despite their fascinating physical properties, commercial applications of carbon nanotubes are mainly limited to composites and breakthrough is yet to be realized. Integration, up-scaling or maintaining the performance of individual nanotubes in macroscopic devices is seemingly an obstacle. In this research, we are aiming at contributing to the realization of a potentially revolutionary idea, a brainchild of Richard E. Smalley, to reach the actual performance of conventional wiring materials such as copper and aluminum with the use of carbon nanotubes. We describe a technique to pull macroscopic wires of carbon nanotubes that have fusing current values only an order of magnitude lower than those are for copper wires with similar diameter. We also show simple wet chemical routes to increase the electrical conductivity of nanotube networks. Based on the results, we anticipate that with a proper combination and optimization of the two techniques, we will be able to bring a vision to reality.

Molecular plasmonics – biomolecules meets the colourful world of nanoparticles (O32)

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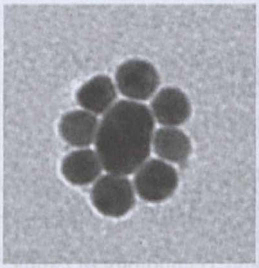
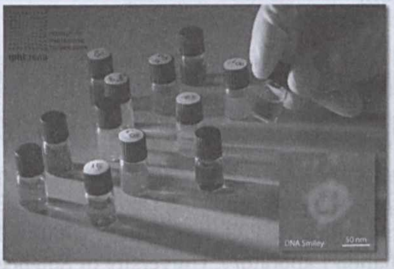
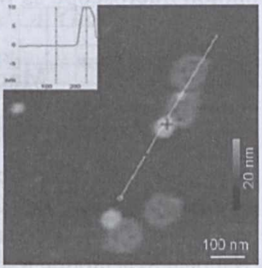
Nanoscale objects, especially metal nanoparticles offer optical behaviour completely different from bulk material based on their high surface-to-volume-ratio and effects based on their nano confinement behaviour. So these nanostructures can be allow novel readout principles for future biosensings and labelling techniques are nice antennas for optical nano biomanipulations or parts in novel photonic devices. Metal nanoparticles show by interactions with electromagnetic field well defined localized surface plasmon resonance (LSPR) based on the collective oscillation of their conduction electrons. This mostly macroscopic visible effect (color) is exact adjustable in the UV- to the NIR range by simple chemical synthesis with the parameters: material, shape and dimension. Especially, the particles in the visible spectral range offer an easily detectable optical signal. All changes in the surrounding media can be easily detected by the shift of the plasmon resonance band.[1,2] Sensor devices in ensemble and also below at the single particle level can be realized.







To enhance the sensitivity of these plasmonic transducers more complex structures are advantageous, they induce a local field-enhancement in form of hot-spots. For this biomolecules, like nucleic acids can be utilized. DNA shows a large potential for bottom-up construction principles in Nanotechnology.[3] Their sequence coded in the member of nucleotides and form so a well-defined biomatrix. The proposed geometrical arrangement is realizable using molecular self-assembly in parallel. One of the most innovative techniques for molecular constructions last years is the DNA-origami method, founded by Paul Rothemund.[4] The combination of this molecular technique with the nanoparticles opens new possibilities for future Plasmonics.

Acknowledgement: Financial support: DFG FKZ FR 1348/12-1, BMBF 16SV5386K, V4MNI014.

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MP-SPR – a new optical characterization method for ultrathin films (O33)

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Keywords: MP-SPR, ultrathin film, thickness, refractive index, molecular interactions

Surface Plasmon Resonance (SPR) has been used few decades for label-free detection and characterization of biochemical kinetics and affinities for many different types of analysts. However, the physical phenomena are not limited to measuring only biochemistry, but can be applied to many other different types of characterization.[1]

Multiparametric Surface Plasmon Resonance (MP-SPR) can be utilized to determine unique refractive index *(RI)* and thickness *(d)* of ultrathin films (d 0.5–100 nm) without knowledge of the RI of the material. These are important properties for many thin film coating industries and applications, such as insulation layers and antifouling coatings, but also important for biological and biomaterials basic research, such as determining lipid bilayer properties. The new method allows measurement of these properties for both dielectric layers, but also for metals and metal-like coatings that are difficult to measure with other optical methods.

Traditional optical methods, such as SPR and ellipsometry, require prior knowledge of either *RI* or *d* from other sources for accurate characterization of dielectric layers. This is because the measurements result in continuum answer, where *RI* and *d* depend from each other.[1] Two new methods utilizing MP-SPR have recently been introduced, either measuring in two different media (2M) with high *RI* difference, such as air and water,[1,2] or measuring at two different wavelengths (2W) of light,[2] such as 670 and 780 nm. The recent publications in this area show that the two methods can be applied to measure the properties of ultrathin films.

Strongly light absorbing materials, such as metals and semiconductors, have been difficult to measure with traditional thin film measuring optical methods, such as ellipsometry because they are mostly non-transparent materials.[3] However, for Plasmon generation needed for MP-SPR this is not as crucial issue. Also multilayer films, such as thin films with an adhesion layer, are challenging for ellipsometric methods,[3] while being clearly distinguishable from surface plasmon measurements as they change the overall shape of the SPR angular spectra measured in MP-SPR.[1,4]

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Nanocluster Bi-doped CdO thin films for optoelectronic applications (O34)

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Keywords: nanostructure metal oxide semiconductor, thin films, sol gel method

The nanostructure Bi-doped CdO thin films were prepared using sol gel spin coating method. The morphology and optical properties were investigated using Atomic Force Microscopy (AFM) and UV visible spectroscopy. The AFM results indicate that the CdO films are formed from the nanoparticles and the grain size of the films is changed with bismuth doping level. The optical band gap values of undoped and Bi-doped CdO films were determined by optical absorption method. The band gap value of undoped CdO film was found to be 2.589 eV, on the other hand, the band gap values of Bi-doped CdO films were found to be in the range of 2.657–2.684 eV. The band gap value of the CdO films is increased with the content of Bi dopant. It is evaluated that the optical band gap and grain size of the CdO film could be controlled by Bi-doping.

Nano-hydroxyapatite composites for medical applications (O35)

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Keywords: nano-hydroxyapatite, biocomposites, bone remodelling

Hydroxyapatite, $(Ca_{10}(PO_4)_6(OH)_2$ is chemically similar to the mineral component of bones and teeth. HAp is among of the few materials that are classified as bioactive, meaning that it will support bone ingrowth and osseointegration when used in orthopaedic, dental and maxillofacial applications. Hydroxyapatite may be employed in forms such as powders, porous blocks and hybrid composites to fill bone defects or voids. These may arise when large sections of bone have had to be removed or when bone augmentations are required (e.g. dental applications). In this work, nano-hydroxyapatite (nHA) was successfully produced by using recycled eggshell and phosphoric acid. The observed phases of the synthesised materials were dependent on the mixing ratio (wt.%) of the calcined eggshell and phosphoric acid, the calcination temperature and the mechanochemical activation method (e.g. attrition milling). nHA bioactivity was evaluated in animal (rabbit and mouse) models. Sixteen 4-month-old New Zealand white rabbits with an average weight of 2.8 kg (range 2.5–3.0 kg) were used in experiments. After bilateral parietal bony defects formation (diameter: 8.0

mm), nHA was grafted. The control was unfilled defect. The bone regeneration was evaluated by micro-computerized tomograms (μCT) and histomorphometric analysis at 4 and 8 weeks. In conclusion, nHA from eggshell showed much more bone formation compared to unfilled control group in both μCT analysis and histomorphometric analysis. Considering that the eggshell is easily available and cheap, nHA from the egg shell can be good calcium source in tissue engineering.

Nanoparticles: Toxicity and penetration across biological barriers (O36)

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Keywords: blood-brain barrier, culture model, drug delivery, drug targeting, microvesicle, nanopolymer, toxicity

Nanoparticles provide new opportunities for drug delivery and therapy. Two major aspects, toxicity and penetration across barriers of the body need to be determined to assess the therapeutic potential of nanoparticles. Different *ex vivo* and *in vitro* cell culture based models of the skin, nasal, lung, intestinal and blood-brain barriers have been established in our laboratory to study the biological effects of potential nanomedicines. Three different types of nanoparticles were tested. Amorphous nanoparticles from the antiinflammatory drug meloxicam were obtained by co-grinding with polyvinylpyrrolidone. Nanosized bilayered vesicles of non-ionic surfactants bearing glucose and amino acid ligands were prepared to specifically target solute carriers on the blood-brain barrier.[1] Poly(ferrocenyl silane) redox responsive polymer nanocarriers were also studied.[2] Toxicity was meausred by MTT dye reduction assay, release of the cytoplasmic enzyme lactate dehydrogenase and real-time, label free monitoring of cellular events. Quantitative information on cell viability and intercellular adherence indicating paracellular permeability was obtained by measuring impedance across microelectrodes covered with cells. Co-culture models of the barriers were prepared from primary cultures or human cell lines[3] and used to test the penetration of nanocarriers across cell layers. In the case of the blood-brain barrier a kinetic *in vivo* study in mice was also performed by near infrared fluorescence time-domain optical imaging. The results indicate that (i) toxicity measurements are crucial to define the optimal dose of nanoparticles on living cells, (ii) nanonization of drugs can improve drug dissolution, absorption and pharmacokinetics, (iii) targeting of microvesicles with solute carrier ligands increases their penetration across barriers.

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Nanoporous carbon from unburned carbon in bagasse ash (O37)

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Keywords: bagasse, unburned carbon and nanoporous carbon

Nanoporous carbon materials have been extensively studied in many fields of science and technology. They have excellent textural characteristics, tunable pore structure, thermal and chemical stability and good electrical conductivity. This leads to use in a number of applications as adsorbents, gas storage materials, as electrodes in supercapacitors, as a catalyst and catalyst support. A variety of raw materials including coconut shells, wood, coal as well as various agricultural waste (e.g. rice husk,[1] bagasse,[2] tea-industry waste etc.) have been used for their preparation. Bagasse fly ash is one such waste that could be used to get nanoporous carbon. The ash is generated in sugar mills where the bagasse residue obtained after sugarcane juice extraction is used as fuel in the boilers. The bagasse ash contains approximate 16–33 wt% of unburned carbon that could be easily separated and modified.

In this study, the preparation and characterization of nanoporous carbon from the unburned carbon is described. The unburned carbon was separated from bagasse fly ash through sieving and floatation techniques. The separated carbon was then activated in steam under different conditions to get nano porous carbon. The prepared carbons were analysed using techniques such as electron microscopy and nitrogen adsorption. The separated unburned carbon has a surface area of around 200 m^2/g whereas the activated carbon showed a surface area around 700 m^2/g. DFT analysis of the samples showed pores in the 12 to 15 Å range and in some cases, additional pores in the 7–8 Å range. In contrast, the unactivated separated carbon had pores in 10–12 Å range and an undeveloped peak at 5 Å.[3] The development of pores was visible and the samples showed presence of mostly amorphous carbon in transmission electron microscopy. The detailed characteristics of the carbon and their performance as adsorbents will be presented.

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A nanostructure pentacene thin film transistor with good performance using sol-gel derived SiO_2 gate dielectric layer (O38)

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Keywords: thin film transistor, pentacene, sol gel method

A low-voltage pentacene field-effect transistor with sol–gel derived SiO_2 gate dielectric was fabricated. The mobility of the transistor was achieved as high as 1.526 cm^2/Vs on the bared SiO_2/Si substrate by a higher dielectric constant. The interface state density for the transistor was found to vary from 3.8×10^{10} to 7.5×10^{10} eV^{-1} cm^{-2} at frequency range of 100 kHz–1 MHz. It is evaluated that the SiO_2 derived by low cost sol–gel is quite a promising candidate as a gate dielectric layer for low-voltage pentacene field-effect transistor.

Acknowledgements: This study is a result of an international collaboration program between University of Tabuk, Tabuk, Saudi Arabia and Firat University, Elazig, Turkey under project no. 4/1433 and international collaboration program between teams at King Abdulaziz University and Fırat University, Turkey.

Novel strategy for cancer cell specific oligonucleotide therapeutics with intracellular environmental condition responsible artificial nucleic acid: Peptide Ribonucleic Acids (PRNA) (O39)

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We have recently proposed a new strategy and a practical tool for cancer cell specific gene therapeutic artificial nucleic acids, named Peptide Ribonucleic Acids (PRNAs) with active *on-off* control of miRNA function corresponding the cancer cell specific intracellular environmental condition. The PRNAs can be actively switching the target miRNA complexation behavior by a low oxygen concentration of the cancer cellular cytoplasm. This strategy utilizes a new category of artificial nucleic acid that carries a ribonucleoside unit tethered to a peptide backbone as a recognition and stimulus-sensitive module. In this artificial nucleic acid called peptide ribonucleic acid (PRNA), the 5'-amino-5'-deoxypyrimidine ribonucleoside unit, which is in the anti conformation in normal cellular cytoplasm condition in the presence of borate, but functions as a built-in switch to be triggered by a low oxygen concentration of the cancer cellular cytoplasm, is attached to the alpha-glutamine backbone as a pendant. Under normal cellular cytoplasm condition, the cis-2',3'-diol of ribose forms a cyclic borate ester with phenyl boric acid moiety of the PRNA to switch the nucleobase orientation from anti to syn through the change in sugar puckering to 2',3'-planar-O4'-exo synchronized with the hydrogen-bond formation between the 5'-amide proton of ribose and the 2-carbonyl oxygen of pyrimidine nucleobase. The results obtained in these studies are promising, validating that the original alpha-PRNAs with anti-oriented nucleobases form stable complexes with the target miRNA under low cytoplasm pH (pH = ca. 6.5) of a low oxygen concentration of the cancer cell, which are readily dissociated under normal cellular cytoplasm pH (pH = ca. 7.2). This means that the PRNA strategy can be used as a powerful tool for on-off switching the miRNA complexation behavior, which is potentially applicable to the cancer cell specific oligonucleotide-based gene therapeutics of the next generation.

Nevertheless, RNA specific cleavage activities of PRNA-RNA complex with RNase H might be moderate due to a lack of negative charge of the PRNA backbone and unnatural double helical structure of PRNA-RNA complex. RNase H activities of antisense molecules would be one of the most crucial factors for practical antisense, siRNA, and miRNA related drugs (see References). Thus, in this study, we have been design PRNA-DNA chimera, in which both PRNA and DNA domains work as recognition sites for the complementary DNA and/or RNAs to form stable complex, while

DNA-RNA hybrids formed in the DNA domains of DNA-PRNA chimera should be substrates to the hydrolysis by RNase H and PRNA moieties work as recognition control/switching devices and as inhibitor for the hydrolysis of the chimera by nuclease.

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On the equilibrium of nano-systems (O40)

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Keywords: equilibrium, Kelvin, Gibbs, Ostwald, Freundlich

The equilibrium state of nano-systems is an important chapter of nano-sciences and is a basis of any nanotechnology.

The essential question is how to introduce correctly the surface term into the equation for the Gibbs energy. In view of the controversy between the Kelvin and Gibbs equations, even this task has not an obvious solution (in the present talk the Gibbs method is preferred). However, there are many further questions to be addressed when the method of Gibbs for the equilibrium of macro-systems is converted for the case of nano-systems. This talk attempts to give the full list of all those problems, such as: i. the definition of a new, independent thermodynamic variable, ii. the extended phase rule, iii. the size dependence of the interfacial energies, iv. the dependence of interfacial energies on the separation between interfaces, v. the role of the shapes and relative arrangement of phases, vi. the role of the substrate (if such exist), vii. the role of segregation, taking into account its effect on the mass balance within multi-component nano-phases. It is also shown that the well known meaning of the tie line in binary two-phase fields is lost in nano-systems. The issues related to the size limits of materials thermodynamics and the need for a more complete databanks on molar volumes and interfacial energies are discussed.

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Optical spectroscopy of "soluble" nanocarbon: Nanodiamond and graphene oxide (O41)

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Keywords: Raman spectroscopy, luminescence, nanocarbon, nanodiamond, graphene oxide

Nanodiamond (ND) possesses a number of unique properties. First, it is "soluble", i.e. forms stable colloids in water and other polar solvents. Furthermore, it is coloured (black, brown or yellow, depending on concentration). Detonation nanodiamonds, due to the small particle size (<4 nm), have a large surface area. The ND surface is hydrophilic, and may carry functional groups, which gives rise to promising applications: drug delivery, cell imaging, anti-friction additive etc.[1] For the past decade science faced a number of problems about ND:

- What is the origin of colour?
- What is the surface structure? Does it have sp2 or sp3 termination?
- What could be the origin of blue luminescence of ND, which is observed on surface passivation?[2]

Understanding of the surface structure and chemistry of ND is important for both fundamental and applied science. We investigate 4 nm (detonation produced) and 25 nm nanodiamonds (made by CVD) as materials with different surface-to-volume ratio to address these questions.

Another promising nanocarbon material is graphene oxide (GO). It also can easily form water colloids. The GO has conjugated sp2 clusters in its structure along with oxygen-grafted sp3 carbon.[3] In this work we take it as a model compound for spectroscopy investigation. We use Raman, hyper-Raman, infrared, UV-visible and luminescence spectroscopy to analyse the structure of ND and GO.

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Photocurrent from planar strips of multi wall carbon nanotubes (O42)

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Keywords: carbon nanotube, photocurrent

Photocurrent measurements derived by light excitation have been reported in different configurations exploiting carbon nanotubes (CNTs).[1–3] The study of light/CNT interaction offers opportunities to observe quantum confinement and new photophysical effects related to low dimensionality, opening the route to the development of new nano-optoelecronic devices. We report a study of photocurrent generation from a planar device made by growing simultaneously different strips of multi-wall carbon nanotubes (MWCNTs) onto quartz substrates.

MWCNT have been synthesized at 500°C and 750°C by thermal chemical vapour deposition (CVD) of acetylene (C_2H_2) gas, in ammonia (NH_3) atmosphere, onto nickel (Ni) catalyst nanoparticles. Gold (Au) electrodes have been evaporated on the ends and in the middle of each strip. The whole surface of the sample has been illuminated using a halogen lamp by means of an optical fiber and each MWCNT strip has been illuminated using a spectrophotometer beam. High photocurrent measurements have been obtained for the two samples and compared. We have shown that the photocurrent of all strips depends on the light spot position.[4] The highest photo-response has been obtained when the light spot was close to the electrode negatively biased. No experimental evidence can be found that the Schottky barriers have been formed at the conctact regions (nanotube-metal heterojunctions). We have also investigated photoconductivity properties of MWCNTs under ultraviolet, visible and near-infrared radiation using a spectrophotometer beam as a light source. It has been observed that the dark current versus bias voltage (I_d–V_{pol}) characteristics of each strip have an Ohmic behaviour, and the presence of all different radiation induces a photocurrent in each strip. The spectral photoresponse increases with increasing photon energy and is strongly correlated to the absorbance. These preliminary photocurrent measurements have demonstrated the ability of our devices to work as large area detector for white light as well as monochromatic incident radiation.

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Plasmon resonance frequencies and damping rates as a function of size of gold nanospheres (O43)

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Keywords: surface plasmons, nanoparticles, plasmon resonance frequencies and damping rates, size dependent plasmon properties, nanophotonics, plasmonics

Metal nanostructures, which have the capacity to resonate with electromagnetic waves, offer many interesting possibilities both in terms of fundamental sciences and applications. Noble metal nanoparticles are examples of such structures, as they support surface plasmons (SPs) in the optical frequency range. Metal nanospheres are the simplest and the most fundamental structures for studying the basis of plasmon phenomena. Controlling the plasmon properties is not possible without knowing the direct dependence of plasmon resonances and plasmon oscillation damping rates (damping times) on particle size. Still it is believed that existing theories do not allow the rigorous, direct calculation of such size characteristics.

We present the SP resonance frequencies and damping rates as a function of size up to uncommonly large particles of radius 1000 nm,[1,2] which could serve as a convenient tool in optimization of plasmon properties of noble-metal particles for scientific and technological applications. Our results show, that the significant increase in damping rates is followed by noteworthy decrease for larger particles along with substantial red-shift of plasmon resonance frequencies with increasing particle size. We demonstrate unexpected reduction of the multipolar SP damping rates in certain size ranges.[2] This effect can be explained by the suppression of the nonradiative decay channel resulting from the lost competition with the radiative channel.

We also show that experimental dipole damping rates,[3,4] and the resulting resonance quality factors can be described in a consistent and straightforward way within our modelling extended to particle sizes still unavailable experimentally.

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Plasmonic nanoparticles for photocatalysis and biomedical applications (O44)

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Keywords: silver, gold, nanoparticles, hybrid materials, biomolecules, plasmonic coupling, surface plasmon resonance spectroscopy

Plasmonic noble metal nanoparticles (Ag and Au) are able to sensitise photocatalysts in visible light by modifying the TiO_2 surface with different (0.1–0.5 wt%) loading. Modifications with silver and gold lead to a change in the optical properties due to the plasmonic light absorption on TiO_2 surface. The Ag- and Au-modified plasmonic TiO_2 can be excited by the incoming light without much loss of the photon energy. We have theoretically also studied and optimized the field enhancement and temporal response of single and coupled bimetal Ag/Au core–shell nanoparticles(NPs). We synthesized small bimetal Ag/Au core–shell NPs and compared their optical response with pure Au and Ag NPs and numerical results. Very high-field enhancements in nanoplasmonic field were demonstrated using the fine element calculation methods. The TiO_2 photocatalysts were also functionalized by core-shell Au/Ag NPs. The synergistic effect was established in the photocatalyical processes using solar light or LED light source ($\lambda = 405$ nm).

Gold surfaces and nanoparticles/nanorods were functionalized by biomolecules. Lysozyme stabilized gold nanodispersions and bilayered gold nanorod films were prepared and their optical properties (photoluminescence) were measured. The plasmonic coupling effect takes place between the gold nanorods and the lysozyme protein.

The surface plasmon resonance spectroscopy (SPR) on Au film was used for determination of the interaction between the biomolecules (proteins and drug molecules). Adsorption binging isotherms and energy can be determined. These SPR experiments on nanoscale are very useful to give quantitative data to the controlled drug delivery in nanomedicine. Transport of drug molecules and bioconjugated systems across the cell membrane is a key factor fro drug delivery systems. We examined the penetration/incorporation of gold functionalized NPs through Langmuir phospholipid films. The surface pressure was measured and AFM and FTIR characterization are given for the gold nanohybrid-lipid membrane films.

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Polymer properties enhancement by hybrid nanofillers (O45)

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Keywords: nanotube, epoxy, composite, fracture toughness

Both carbon nanotubes (CNT) and graphene nanoplatelets (GNP) possess excellent electrical/thermal conductivity as well as mechanical properties, which make them ideally suited as fillers to enhance properties of epoxy composites. However, the high aspect ratios of these objects along with the strong vdW attraction between them result in CNT entanglement and in GNPs stacking to graphite flakes. Furthermore, the chemically inert nature of carbon based nanofillers leads to poor dispersability and weak interfacial interactions with the matrix.[1] The present study aims at fracture toughness enhancement of CNT-epoxy composites obtained by surfactant-assisted dispersion of GNPs and CNT dispersions at high concentrations in water.The dispersion is then lyophilized and integrated in an epoxy matrix. The effect of nanofillers addition on the thermomechanical, mechanical and electrical properties of CNT–GNP-Epoxy nanocomposite is then evaluated. We employ a variety of surfactant-assisted exfoliation procedures to obtain a stable dispersion of GNP and CNT in water. The solution is first characterized by cryo-transmission electron microscope (water/CNT solution) where individual CNTs are found. The solid composite (Epoxy/CNT after hardening) is microtomed and imaged by TEM at room temperature indicating no CNT aggregation.

The dispersions stability and the final concentration are determined by UV-VIS spectroscopy and thermogravimetric analysis. Excellent dispersions, using nonionic (polyoxyethylene octyl phenyl ether) and protein-based surfactants (β-Lactoglobulin), are obtained in both water and Epoxy. The biding of the dispersant to the CNT is rather weak, as indicated by self-diffusion NMR spectroscopy.[2] Finally, the fracture toughness is found to increase by 130% upon loading the epoxy matrix by 0.15 wt% CNT (Figure 1).

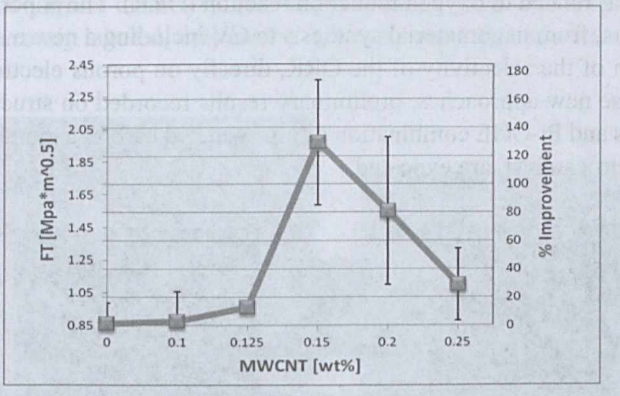

Figure 1. Fracture toughness (FT) of epoxy loaded by carbon nanotubes filler

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Porous nanostructures based on carbon nanotubes and capped platinum electrocatalysts through bottom-up approach: Model and efficient electrodes structures for fuel cells (O46)

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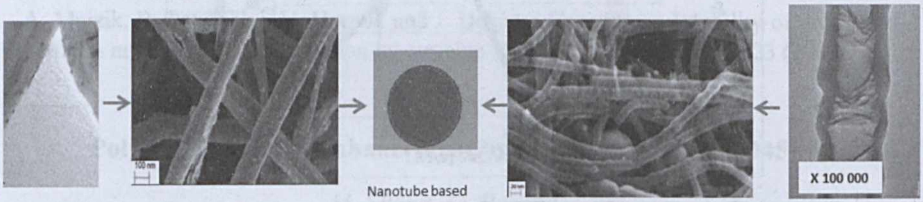
Keywords: nanoparticle, carbon nanotube, nanostructure, electrocatalyst, energy conversion, fuel cell

This paper provides an overview of our research over the past few years on the elaboration and characterization of porous electrodes for fuel cells, using a bottom-up approach. It involves the synthesis of various original Platinum Organically Grafted Electrocatalalysts (Pt-OGE) and carbon nanotubes (CNT), and the formation of model and efficient porous electrodes on carbon felts, with Pt loading from 0.1 $\mu g_{Pt}.cm^{-2}$ to few hundreds.[1] Thanks to the high degree of control offered by the bottom-up approach at each step of the process, we determined by cyclic volammetry (CV) a new feature parameter:[2,3] the specific area of porous electrode, ($ADiffO_2$ in $m^2.g^{-1}$ of electrocatalyst) related to oxygen reduction reaction (ORR). The paper presents these original results, from nanomaterial synthesis to CV including a new method allowing determination of the selectivity of the ORR, directly on porous electrode structures. Based on these new approaches, preliminary results recorded on structures based on carbon blacks and Pt-OGE combination or nitrogenated carbon nanotubes, as non noble ORR electrocatalyst, are evocated.



Platinum based structures

Nanotube based porous electrode formed on carbon felt

Nitrogen doped carbon nanotubes based structures

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Quasi 2-dimensional actin models: Is the bundling irreversible? (O47)

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Actin is one of the most abundant and critical components of the cytoskeleton of eucaryotic cells, contributing to the mechanical properties of cells such as shape, adhesion and response to external mechanical stimuli. In filamentous form it is a semiflexible polymer, which has been intensively studied in-vitro constructing three dimensional gels in droplets or single filaments in confined (few micron high) spaces. Such reconstructed networks allow studying the behavior of the filaments, such as their interaction, network formation and mechanical properties in a controlled physical-chemical environment. In our work we use microfluidic devices to construct thin, quasi two dimensional networks of actin morphologically approximating parts of the cellular actin cortex or stress fibers in the cytoskeleton. Though the individual filaments are about 8 nm in diameter, their length is in the order of 20–30 micrometers, they are fluorescently labeled, thus can be observed using high resolution optical microscopy.

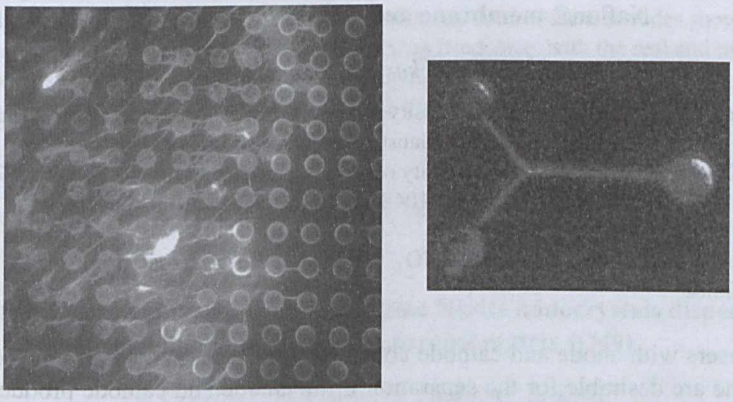

Figure 1. Example of a 2D actin network on a micropillar scaffold (left) and single filaments on a particle anchor set (on the right) held by holographic optical tweezers

Applying an elastic scaffold, such as elastic micropillars or microparticles trapped by multiple optical tweezers, one can form networks with stiff anchoring points, morphologically similar to the bottom cytoskeletal layer of an adhering cell. The topology of the network is controlled by the local flow conditions as well as the presence of crosslinker agents.

In our research we have created thin, quasi two dimensional networks of actin from single filament level up to complex random meshes formed by in-situ polymerization upon micropillar arrays. The filaments are attached to the surface only at the pillar tops or the microbeads, but stand free in between. Bundling actin using various biochemical agents (actin binding proteins and divalend cations) showed a zipping-like bundling mechanism, enforced by the crossed or splayed configuration of the filaments in the network. Measuring the forces acting during the bundle formation at single filament level, we have detected values up to 0.1–0.2 pN when magnesium or calcium ions were employed. The concentration dependence of these forces shows a saturation type curve. Interestingly, in all of our experiments the bundling process was found irreversible, thus the frontier of the bundling was moving in one direction only. The resulted network is a soft elastic system, where the diffusion is hindered by the anchoring points, resulting a broader band rubber plateau than what was observed in three dimensional gels in previous literature.

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A solid-state photoelectrochemical water splitting cell with a composite Nafion® membrane and gaseous reactants (O48)

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Keywords: water splitting, hydrogen, TiO_2, solid-state, charge transfer, impedance spectroscopy, Nafion®

Electrolysers with anode and cathode compartments separated by an ion conducting membrane are desirable for the separation of the anode and cathode products. If the membrane acts as a support for the electrodes (e.g. polymer electrolyte membrane water electrolyser), additional advantages of device compactness and a short travel path for ions are obtained. Photoelectrochemical (PEC) water electrolysis, which uses light energy as a source of electrical energy, has the potential of making hydrogen production viable in such a device if there is efficient photogeneration and utilisation of electron hole pairs.

We report, for the first time, on a Nafion® $_+ Mo_{0.5}W_{0.5}O_3 \cdot 1/3\ H_2O$ composite membrane for PEC water splitting, using gaseous water/methanol, as opposed to liquid reactants.[1] Oxidising gaseous feedstock at the anode is more favourable from thermodynamic view point. The anode and cathode catalysts are nanoparticles of TiO_2 or WO_3 (photocatalysts) and Pt-C (electrocatalyst), respectively (Fig. 1a). Current-voltage and chronoamperometric measurements indicate that photocurrent is produced upon illumination, even without applied external voltage. From electrochemical impedance spectroscopy (EIS) studies, we show that photogenerated charge species accumulate at the electrodes upon illumination, leading to increase in the resistance and capacitance of the electrodes with increasing light irradiance, in spite of a corresponding increase in overall cell photocurrent (Fig. 1b–c). As an example, an irradiance of 33 mW/cm^2 increased the resistance and capacitance at the electrodes by 50% and 190% respectively, while increasing the cell's photocurrent significantly (inset of Fig. 1b). Ongoing studies aimed at eliminating this charge accumulation, which is vital for improving the efficiency of the device, are highlighted.

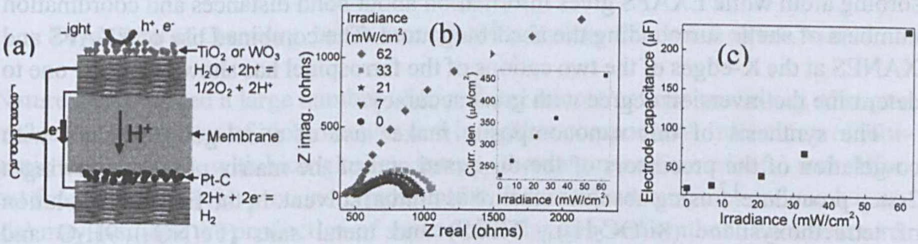

Figure 1. (a) Schematic of the PEC cell, with reactions at the electrodes shown, (b) EIS spectra of the electrode processes at varying irradiance, with the real and imaginary components of the impedance on x- and y-axes, respectively. The inset shows the overall current density vs irradiance, (c) Electrode capacitance vs irradiance

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The study of the inversion degree in zinc ferrite nanocrystals dispersed on a highly porous silica aerogel matrix (O49)

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Bulk zinc ferrite is a normal spinel with Zn^{2+} cations occupying tetrahedral sites and Fe^{3+} cations occupying octahedral sites. Therefore, it is not magnetic at room temperature, with a $T_{Néel} = 10$ K. However, a rearrangement of the cation distribution has been observed when this ferrite is at the nanoscale and a partially inverted structure is obtained, which is responsible for an enhanced magnetization. Therefore, this is an ideal system to study the effect of particles size on the distribution of cations in ferrospinels.

Several techniques can be used to study the inversion degree, such as X-ray (XRD) and neutron (ND) diffraction and Mössbauer spectroscopy. However, the effectiveness of XRD is limited by the similarity of the scattering factors of the cations, while Mössbauer spectroscopy is effective in determining the environment of Fe^{3+} ions but does not provide information on the bivalent cations and is not very effective for dilute samples.

On the other end, X-ray Absorption Spectroscopy has been shown to be a very powerful tool to determine the cation distribution in ferrite spinels, since it is ideal for studying multicomponent dilute and disordered materials, being element specific and sensitive to the local structure. Both Extended X-ray Absorption Fine Structure (EXAFS) and X-ray Absorption Near Edge Structure (XANES) provide valuable information: XANES gives information on site symmetry and oxidation state of the absorbing atom while EXAFS gives information about bond distances and coordination numbers of shells surrounding the absorbing atom. The combined use of EXAFS and XANES at the K-edges of the two cations of the ferrospinel has shown to allow one to determine the inversion degree with great accuracy.

The synthesis of this nanocomposite makes use of a sol-gel procedure with co-gelation of the precursors of the dispersed and of the matrix phases following a 2-step procedure[1,2] using absolute ethanol as mutual solvent. In the first step a solution of tetraethoxysilane ($Si(OC_2H_5)_4$, TEOS) and metal salts ($Fe(NO_3)_3 \cdot 9H_2O$ and $Zn(NO_3)_2 \cdot 6H_2O$) are prehydrolyzed by adding a hydrolyzing acidic solution of nitric acid. In the second step, a gelifying basic solution containing urea (NH_2CONH_2) is added to the pre-hydrolyzed sol to promote a fast and homogeneous gelation, which occurs in less than 2 days. In order to obtain aerogels with highly extended and open porosity (up to 98%), low densities and high inner surface areas, the wet gel undergoes supercritical drying in an autoclave (Parr, 300 cm^3) to avoid the capillary forces at the liquid/vapor interface responsible for shrinkage and cracking of the original porous structure. The sample is then thermally treated up to 900°C in air.

EXAFS and XANES spectra were recorded at beamline 11.1 (XAFS) of the ELETTRA synchrotron (Trieste, Italy). Spectra at the Fe (7112 eV) and Zn (9659 eV) K-edges were acquired at room temperature in transmission mode using a Si (111) monochromator on the nanocomposite sample submitted to three different thermal treatments, 750°C for 1 h, 750°C for 6 h, 900°C for 1 h and on two $ZnFe_2O_4$ bulk samples, one prepared by us, and one commercial sample provided by Alfa Aesar.

Both XANES and EXAFS results indicate that the aerogel samples are partially inverted and that the degree of inversion decreases with increasing particle size. In particular, the degree of inversion *i* was determined with great accuracy by fitting the fraction of tetrahedral (A) and octahedral (B) sites occupied by Fe^{3+} and Zn^{2+}. The results of the fitting indicate that only the bulk zinc ferrite with the largest nanoparticles is a normal spinel, while some degree of inversion is present in all the other samples, the value being 0.21 for both the commercial bulk sample, and the nanocomposite thermally treated at 900°C for 1h, and increases further in the samples thermally treated at 750°C, the values being in this case 0.29 and 0.41 for the sample treated for 6 h and for 1 h, respectively.

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Supramolecular directed assemblies of biotemplated metal/semiconductor nanohybrids (O50)

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Nature has designed a large number of functional nanostructures consisting of supramolecular aggregates of biomolecules and inorganic components. Interaction of inorganic nanoparticles with biological systems possessing nanodimension(s) and different functionalities (viz. proteins, lipids, antibodies, antigens, enzymes and nucleic acids) may facilitate the production of supramolecular directed synthetic nanostructures of varied dimension with changed physicochemical properties.

In recent years, there has been an enormous interest in making nanohybrids of biomolecules with metal/semiconductor nanostructures specifically to replace the fluorescent organic dyes employed presently as biomarkers. Moreover, these systems have several added advantages over organic dyes as regards to their tunable optical and fluorescing properties, higher solubility, and enhanced chemical and photostability. Among different biomolecules, functionalized biopolymers have lately been employed extensively for templating of nanomaterials. These consist of long range nanoscale order which could be tailored to fabricate artificial nanostructures with tunable properties.

Synthesis of colloids by using chemical methods provides an interesting methodology to grow a variety of nanostructures in solution using bottom up approach. Colloidal nanostructures with distinctive size tunability, manipulative surface characteristics and charge demonstrate an enormous potential to mediate the synthesis of nanohybrids using biomolecules as template. Integration of the functionalized biomolecules to inorganic colloidal nanomaterials is a challenging area of research to design new materials of required dimension/morphology with enhanced physicochemical properties, surface characteristics and increased photostability. An understanding of the interaction of semiconductor quantum dots with biomolecules through its various functional sites may provide a key to optimize their nucleation and growth needed for the fabrication of new nanostructures.

The present lecture will focus on the potential of biomolecules as template for the synthesis of nanohybrids comprising colloidal semiconductor and metal nanoparticles. Several biotemplated nanosystems consisting of metal chalcogenides and metal nanoparticles will be discussed. In the presence of biomolecules the nucleation and growth of inorganics has been observed to differ significantly to yield quantized nanostructures with novel optical, emission and magnetic properties. Self-assembly of these nanostructures demonstrates some interesting changes in their morphology and dimensionality from Q-dots *to* nanowires/nanofibre/nanotubes associated with further enhancement in their properties. These changes have been attributed largely to increased interfacial and polar interactions. Different schemes explaining these interactions will be presented. A correlation between surface morphology, electronic properties of these materials and the mechanism of these processes will be discussed. The production of quantum confined nanostructures with a control of dimensionality/shape and subsequent organization into hierarchical system with tunable properties may find potential usages in the fabrication of advanced materials for optical, electronic, magnetic, solar energy conversion and biomedical applications.

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Surface modification of aerosol nanoparticles for materials applications (O51)

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Keywords: aerosol, nanoparticle, surface modification

The surfaces of aerosol particles, especially nanometer-sized aerosol particles, present a fascinating and compelling challenge to the materials scientist. Aerosols have become increasingly important in the synthesis of certain nanostructured materials.[1,2] At the same time, recent advances in instrumentation have created new opportunities for studying chemical processing. It is now possible, for instance, to monitor adsorption or desorption of monolayer quantities of material on an authentic aerosol. This presentation will describe the potential use of aerosols for high-yield synthesis of nanparticles for materials and biomedical applications, explored through examples out of our laboratory. In one study, ZnO aerosol nanoparticles were synthesized via thermal decomposition of an organometallic precursor. The interactions of the simple amine functional groups with the surfaces of aerosol ZnO were investigated and shown to lead to the formation of amide monolayers. In another study, serial reactor consisting of a spark particle generator coupled to a collison atomizer was used to fabricate the new materials of potential biomedical application. The materials included nanomagnetosols (comprising iron nanoparticles, the drug ketoprofen, and a Eudragit shell), hybrid nanogels (comprising iron nanoparticles and an N-isopropylacrylamide, NIPAM, gel), and nanoinorganics (gold immobilized silica) . A fourth hybrid material, consisting of iron-gold nanoparticles and NIPAM) was obtained via an aerosol into liquid configuration, in which aerosol iron-gold particles were collected into a NIPAM/ethanol solution and then formed into nanogels with NIPAM under ultrasonic treatment. The strategies described in this work are potentially generalizable as new platforms for creating functionalized nanoparticles and nanocomposite materials, using only simple starting materials in a single pass reactor and under low temperature conditions.

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Synthesis and surface modification of nanoparticles for theragnostics (O52)

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Keywords: theragnostic, bioconjugation, ferrofluids

Composite nanostructures containing a superparamagnetic material represent a versatile platform for the design of multifunctional tools for biomedicine, ranging from anticancer treatment, cell imaging and magnetic separation.[1] In particular, iron oxide superparamagnetic nanoparticles offer the privileged status of being accepted for clinical purposes.

In this work, multifunctional ultrasmall superparamagnetic iron oxide (USPIO) coated by either biopolymers, non-toxic commercial dispersants, silica or gold were tested as contrast enhancers in magnetic resonance imaging (MRI) and as magnetic hyperthermia mediators. In particular, synthetic protocols were developed in order to tune the nanocrystal size and shape. XRD, TEM, FT-IR, TGA, N2-Physisorption and DLS techniques were used to gain insights on the structural and morphological features of the materials as well as on the features of the coating. SQUID magnetometry has been used to investigate the magnetic behaviour of the nanoparticles by zero field cooled-field cooled measurements as well as the field dependence of the magnetization at low temperature. NMR-Dispersion (NMRD) profiles, i.e., the measurements of proton nuclear r_1 (longitudinal) and r_2 (transverse) relaxivities as a function of frequency were collected in order to gain insights on the ability of the materials to act as contrast agents for MRI. The potential of the nanostructures in magnetic hyperthermia was assessed by Absorption Rate (SAR) measurements.

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Textile and antifungal behavior of a cotton woven support to ultrasonically deposited copper oxide nanoparticles by means of two different methods (O53)

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Keywords: nanoparticles, copper oxide, antifungal effect, medical textiles, ultrasonication, *Candida albicans*

The extent use of textiles from traditional to modern applications transformed entirely in the last 50 years the textile industry. New fibers obtained from natural sources or produced by innovative technologies emerged on the market especially in the medical, sport and technical sector reshaping our vision about the structural and functional limits of textile elements (fibres, yarns, plane products).

In the health care sector a special attention is given today to all types of products that are able to lower the risk of infection with pathological agents like bacteria and fungi. In hospitals, the nosocomial infections are still an important problem, in the same time with the development of microorganism resistant to normal antibiotic therapy. Thus, functionalized materials with antimicrobial properties started to be developed, and the approaching are made from different levels of the textile support: incorporation of the antimicrobial agent during the spinning process, attaching it on the fibers or yarns, applying biocidal biomolecules or other types of substances by many techniques on the 2D textile support, etc. Moreover, researcher all over the world are trying to obtain the antimicrobial effect by using natural and ecological substances.

We present part of a work that is carried on a FP7 project where an ultrasonical technique is used to deposit nanoparticles of metal oxides on different textile supports. The results obtained after the deposition of copper oxide derivated from two chemical forms, from nanopowder and from copper acetate on a cotton 100% woven show a slightly different pattern of action between them especially in the case of the antifungal effect. Structural textile characteristics were analyzed through physical, physico-mechanical, SEM, AAS analysis. The antifungal effect was demonstrated for *Candida albicans*.

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Time resolved optical measurements on different architectures of carbon nanotubes as a basis of new photovoltaic devices (O54)

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Keywords: carbon nanotubes, time resolved optics, exciton dynamics

In these last twenty years carbon based materials have been among the main actors of a fundamental match played in the research field on solar cells and sensor devices.[1] In general the optical devices contain Carbon Nanotubes (CNT) ensembles, combined with several other systems (nano-particles, molecules, metallic connectors, substrate...). Therefore it is essential to undertake an experimental analysis of the complex CNT ensembles as a preliminary step toward a deeper understanding of the composite systems.

In this framework, a fundamental knowledge of the charge carriers dynamics, charge transfer[2] and charge transport into and between the different parts of the whole system is necessary in order to achieve the goal of increasing the efficiency, choosing the better configuration and the most useful components.

Besides Single Wall Carbon Nanotubes (SWCNTs), Multi Wall Carbon nanotubes (MWCNTs) represent a very promising challenging materials for several technological applications. For example, their enhanced conductivity constitutes a huge benefit for different technological aims. At the same time, open issues have to be addressed in order to understand the MWCNT electronic structure and improve their optical response.

In this talk time resolved optical analysis are carried out on different CNT architectures: vertically aligned SWCNT and vertically and horizontally aligned MWCNTs. In particular time resolved optical techniques allow to follow the dynamics of the photoexcited carriers in the CNT ensembles.

One of the main result concerns the MWCNT transient optical response, which reveals a SWCNT-like rather than a graphitic-like behavior. This result can clarify an old open question about the nature of MWCNT electronic structure.

Time resolved techniques, revealing, linear and non-linear excitonic effects both in SWCNT and MWCNT aligned systems can open, in particular, interesting perspectives in the use of MWCNTs.

These measurements represent the initial step of a project whose ultimate goal is to improve the efficiency of photovoltaic devices based on SWCNTs or MWCNTs systems, in which different CNT architectures are combined with nanoparticles or organic groups.

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Universal approach to covalent immobilization of silver nanoparticles on solid substrates (O55)

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Keywords: covalent immobilization, silver, nanoparticles, universal approach

Over the last twenty years, the silver nanoparticles have become one of the most intensively studied materials due to its possible application in several fields such as catalysis, SERS, and as an antibacterial agent. The already published studies proved that AgNPs perform similar or even greater antibacterial and antifungal effect than more toxic ionic silver at comparable or higher concentration[1,2] and at the same time bacterial resistance against the Ag NPs has not been proved. These two facts predetermine the AgNPs usage of the applications in medicine, for the treatment of environmental issues, or as disinfection agents

The objective of our research is to suggest a synthetic approach of a composite preparation in which all disadvantages of previous methods (i.e. aggregation of the particles, release of the NPs into the environment, etc.) would be eliminated. The attention will be also paid to the universality of the suggested approach and to the fact that it must be environmentally acceptable, i.e. the system, in which the immobilization is realised cannot involve toxic chemicals or its traces. We have chosen several substrates (non-woven fabric, catheters, hypodermic needles) that can be interesting from the application point of view and modified them by branched high-molecular synthetic polymer (polyethylenimine – PEI). This polymer is sufficiently adhesive to different materials and at the same time it can offer its reducing power,[3] throughout which the silver precursor is reduced and the generated AgNPs are at the same time immobilized to the surface. Only such composite materials can be used in variety applications because the deposited AgNPs are aggregation free and additionally they can provide the antibacterial action even when the substrate is mechanically stressed.

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Unravelling the correlated electronic and optical properties of tailored low dimensional carbon hybrids (O56)

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The presentation will give an overview on our current research focus on the electronic properties of carbon based low dimensional hybrid structures. These properties are strongly influenced by basic correlation effects and have a broad and promising application potential. Archetypical examples of these systems are functionalized graphene, graphite and single wall carbon nanotubes (SWCNT) which are determined by the local arrangement of their sp^2 hybridised carbon atoms, such that their character is either a zero gap semiconductor, semi-metallic, insulating, semiconducting or metallic. Examples of our recent work on how one can unravel the underlying electronic structure using high energy spectroscopy (electron energy-loss, (resonant) photoemission and X-ray absorption spectroscopy) and optical spectroscopy (resonant Raman and Photoluminescence) as a probe will be presented. Special emphasis will be given to the influence of basic correlation effects and local field corrections on the electronic and optical properties of graphite, graphite intercalation compounds and functionalized SWCNT hybrids. The latter include examples for the three alternative doping routes, namely, substitution and side wall functionalization (e.g. via the chemisorption of reactive gases like nitroxides), intercalation and endohedral doping (e.g. by filling with fullerenes and metallocenes) as well as examples for the growth of defined inner tubes from the different precursors via nanochemical reactions. Different pathways to tailor these carbon hybrids regarding the complex interplay between charge transfer and hybridisation towards optimized optical quantum yield and defined conductivity will be emphasized.

In addition for metallic tubes, exhibiting a Luttinger liquid behavior, changes in basic correlation effects, will be discussed in the framework of a dimensionality cross-over which causes a change from a one-dimensional metal to a normal Fermi liquid for functionalized SWCNT hybrids.

The detailed understanding of these fundamental electronic properties of functionalised graphite/graphene and SWCNT hybrids is the key to their future success in for instance nanoelectronic and different transport/optical based sensor applications.

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Vibrational spectroscopic methods applied to self-assembled nanostructures (O57)

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Keywords: ATR, IRRAS, Raman

Vibrational spectroscopy is mostly used as an analytical tool in organic chemistry. Its significance grows in hybrid systems because weak interactions during self-assembly can influence the bond strengths and/or symmetry of the participating molecules. As a consequence, the vibrational spectrum can show high sensitivity to even small distortions or deformations.

I will present several types of secondary bonds: hydrogen bonds, surface adsorption and π-π interactions, which can be investigated by vibrational spectroscopy. Besides the common absorption technique, special methods are employed for this purpose, attenuated total reflection (ATR) and infrared reflection-absorption spectroscopy (IRRAS). Materials investigated in this way range from simple semiconductor systems (Si surfaces and various oxides) to uracil-type nucleic acid model systems[1] and carbon nanotube hybrids with molecules adsorbed[2] or encapsulated. In the latter, a combined ATR/Raman method will be presented to decide whether the small molecules are encapsulated or adsorbed on the nanotube surface.[3]

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ZnO nanofiber films for UV sensor applications (O58)

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The Cu-doped ZnO thin films were grown onto glass substrates by sol–gel spin-coating technique. The Cu dopant ratios were less than 10%. The prepared $Zn1_{-x}Cu_xO$ thin films were analyzed by X-ray diffraction (XRD) and atomic force microscopy (AFM). The XRD pattern of Cu-doped ZnO thin films indicates the existence of a ZnO single phase with a hexagonal wurtzite structure. AFM measurements confirmed the decrease in particle size observed from XRD data due to the incorporation of Cu atoms in ZnO lattice and also showed that the surface of the undoped ZnO film was turned from the nanorods into nanofibers after the incorporation of Cu ions into ZnO.

The obtained results indicate that Cu-doped ZnO thin films could be used in many research, environmental, industrial, and technological applications.

ZnO nanopowder based on quartz crystal microbalance humidity sensors (O59)

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Undoped and Sn-doped ZnO nanopowder samples were prepared by Sol-gel method. The crystalline structure and surface morphology of the samples were analyzed by X-ray diffraction (XRD) and Atomic Force Microscope (AFM). X-ray diffraction results indicate that the samples have a hexagonal wurtzite and polycrystalline structure. Quartz Crystalline Microbalance (QCM) technique was employed to investigate sensor features of the produced ZnO nano-systems. Sensor features of the pure and Sn-doped ZnO nano-systems were investigated under changing humidity conditions depending on the change in frequency. The obtained results suggest that the pure and Sn-doped ZnO nanopowder samples can be used in humidity sensor applications.

Nitrogen-containing CMK-3 carbon nanorods with different length as efficient cathode for oxygen reduction reaction (O60)

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Keywords: N-containing, CMK-3, nanorods, carbon, cathode, oxygen reduction reaction, fuel cell

Proton exchange membrane fuel cells (PEMFCs) are receiving widespread attention as a promising power technology due to many applications in portable, stationary power sources and automotieve energines.[1] Platinium (Pt) is the most commonly used electrocatalyst for the four-electron oxygen reduction to water in acidic environments with low overpotential and high stability.[2,3] However, Pt is a precious metal of low abundance, and it is thus of great interest to develop Pt-free cathode catalysts for PEMFCs. In this study, the polypyrrol based nitrogen-containing CMK-3 carbon nanorods with different length successfully synthesized via chemical vapor infiltration. SBA-15 silica nanorods with different length were used as the template, and pyrrole was employed as nitrogen precursor together with iron (III) chloride as a catalyst. The N-containing CMK-3 carbon nanorods with different length were prepared and examined for their ability as electro catalyst for oxygen reduction reaction (ORR). Cyclic voltametery (CV) and ring rotating disc electrode (RRDE) tests show the Pt-free N-containing CMK-3 carbon nanorods prove to be effective electro catalyst or the four-electron oxygen reduction along with excellent stability comparable to the state of art Pt/C in alkaline conditions

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POSTER PRESENTATIONS

P001 – The adsorption and diffusion properties of Li^+, Na^+ and K^+-ions on graphene surface under the effect of external electric field

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Keywords: graphene, ion diffusion, electric field

In our earlier works the investigations of non-covalent interactions between carbon nanotubes (CNTs) and aromatic molecules have been performed [see e.g. Peles-Lemli et al. (2010)[1]]. Vibrational dynamics calculations showed that the tubular conformation change of the CNT could affect both this weak interaction[2] and the CNTs' adsorption on CeO_2 islands grown on sapphire substrate.[3] Furthermore, we have reported a new method,[4] how to generate graphene-CeO_2-sapphire layer. This system with electrochemical modifications could be a potential surface of ion diffusion controlled by external electric field. In this way, we might be able to get transported ions selectively by changing the applied perpendicular and parallel electric fields. To reach the practical benefits of this method, it is necessary to clarify the diffusion and adsorption mechanism of the ions on graphene layers. In this work the interaction between alkali ions and the graphene surface with the absence and the presence of external electric field applied perpendicular to the graphene surface was investigated. Results show, that the electric filed push close the positive charged ion to the graphene surface, where the Coulomb repulsion results higher energy barriers on the investigated diffusion pathways. The Li^+-ion with the smallest ionic radius diffuse the fastest under neutral field, at the same time, its diffusion is the slowest under electric filed. These effects are applicable in the design of electronic devices designed to nanoscale.

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P002 – Adsorption mechanisms of organic compounds on multiwalled carbon nanotubes

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Keywords: carbon nanotubes, hydrophobic organic compounds, adsorption mechanism

In this work we studied the adsorption of a set of organic compounds (OCs) by multiwalled carbon nanotubes (MWCNTs) from aqueous solution. In total, adsorption parameters for seven OCs (hexane, benzene, toluene, 1,2,3-trichlorbenzene, 1,2,4-trichlorbenzene, fluoranthene and pyrene) were determined for two different MWCNTs: the pristine (original, as-received) MWCNTs (OMWCNT) and functionally modified MWCNTs by acid treatment (FMWCNT) to probe the influence that oxygen containing functional groups exert on MWCNTs sorption properties.

All adsorption isotherms were performed in conventional batch adsorption experiments. The background solution was 0.01 M $CaCl_2$ in doubly distilled water with 100 mg/l NaN_3 as a biocide. The amount of MWCNTs in each experiment corresponded to a sample/solution ratio that resulted in 20-80% uptake of given OC. The procedure was as follows: flasks containing premeasured adsorbent and background solution were agitated at ultrasonic bath for 30 min before a certain volume of methanol stock solution of OC was spiked and equilibrated at room temperature by continuously shaking for 3 h. The flasks were allowed to settle for 24 h and a sample of clear supernatant was removed for gas-chromatographic determination of the OC equilibrium concentration.

All adsorption isotherms well fitted Freundlich model. The nonlinearity of isotherms ranged from 0.418 to 0.846. Both MWCNTs have a higher adsorption affinity for OCs of large molecular size (trichlorbenzenes, fluoranthene, pyrene) relative to those of smaller size (benzene, toluene and hexane) possibly due to their large contact area with the surface of adsorbent. However, direct comparison of adsorption affinities could not be made because of their different units as a result of the nonlinearity of the adsorption isotherms. Therefore, distribution coefficients (K_d) were calculated at a selected equilibrium concentration (100 µg/L). The results showed that K_d values for both adsorbents increased in the order benzene < toluene < hexane < 1,2,3-trichlorbenzene < 1,2,4-trichlorbenzene < pyrene < fluoranthene, showing a good correlation with compound's hydrophobicity (K_{OW}). These results suggest that hydrophobic interactions have a significant role in the overall adsorption mechanism of OCs on both investigated MWCNTs.

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P003 – Antimicrobial effect of silver functionalized TiO_2 coated lamp surface in indoor air sample using LED light sources

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Keywords: antimicrobial, reactive lamp, photocatalyst, photo reactor, LED light, silver

The development of sterilizing methods is an important step to prevent the spread of pathogens in hospital and health care settings. Varied disinfectants have been used to kill pollutants and microorganisms on the surface and in the air. It is already known that TiO_2 can be activated under UV-light irradiation and has a pronounced antimicrobial activity because of producing highly reactive radicals. The photocatalytic effect of noble metal functionalized TiO_2 has been presented in many studies. The wavelength of the light source of photocatalysis can be extended to the visible light region with plasmonic catalyst so the noble metal functionalized surface can be widely used in air sterilization.

In this study we present the antimicrobial effect of silver functionalized TiO_2 coated lamp (reactive lamp) in indoor air sample. The inner surface of the reactive lamp was prepared using the spray coating technique. The silver functionalized TiO_2 was activated with LED-light source (λ = 405 nm) inside the lamp to express the antimicrobial effect of the lamp when it is turned on. The antimicrobial activity of the reactive lamp was investigated in a closed photo reactor using RCS PLUS air sampler.

Parallel experiments were investigated with a photocatalyst-free lamp and without lamp. Colony forming units were counted on nutrient agar (HYCON Agar Strips TC) and compared to the null-point sample. Two parallel experiments were carried out in each case and the counts of different adhering bacterial/fungi colony forming units were averaged.

We found an antimicrobial effect by using reactive lamp; the percent reduction of the colony forming units was 69.65% after 24 h illumination and 96.27% after 48 h illumination. Using photocatalyst-free lamp, the percent reduction of the colony forming units was 23.25% after 24 h illumination and 23.02% after 48 h illumination. According to the investigation without a lamp the percent reduction of the colony forming units was 26.92% after 24 h illumination and 38.46% after 48 h illumination. After 16 days light activation the reduction of the colony forming units was 92.45% after 48 h illumination in the photo reactor.

The results showed that the antimicrobial effect of the reactive lamp was sufficiently high; the reactive lamp was able to kill a wide spectrum of bacteria and fungi in indoor air sample after a 48 h operation.

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P004 – Applicability of MWCNTs and iron modified MWCNTs for removal of selected neonicotinoid insecticides in aqueous solution under natural insolation

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Keywords: Fe-MWCNT, MWCNT, neonicotinoid insecticides, removal, natural insolation, HPLC-MS/MS

In recent years, immobilized iron species on solid supports as promising heterogenous catalysts, attracted more and more attention. The supports can be organic and inorganic materials such as zeolit, activated carbon, multiwall carbon nanotubes (MWCNTs), TiO_2, clays, etc. Some of them like iron modified clay, zeolit, and TiO_2 were successfully applied for removal of widely used imidacloprid[1] and thiacloprid[2] neonicotinoid insecticides. MWCNTs are effective adsorbents for organic chemicals in water treatment, and additionally their decoration with Fe_2O_3 or Fe_3O_4 particles are efficient for combined removal (adsorption and degradation) of hazardous phenolic compounds[3] and 17 α-methyltestosterone.[4] In this work we compared the efficiency of MWCNTs with iron decorated MWCNTs for removal of selected neonicotinoid insecticides (chlotianidin, thiamethoxam, acetamiprid, thiacloprid, and nitenpyram) from aqueous media in one month time interval under natural insolation. Furthermore, parallel stability experiments were performed with the same concentrations of neonicotinoids under the same experimental conditions, but without MWCNTs. For all investigated systems the sampling was performed daily, and the samples were analysed by optimised HPLC-MS/MS method. It was found, based on the stability study, that all investigated neonicotinoids, except nitenpyram, were degrading pretty slowly over a two weeks period, confirming the need for their removal from systems. MWCNTs, depending on the structure of insecticides, gave removal efficiency between 40 and 60%, while the iron decorated ones showed activity higher than 87% in the case of all investigated neonicotinids.

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P005 – Application of the supercritical fluid technology for the micronization of active pharmaceutical ingredients

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Keywords: supercritical fluid technology, micronization, active pharmaceutical ingredients

Supercritical fluid technology is a novel approach for extraction, separation, reaction and particle formation. We apply this method on the re-crystallization and micronization of active pharmaceutical ingredients (APIs). The main advantages of this technology include its simple and fast process without traditional organic solvent contamination or thermal degradation effect. Carbon dioxide is the most commonly used supercritical fluid. Based on the solubility of API in supercritical carbon dioxide, either the supercritical antisolvent (SAS)[1,2] or rapid expansion of supercritical solution (RESS)[3] method is chosen to reduce the mean particle size of the API in the re-crystallization procedures. The product may have different morphologies and polymorph forms that can contribute to the enhancement of the dissolution rate and the more suitable formulation of pharmaceutical compound.

Hydrochlorothiazide (HCT) is taken as a model API in our SAS experiments. The original mean particle size of this API was 180 mm. It was dissolved in acetone and then injected through a coaxial nozzle with supercritical carbon dioxide into a high pressure column. The API was re-crystallized due to decreased solubility during the fast volume expansion. At an optimal process condition, 120 bar and 318 K, the resulting product has a significant mean size reduction to 670 nm. The dissolution rate of the SAS treated HCT was 3 times faster than the original API in a simulated gastric buffer solution. Erlotinib hydrochloride is an anti-cancer API and is taken as another example using the SAS process. The original erlotinib hydrochloride has a mean size of 20.7 mm. After the SAS process at 100 bar and 308 K, the micronized erlotinib hydrochloride depicted a mean particle size of 980 nm. It also changed from the original crystal form B to another polymorph form E or A. The micronized erlotinib hydrochloride showed an enhanced dissolution rate in a simulated gastric buffer solution by 3 to 4 times. It is also presented that several anti-oxidant particles can be micronized from 18 mm to 150 nm with polymorph transition by employing the SAS process.

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P006 – Biosensors prepared for detectation of aflatoxins in corn matrix

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Keywords: aflatoxin, cyclodextrin, biosensors, gold

The aim of this work is to develop a new selective sensor for detection of aflatoxins. Aflatoxins are carciogenic and harmful for gene and occur in nature. The aim of our work to detect this toxin with selective sensors. We use functionalised gold nanoparticles and gold nanofilms to develop sensors. The functionalisation of good surface can be prepared with cyclodextrines which are modified by thiol or fluorescent groups.

Identification and characterization of citrate and aminodextran reduced gold nanoparticles were performed by their XRD diffractograms, UV-Vis spectra and TEM images. We could establish uniform conductive films on silica crystal and glass surfaces by spray-coating technology from the prepared gold nanodispersion if the SiO_2 surfaces were treated previously by PEI (positively charged layer). These specifically produced films are suitable for biosensors.

The maximum absorbed amounts of β- and γ-CD (cyclodextrin) on gold thin films were determined from SPR and QCM measurements. These were 25 ng/cm^2 from SPR results and the binding was physisorption. We have modeled in QCM measurements the surface which was prepared by spray-coating. First the gold surfaces were treated by PEI after the deposition of gold nanoparticles and then they were measured after the attaching of cyclodextrins. The absorbed amount of PEI was 185 ng/cm^2 while the amount of gold was 250 ng/cm^2. Cyclodextrins attached by physisorption (maximum absorbed amounts: 150 ng/cm^2) as expected like SPR measurements and unlike thiol groups modified cyclodextrins.

The attachment of aflatoxin molecules to cyclodextrin modified gold thin films was studied by SPR and QCM measurements. For comparison a quantitative analysis of aflatoxin molecules on surfaces of modified gold nanoparticles will be done by ELISA (Enzyme-Linked ImmunoSorbent Assay) method. Validation of thiol modified gold nanosensors on silica crystal will be performed by HPLC-MS method.

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P007 – Boron doped single-walled carbon nanotubes from high vacuum CVD and density gradient ultracentrifugation towards doped semiconducting nanotubes

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Keywords: single-walled carbon nanotubes, boron doping, density gradient ultracentrifugation, metallicity sorting

One of the advantages of single walled carbon nanotubes (SWCNTs) is given by the possibility to functionalize them as a path to control their electronic structure. The experimental limitations to produce samples with direct heteroatoms substitution (i.e. B, N, P) are still not overcome. Moreover, the presence of both metallic and semiconducting SWCNTs in a sample has slowed their application in electronic devices as well as the detailed study of the physical properties of a specific nanotube species.

In this contribution, we employed high vacuum CVD for the high yield production of B-doped SWCNTs[1,2] and a modified density gradient ultracentrifugation (DGU) to obtain semiconducting-enriched doped tubes. The raw material was doped in-situ with a B content below to 0.5% at. We have observed that the samples' metallic nature was enriched and the overall purity was improved, not only maintaining the crystalline structure but keeping the morphological characteristics and dopant incorporation in the starting material. Transmission electron microscopy (TEM), Raman, optical absorption and core level photoemission spectroscopy were used to monitor the sample quality regarding purity bonding environments and defects concentrations.

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P008 – Bulk Al-Al_2O_3 nanocomposites – Study of their nanosintering with respect to densification and grain growth

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Keywords: aluminum, alumina, nanocomposites

The property improvements of nanocrystalline materials have been attributed to the novel characteristics of grain boundaries coupled with drastic refinements in grain size. The added advantage of nanocomposites is that their properties can be tailored by varying their composition and grain microstructure to suit a particular application making their applications more wide and versatile with improved performance. Al-Al_2O_3 are important metal-ceramic composites possessing high wear resistance, low CTE and improved mechanical properties over a wide range of temperatures. In view of the background mentioned, this work proposes to synthesize bulk nanocomposites of Al-Al_2O_3 (with varying weight fraction of Al_2O_3) in two stages (i) synthesize Al-Al_2O_3 nanocrystalline composite powders using high energy ball milling followed by (ii) consolidation of these nanopowders using rapid sintering at high pressures. An expected outcome of this research work is the development of "rapid sintering at nearly-isostatic high pressures" as a consolidation technique of nanopowders, which is economical, fast and yields nanocomposites with near-theoretical density with minimal grain growth leading to improved properties.

P009 – Carbon nanotubes quench singlet oxygen generated by photosynthetic reaction centers

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Keywords: carbon nanotubes, photosynthesis, singlet oxygen

Photosensitizers may covert light into formation of reactive oxygen species (ROS) including, e.g., singlet oxygen ($^1O_2$), superoxide anion (O_2–), and hydroxyl radicals ($^{\cdot}OH$), chemicals with extremely high cyto- and potential genotoxicity. Photodynamic ROS reactions are determinative in medical photodynamic therapy (cancer treatment with externally added photosensitizers) and in reactions damaging the photosynthetic apparatus of plants (via native pigments). The primary events of photosynthesis take place in the chlorophyll containing reaction center protein complex (RC), where the energy of light is converted into chemical potential. ROS are formed under conditions when RC photochemistry is limited (by excess light and/or by impaired photochemical processes). $^1O_2$ production in RC preparations under excess irradiation is well documented.[1–3] In plant physiology, reducing the formation of the ROS and thus lessening photooxidative membrane damage (including the RC protein itself) and increasing the efficiency of the photochemical energy conversion is of special interest. Carbon nanotubes, in artificial systems, are also known to react with singlet oxygen.[4]

To investigate the possibility of such quenching *in vivo,* we studied the effect of carbon nanotubes on $^1O_2$ photogenerated in photosynthetic RCs. 1,3-diphenylisobenzofuran (DPBF), a dye responding to oxidation by $^1O_2$ with absorption change was used to measure $^1O_2$ concentrations after excitation of either a photosensitizing dye (methylene blue) as a model system or photosynthetic RCs in the presence of carbon nanotubes. Our results indicate that the $^1O_2$ induced absorption change of the DPBF at 420 nm decreased in the presence of carbon nanotubes, suggesting that carbon nanotubes potential quenchers of this ROS *in vivo,* too.

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P010 – Catalytic activity of molybdenum nanoparticle decorated carbon aerogels

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Keywords: carbon aerogel, nanoparticle, hydrogenation, molybdenum carbide

Carbon aerogels that are simultaneously micro-, meso- and macroporous offer advantages over other forms of porous materials for catalytic applications that demand rapid access to the internal surface. Polymer precursors for such carbons can be prepared from resorcinol and formaldehyde by a sol/gel process under controlled conditions. Carbonization enhances the microporosity while the porosity in the wider range is conserved.[1] The synthesis route offers several opportunities for introducing metal ions that can improve the catalysis or gas purification efficiency of the porous carbon.

The precursor hydrogel was prepared by using sodium carbonate as catalyst. Drying was performed after substituting the water by acetone, which was then replaced with CO_2 under supercritical conditions. A detailed description is given elsewhere.[2] The polymer aerogel was then impregnated with a solution of $(NH_4)_6Mo_7O_{24}.4H_2O$ and carbonized to yield carbon aerogels with highly dispersed molybdenum nanoparticles. The carbonization step reduced the Mo into various carbides.

The catalytic activity of the Mo decorated carbon aerogel was tested in the hydrogenation reaction of a model biomass. The molybdenum nanoparticles significantly reduced the amount of gaseous products (CO, CH_4) and enhanced the yield of high value products such as acetone, acetaldehyde and ethyl acetate.

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P011 – Cell culture and *in vivo* study of microvesicles for drug delivery across barriers

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Keywords: blood-brain barrier, brain endothelial cell, drug delivery, microvesicle, solute carrier

Efficient drug delivery across biological barriers, like the intestinal and blood-brain barriers is a central problem in the pharmaceutical treatment of disorders.[1] Most pharmaceutical drug candidates, hydrophilic molecules, biopharmaceuticals, and efflux transporter ligands have a low permeability across barriers. To solve this unmet therapeutical need colloidal drug delivery systems utilizing physiological transporters of the barriers hold a great promise. The aim of our study was to test nanosized, biocompatible and biodegradable vesicles which can incorporate both hydrophilic and hydrophobic drug cargos and present on their surfaces ligands for solute carrier (SLC) proteins. Glucose analogues and amino acids were used to achieve increased specificity and efficacy for drug delivery across barriers. Bilayered microvesicles of non-ionic surfactants, niosomes are able to encapsulate solutes and serve as potential drug carriers. Niosomes with an average hydrodynamical size of 200 nm were prepared containing different ligands and their combinations, and Evans blue-albumin as a model molecule. Human Caco-2 intestinal epithelial and D3 brain endothelial cells, a model of the blood-brain barrier,[2] were used for toxicity measurements by colorimetric methods and real-time cell microelectric sensing, permeability experiments and morphological examinations. The presence of glucose and amino acid ligands on microvesicles increased the uptake of Evans blue-albumin to the cells and its penetration across the cell layers. A kinetic *in vivo* study in nude mice by eXplore Optix, a near infrared fluorescence time-domain optical imaging demonstrated the elevated accumulation of Evans blue-albumin in the brain after the intravenous injection of glucose analogue and amino acid labeled niosomes. These results indicate that microvesicles labeled with SLC transporter ligands can be used for targeting hydrophilic biomolecules across barriers.

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P012 – Characterization of luminescent silicon carbide nanocrystals by photoluminescence and surface infrared spectrocopy

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Keywords: nanocrystals, silicon carbide, surface infrared spectroscopy

Fabrication of nanosized silicon carbide crystals is a crucial aspect for many biomedical applications. We report the characterization of silicon carbide nanocrystals synthesized by the reactive bonding method followed by electroless wet chemical etching.[1] Our samples show strong violet-blue emission in the 410–450 nm region, the wavelength depending on the used solvents. Infrared measurements unraveled the surface bonding structure of the fabricated nanoparticles being different from silicon carbide microcrystals. Attenuated total internal reflection infrared spectroscopy was used to reveal the complex nature of the surface geometry of the nanocrystals, which provides numerous surface terminations to interact with the surrounding solvent molecules. Surface related bands characteristic of Si-O-Si, C-O-C, CH as well as COOH and COO- was revealed. The functionalization of these surface terminations is feasible with chemical methods for further applications. This might give an opportunity to use standard chemistry methods for biological functionalization of such nanoparticles.

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P013 – Characterization of the chemical bonding between Al_2O_3 and nanotube in MWCNT/Al_2O_3 nanocomposite

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Keywords: carbon nanotubes, alumina, chemical interaction

This work investigates the possible chemical bond formation between functionalized carbon nanotubes and alumina, in multi-wall carbon nanotubes/alumina nanocomposite (MWCNT/Al_2O_3), with the aid of spectroscopic analysis. For this purpose, the nanocomposite MWCNT/alumina was synthesized via hydrothermal treatment. Different characterization techniques, scanning electron microscopy, energy dispersive X-ray spectroscope, X-ray diffraction, Fourier transformed infrared spectroscope and high-resolution transmission electron microscopy, have been used to investigate the interaction of the nanocomposite. XRD data confirmed the main alumina phase on the nanotube was $\alpha - Al_2O_3$, with 12 nm average crystallite size. The presence of a shift in the carbonyl peak between oxidized nanotube and the nanocomposite, from 1710 cm^{-1} to 1630 cm^{-1} indicates the formation of chemical bond between alumina and CNT tips. The study predicts the possibility of covalent chemical bonding between alumina and the nanotube.

P014 – Comparative investigation of photodegradation of oxalic acid and phenol over TiO_2/MWCNT photocatalysts

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Keywords: TiO_2, MWCNT, photocatalysis

TiO_2-based photocatalytic oxidation is a highly efficient method to decompose pollutant compounds.[1,2] Previous studied has shown these photocatalysts can be enhanced by coupling TiO_2 with multiwall carbon nanotubes (MWCNT) in the form of a nanocomposite.[3,4] Also, the adsorptive property of these composites plays an important role in the photocatalytic process and can enhance their performance.

TiO_2/MWCNT composite photocatalysts were synthetized with different MWCNT content by hydrolysation of titanium containing precursor adsorbed on the surface of functionalized MWCNT. Annealed catalysts were characterized with TEM, XRD, BET and Raman spectroscopy. XRD and Raman results showed that annealing the amorphous titanium-oxide-hydroxide resulted only anatase-phase titanium dioxide. This is the preferred phase as it is more photocatalytically active than all other TiO_2 phases. TEM revealed that anatase nanoparticles (around 10–20 nm in diameter) were bound onto the surface of MWCNTs. The prepared composite photocatalysts has quite high specific surface area (>100 m^2/g) according to BET measurements.

Photocatalysts were tested in liquid-phase photocatalytic reaction using sol-gel prepared TiO_2 and Aeroxide P25 as references. The choice of model compounds was based on their affinity to aromatic and polar surfaces (phenol and oxalic acid respectively). The concentration of the model compounds was measured by HPLC technique.

The measurements showed that photocatalytic activity does depend on the model compound and MWCNT content. The composite containing 5 wt% MWCNT resulted the highest photoactivity in case of the oxalic acid.

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P015 – Comparison in physico-chemical properties in In and Ga doped Ge-Te glassy chalcogenides

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Keywords: chalcogenide glasses, glass formation, physico-chemical properties

The present paper reports for the first time the effect of In and Ga addition to some physico-chemical characteristics into Ge-Te matrix, such as density (ρ), calculated by the formula described by Kashchieva et al.,[1] compactness (δ), molar volume (Vm).

Their correlation with the average coordination number (Z) has been discussed. The number of constraints per atom (Nco) as a function of the average coordination number has been calculated by some theoretical arguments and the average bond energy <E> was received according to Tichy equations.[2]

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P016 – Controllable preparation of silver small particles for electronics

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Keywords: silver, small particles, electronics

As a good conductor, silver powder is the main element of conductive pastes. With the development of microelectronic industry, the size and shape controlled fabrication of silver micro/nano particles is more important. Here we would introduce the controllable synthesis of super-small particles of silver, particularly, the precipitation of multi-injects and process control method.

Furthermore, a relatively high concentration (0.093 M) of silver nanoparticles sized 5 nm was directly synthesized in water phase. The ink (20% silver) prepared with the silver nanoparticles could be written on weighing paper by a pen-on-paper paradigm. The influence factors of the conductivity of the patterns from the ink were studied.

P017 – Controlling gas sensitivity of spinel ferrites

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Keywords: Spinel ferrite, gas sensors, sol-gel

Recently it was found, that gas sensitivity of spinel ferrite transition metal oxide nanomaterials is affected not only by chemical composition and microstructure but also by faults and defects in the structure. Concentration of the point defects such as cation or oxygen vacancies can be regulated by replacing trivalent iron ion in tetrahedral site in the inverse spinel structure with divalent non-transition metal ions (Me^{2+}), thus changing the type of structure to mixed or normal. Also, cation and oxygen vacancies can be introduced or extinguished varying iron ion stoichiometry, synthesis parameters or method, as well as annealing conditions.[1–3]

Present work shows ways towards a more sensitive inverse and normal spinel type ferrite gas sensor materials including formation of 3D and 2D nanostructures. Spinel type ferrite gas sensor materials were synthesized by using sol-gel combustion and spray pyrolysis methods. For characterization of gas sensor material, X-Ray diffraction, scanning electron microscopy, DC resistance and impedance spectroscopy (IS) measurements were employed.

The tuning of sol-gel auto combustion reaction character results with formation of nanoparticles with different size, nature of agglomerates (primary or secondary), as well as impurity and defect content. Spray pyrolysis derived stoichiometric and non-stoichiometric spinel ferrites with nanosized 2D structures with different thicknesses ranging from nano- to micro-. Complex impedance spectra enabled to separate electric properties of different phases (grain and depletion layer) of the ferrite gas sensor materials. Also, IS helps to find equilibrium between optimal concentration of the surface oxygen species and charge carrier (defect) concentration.

Overall, gas sensitivity is higher for n-type zinc ferrite than nickel or nickel-zinc ferrites and increases with increasing concentration of oxygen vacancies. Thin film gas sensors possess faster response-recovery behaviors and higher sensitivity.

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P018 – Crystallization and dielectric properties of barium titanate precipitated in inverse sodium-aluminoborosilicate glasses with high concentration of iron oxide

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Keywords: barium titanate, iron oxide, crystallization, microstructure, dielectric constant

Multicomponent glasses and glass-ceramics with high concentrations of alkaline earth and 3d-transition metal oxides are interesting due to their ability to exhibit simultaneously electric and magnetic ordering and thus, behave as multiferroic materials. The occurrence solely of the ferroelectric phase, especially if $BaTiO_3$ is precipitated, may also be of practical significance. In case of barium titanate crystallization, the synthesis products in the latter systems can undergo numerous phase transitions within the temperature interval of application. The tetragonal $BaTiO_3$ is ferroelectric, while the cubic one exhibits high dielectric constant and is not ferroelectric, which results in isotropic dielectric properties. The cubic modification is used as a dielectric in multilayered capacitors for energy storage and depending on its optical properties, it is a promising candidate for UV lasers in optoelectronics.

In the present work the synthesis, phase formation, microstructure and dielectric properties of the glasses and glass-ceramics, obtained in the system $Na_2O/TiO_2/BaO/Al_2O_3/B_2O_3/SiO_2/Fe_2O_3$ are reported. The characteristic temperatures of the samples are determined by differential thermal analysis and dilatometry. X-ray diffraction is used for phase identification. Different time-temperature programs are applied to the obtained glasses and crystallization mainly of cubic $BaTiO_3$ is observed. The microstructure of the prepared glass-ceramics is studied by scanning electron microscopy and the formation of spherical $BaTiO_3$ particles with sizes varying from 100 nm to some μm is established. The dielectric constants are determined at room temperature as a function of frequency by means of impedance spectroscopy.

P019 – Development of low-temperature sol-gel synthesis of TiO_2 to provide self-cleaning effect on the textile materials

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Keywords: titania, sol-gel synthesis, textile, cross-linking agent

During the past decade the titania-based coatings with high specific surface area and narrow pore size distribution provided new prospects for practical application in solar energy transformation, photocatalysis, water and air cleaning and processing as self-cleaning, photochromic, and superhydrophobic/hydrophilic coatings. A promising direction in modern materials technology is obtaining textile materials possessing dirtproof and oilproof properties, displaying hydrophobic, bactericidal effects, having an increased thermal stability and acid and base resistance. Of importance are developments devoted to obtaining "smart textiles" showing an ability to self-cleaning from organic pollutions under the influence of light as well as high bactericidal activity.

This work is devoted to the development of "smart textiles" with high photocatalytic activity in the reactions of the decomposition of organic compounds on the basis of the proposed new method for producing cotton fibers modified with TiO_2 nanoparticles. For cross-linking of titania nanoparticles with cotton the 1,2,3,4 butane tetracarboxylic acid (BTCA) was used as a spacer. The peculiarity of the formation of photoactive titania nanoparticles is related to developed low-temperature sol–gel synthesis, which allows to obtain titania hydrosol consisting of partially crystallized nanoparticles of anatase – brookite modification at temperatures below 100°C. Self-cleaning effect of the textile materials modified titania nanoparticles was evaluated by the decomposition reaction of rhodamine B under UV-irradiation.

Application of the obtained TiO_2 hydrosol for textile fabric processing allows to reach uniform distribution along the entire cotton fiber surface due to the small size of particles and high sedimentation ability. It is shown that fabric modification with titania hydrosol without using 1,2,3,4-butanetetracarboxylic acid as a cross-linking agent does not lead to strong fixation of nanoparticles on the surface of a cotton fiber. On the contrary, IR spectroscopy reveals that upon adding BTCA as a cross-linking agent and sodium hypophosphite as a catalyst of cross-linking reaction to TiO_2 hydrosol, an absorption band shift from 1642 to 1660 cm^{-1} is observed testifying the formation of the Ti-O-C bond. The cotton fibers processed in this way exhibit high self-cleaning properties and maintain them even after five cycles of washing.

Thus, an application of a sol containing titania nanoparticles allows to substantially improve self-cleaning properties of textile materials.

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P020 – Development of smart hydrogel fims for treatment of bacterial infections on mucosal surfaces

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Polymer hydrogel is a network of hydrophilic macromolecular system that can swell in water and hold a large amount of water while maintaining the structure. These polymer or polymer-hybrid materials are also termed "intelligent or smart gels", because depending on their chemical composition and network structure, they perceive changes in one or several environmental parameters and respond with a functional reaction.[1,2] Due to the properties of this material it has a number of advantages for drug delivery applications.[3] pH-sensitive hydrogels are probably the most commonly studied class of environmentally sensitive polymer systems in drug delivery research.[4]

Our objective is the preparation of a pH-sensitive hydrogel, whose swelling at pH values higher than 4.5–5.5 is significantly enhanced as compared to lower pH values, in order to enable the release of active agents (e.g. PVP-iodine, Ag or Ag-Cu nanoparticles alloys and other biocidal substances) encapsulated within the gel matrix into the environment.

The pH-controlled release of the antibacterial nanoparticles reduce the effects of microbial inflammation thus the developed pH-sensitive hydrogels and composites are advantageously applicable for prevention and treatment of female genital infections.

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P021 – Different synthesis approaches improving the photocatalytic performance of titanium dioxide photocatalyst nanoparticles for water purification and hydrogen production

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Keywords: photocatalysis, titanium dioxide, polyhedral shape, particle size, doping methods

Titanium dioxide photocatalysts can be used for the removal of toxic organic compounds and bacteria from water under solar or artificial irradiation in the UV and visible range. Our research is focused on the development of titania photocatalysts with improved activity tuning the most important material properties, such as the particle size and shape, and the light absorption characteristics by doping.

Our observations confirmed that the water remediation efficiency depends on the particle size and the specific surface area of the photocatalysts. This property is also substrate dependent thus we paid attention to use ill-adsorbing (such as phenol) and strongly adsorbing substrates (such as oxalic acid) for characterization. Ill-adsorbing substrates are most rapidly degrading on larger titania nanoparticles with 20–50 nm primary particle size under UV irradiation. Bare titanium dioxide nanoparticles can be prepared in this size range via flame hydrolysis method with optimized hydrogen-oxygen molar ratio and $TiCl_4$ vapour feeding rate in the flame. Similarly efficient photocatalysts were also made with our newly developed rapid heating and short exposure

(RHSE) calcination method that was applied on sol-gel made titania. The RHSE method using calcination at 600°C for 10 minutes was very efficient producing highly active titania from both $TiCl_4$ and $TiCl_3$ precursors.

Noble metal deposition (Au and Pt) was found to be very efficient for hydrogen production in the presence of oxalic acid under UV light. It has been concluded that the noble metal nanoparticle size is strongly influencing the hydrogen production efficiency.

Nitrogen, iodine and iron doping synthesis methods were optimized for visible light applications. Materials were characterized by XRD, TEM, BET, DRS, XPS, XRF and ICP methods and HPLC, GC and TOC analytical techniques.

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P022 – Control of nano-fibril structure of poly(*p*-phenylene benzobisoxazole) fiber by using multifunctional comonomers

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Keywords: PBO, pentaerythritol, copolymer, fiber, nano-fibril structure, property

Poly(*p*-phenylene benzobisoxazole) (PBO) fibers are known to possess the highest tensile modulus and strength among all commercial synthetic polymer fibers. PBO can be used as reinforcement in advanced composites and has a great potential application in the fields of aerospace, military and general industry. However, the use of PBO fibers in structural application has been highly restricted by their poor compressive property due to the nano-fibril structure.[1]

Among the methods to improve the compressive property of PBO fiber, chemical modification can produce various advantages in PBO compared with the unmodified polymer. A great number of different compounds can be added to the polymerization of PBO to change its nano-fibril structure and properties. Among these chemical modifiers are branching agents such as tri-functional trimethylolpropane or tetra-functional pentaerythritol.[2] The incorporation of small amounts of branching agent leads to the formation of long-chain branches. If the amount of the branching agent exceeds about 1%, crosslinked structures may be obtained.

In this study, we have prepared a series of PBO copolymers by using in-situ polymerization of 4,6-diamino resorcinol dihydrochloride (DAR) and terephthaloyl chloride (TPC) in the presence of pentaerythritol. And then, PBO copolymer fibres are manufactured by in-situ dry-jet wet spinning of the polymerization products. Structure, thermal stability and tensile mechanical properties of the copolymers with different comonomer contents are investigated.

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P023 – The effect of surface defects and functional groups on the sintering and agglomeration of Pd nanoparticles

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The preparation of carbon nanotubes supported catalysts nowadays is a highly popular topic among research groups, since these materials tend to exhibit higher catalytic activity and stability than other metal particles supported on different carbon allotropes or supports. As a result, not only the physical, chemical, electrical and catalytic properties of these materials are studied, but also much effort is taken to better understand the governing mechanisms behind the formation of these composite materials.

There are many different approaches to prepare such materials, such as wet impregnation, ion exchange or supercritical condensation, that are leading to an extensive amount of variables that can significantly change the final product, thus each of them must carefully be chosen to be able to prepare the desired catalyst. Even small changes in some of the parameters, such as metal concentration, temperature or support pretreatment, can alter the quality and/or useful properties of the prepared composite material in quite unexpected ways.

The time spent on the acidic treatment alters the amount of functional groups formed on the surface of carbon nanotubes. The amount of functional groups significantly changes catalyst-support interactions, which affects the size and surface distribution of supported metal particles. Our aim in this work was to determine the immobilizing nature of oxygen containing functional groups, since in many applications catalysts are exposed to high temperatures, where the catalyst suffers a specific type of degradation due to unwanted particle sintering.

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P024 – Electronic properties of metallicity sorted ferrocene filled carbon nanotube hybrids

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Keywords: single-walled carbon nanotubes, functionalization, photoemission and x-ray absorption spectroscopy

In this contribution we present a detailed study of the electronic properties of ultra clean and metallicity sorted single-walled carbon nanotubes filled with ferrocene yielding metallicity sorted hybrids. The complex interplay between the filler and single-walled carbon nanotubes is revealed by site selective high resolution photoemission and X-ray absorption.

The details of the electronic properties especially the internal charge transfer from Fe to the cyclopentadienyl rings of ferrocene and to the SWCNT have been unraveled. An n-type doping of the SWCNT has been detected, with the peculiarity that the metallic tubes are prone up to 30% higher doping than their semiconducting counterparts. Concomitantly, the Fe valency changes from 2 in ferrocene to 2.3 in the ferrocene/semiconducting SWCNT hybrids and to 2.4 in the ferrocene/metallic SWCNT hybrids. Additional resonant photoemission has revealed that this extra charge to the nanotubes is ionic and a finite hybridization between the ferrocene and the fillers can be excluded.[1,2] These results substantiate not only that the internal charge transfer determines the resulting electronic transport properties in the filled 1D carbon hybrids, but they also show that these properties significantly depend on the metallic character of the encapsulating nanotubes, which is an important step towards the regulated and tunable tailored 1D electronic transport properties aimed for nanoelectronic applications.

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P025 – Electronic structure of two isomers of C_{82} fullerene polihydroxylated taking into account Fukui Function

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In the present work, *ab-initio* and semi-empirical calculations at DFT-B3LYP and PM3 levels of theory were performed in order to study the sequential hydroxylation of the isomers 3 and 9 (according to Fowler and Manolopoulos' nomenclature[1]) of C_{82} Fullerene. To obtain the sequential hydroxylation, Fukui Function (in the condensed form) and visualisation of HOMO and LUMO of the carbon atoms of fullerenols (hydroxylated fullerenes) were taken into account. Like C_{60} fullerene, it was found that there was a formation of dangling bonds on structures with an odd number of hydroxyl groups on the fullerene surface, which suggests an enhanced reactivity of these molecules. Nevertheless, the coverings with an even number of groups tend to the reconstruction of π bonds, obtaining less reactive molecular structures. With the adsorption of the first group, a narrow HOMO–LUMO gap (1.28 eV) is observed in comparison with the $C_{82}(OH)_2$ system (1.70 eV), as is found in similar systems, such as C_{60} fullerenol[2,3]. On the other hand, with a coverage of 12 hydroxyl groups, the formation of an amphiphilic molecule, where the location of groups in one side of the C_{82} surface provides a hydrophilic character, is observed, while the uncovered part has a hydrophobic character. This could be important in the formation of Langmuir monolayers. Finally, it is shown that the precise distribution of the OH groups on the fullerene surface plays a crucial role in the electronic structure of the polyhydroxylated fullerenes.

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P026 – Encapsulation and dynamics of spin-labelled insulin in silica matrix intended for oral administration

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Keywords: insulin, spin labelling, EPR, silica, encapsulation

Insulin is a protein drug of great interest for its broad use in the treatment of diabetes mellitus. The major problem associated with oral delivery of insulin is the low bioavailability in the stomach due to the susceptibility to enzymatic attack,[1] together with low permeability across biological membranes. Sol-gel synthesis method enables the encapsulation of protein in silica matrix with minimal manipulation and homogeneous protein distribution. The most techniques frequently used to study the protein structural conformation present significant limitations and are very difficult to be adapted for encapsulated proteins. Electron Paramagnetic Resonance (EPR) combined with the procedure of Site Directed Spin Labelling (SDSL) represents a promising approach, which offers information about the protein structure and protein dynamics, being thus an appropriate method to study the protein behaviour not only in its natural environment, but also encapsulated in silica matrix.

The main purpose of this study was to encapsulate spin labelled insulin into silica microparticles using sol-gel method and to monitor the dynamics and local structure of insulin during *sol* to *dried-gel* transition. Insulin spin labelling was performed using two different spin labels: iodoacetamide (IA) and a bifunctional nitroxide reagent designated RX.[2] Room temperature cw-EPR spectra of the silica encapsulated insulin were recorded to assess the mobility of the attached spin labels, while distances between the spin labels were measured at 160 K. Information about protein distribution in the silica matrix was obtained using DEER (Double Electron Electron Resonance) pulsed EPR technique.

Insulin was successfully spin labelled with high spin label efficiency and low insulin consumption. The results showed that the silica encapsulation guarantees the preservation of the native protein structure during preparation and storage. Silica matrix can effectively isolate individual biomolecules preventing aggregation and insulin denaturation.

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P027 – Engineering nanostructural coatings using Drosophila genetics

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Keywords: *Drosophila,* corneal surface, nanostructural coating, genetic engineering

The corneal eye surface of many insects is covered with pseudo-ordered arrays of nipples – nanostructural evaginations serving anti-reflective and anti-wetting functions.[1] The high diversity of these nanocoatings in various insects provides a rich potential for nanobiotechnological applications. However, controllable engineering of such nanocoatings has so far been lacking. We turned to the famous model insect – the fruit fly Drosophila melanogaster – to utilize the power of genetic engineering for this purpose. Using atomic force microscopy (AFM), we for the first time characterized nipple arrays of wild-type and mutant Drosophila,[2] identifying its corneal nanostructures as paraboloids of ca. 200 nm in diameter and ca. 50 nm in height (see Figure). In order to pinpoint the protein(s) responsible for formation of these nanostructures, we performed exhaustive mass-spectroscopical identification of proteins specifically expressed in *Drosophila cornea*. The respective genes were next knocked-down by eye-

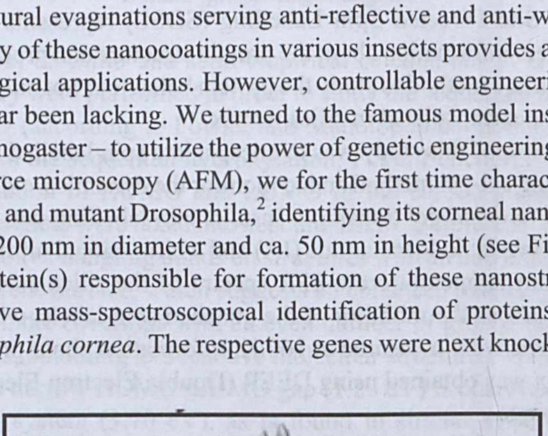

Figure 1.

specific expression of targeted RNAi constructs, and the resulting cornea analysed with AFM. Out of these, retinin mutants had severe reduction in the height and diameter of the nanostructures, revealing a unique role of this protein in formation of corneal nanocoating. Retinin is a member of insect-specific family of small secreted proteins possessing a very high evolutionary diversification rate, becoming the likely candidate for the high diversity of nipple arrays of various insects. Re-expression of different retinin-like proteins in *Drosophila* thus represents an appealing opportunity to engineer artificial nanocoatings. Coupled with analysis of their anti-reflective and anti-wetting properties, this approach will provide significant scientific and technological advances in nanobiotechnology.

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P028 – Enhancing electroremediation by using carbon nanotubes as reactive permeable barrier material – A review

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Keywords: electroremediation, sediment, heavy metals, carbon nanotubes

Electroremediation involves applying a low direct current or a low voltage gradient to electrodes that are inserted into a medium and can be used for remediation of soils and sediment contaminated with organic and inorganic substances. Major processes that influence the contaminants behaviour under applied current are water electrolysis, electromigration, electroosmosis and electrophoresis. In order to improve electroremediation efficacy it can be coupled with permeable reactive barriers (PRB). A PRB is an engineered barrier made of reactive treatment media placed across the flow path of a contaminant that removes/degrades contaminants flowing through it. When a PRB is coupled with electrochemical remediation, the flow of contaminants through the barrier is driven by the electroosmotic flow of pore fluid, electromigration of charged species and/or electrophoresis of charged particles. So far, cobalt coated CNTs were used for enhancing the electrokinetic removal of As(V) from soil.[1] Highly oxidized CNTs where oxygen containing functional groups increase the ion-exchange capability of carbon materials were used for Co(II), Cu(II) and Pb(II) sorption from the aqueous solution.[2] Also, using the carbon-encapsulated magnetic nanoparticles (CEMNPs) showed a high adsorption capacity for Co(II) and Cu(II) from the aqueous solution where the main advantage is easy removal of magnetized material after treatment.[3] Experimental results from different researchers indicate that CNTs can be used for heavy metals sorption and therefore these can be used as PRB material for enhancing the electroremediation of heavy metals contaminated sediment.

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P029 – Entropy driven formation of nanographite layers on the nanostructured cerium dioxyde surface

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Keywords: nanotube, graphite layer, Raman, standing waves

The dispersion of hydroxylated multiwalled carbon nanotubes (MWCNTs) was modified in non-protic acetonitrile solvent using a treatment by ethanol.[1] The dispersion was examined by photoluminescence and Rayleigh scattering methods. In spite of well known very low solubility of nanotubes, our results showed presence of nanotube dimers in the solution with considerable concentration. From this solution phase the MWCNTs were deposited onto the nanostructured CeO_2 films.[2,3] According to preliminary theoretical results,[4] quantum chemical calculations validated the resonant nanotube vibrations, especially for the stationary longitudinal wave at typical surface morphology as the origin of some unexpected property of the Raman signal. High resolution images by both transmission and scanning electron microscopy showed that the nanographite fractions exist in the solution and they were also reorganized on the surface. On the nanostructured surface of specific morphology, the nanographite fractions are deposited into the valleys between the CeO_2 islands and therefore a selective pattern of nanographite was formed. Molecular dynamics calculations highlighted that adsorption and reorganization properties of the nanographite layers have considerable dependence on the morphology of CeO_2 nanostructures. Considering that the CeO_2 surface morphology is fully controlled by the experimental setup of growth, properties of the CNT layers are tunable toward the requirements of practical applications.

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P030 – General toxicity, neurotoxicity, and the corresponding metal levels in rats treated with nanoparticulate and dissolved manganese

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Keywords: manganese, nanoparticle, oral exposure, inhalational exposure, general toxicity, neurotoxicity

Manganese (Mn) is an essential microelement and cofactor in several enzymes in humans. Chronic Mn inhalation can, however, cause a severe, Parkinson-like syndrome, also called manganism. In inhalational exposure, the nanoparticles (NPs) of fumes from welding and other metal industrial processes play an important role, but similar symptoms can also be caused by oral Mn overexposure due to food or drinking water.

In the present study, the two mentioned ways of exposure, and their combination, was examined. Adult male Wistar rats were treated for 3 and 6 weeks, 5 days per week, with 15.0 and 60.0 mg/kg b.w. $MnCl_2$ dissolved in distilled water, administered per os (po.) by gavage. Some animals were further treated for 3 or 6 weeks, with intratracheal (it.) application of 2.63 mg/kg b.w. MnO_2 NPs (Ø 30.9 ± 9.91 nm) suspended in 1% hydroxyethyl cellulose in phosphate-buffered saline. After completion of the treatments, general toxicological, behavioral and electrophysiological examinations were done. The rats' spontaneous motivation was tested in open field, spontaneous and evoked activity of the somatosensory (SS), visual (VIS) and auditory (AUD) cortical areas were recorded, conduction velocity of the tail nerve was measured, and internal doses (tissue Mn levels) were determined.

When nanoparticulate Mn was given it. after the period of po. administration of the dissolved form, certain general, behavioral and electrophysiological parameters were disproportionately strongly affected. On NP administration, body weight gain was significantly reduced in the combination groups. Open field locomotion and rearing was more strongly reduced after 6+6 (po., then it.) then after 6 weeks treatment. Latency of cortical evoked potentials was prolonged in all treated groups. On the SS and VIS evoked potential, latency increase was about equal after 3+3 (po. + it.) and after 6 weeks (po. only) treatment, although the summed dose in the former case was much lower. Tail nerve conduction velocity decreased, and the relative refractory period increased, in the treated groups. In blood, brain, lung and liver samples from the combined treatment groups (3+3; 6+6) significantly elevated levels of Mn were measured.

Exposure to the nanoparticulate form of a heavy metal can add new features to the metal's toxic potential.

P031 – Germaniun functionalization for the development of organic dielectric thin film

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Keywords: functionalization, germanium, diazonium salt, dielectric

For over 40 years, microelectronics has rapidly grown mainly based on silicon technology. Indeed thanks to its low cost, abundance and the insulating, protective and passive properties of its oxide, silicon remains the material of choice for micro and nanoelectronics. Silicon has, however, limitations when looking to high mobility and high frequency operations. Alternative materials such as Ge which presents intrinsic higher mobility and allow operation at higher frequencies, have to be significantly improved since its oxide, unlike SiO_2, is not insulating and impervious enough for real applications. Within this project, we will design, fabricate and evaluate ultra-insulating (High k) thin films based either on self-assembly monolayers on Ge or on grafting of diazonium salts, to give them these viable properties allowing their use in next generation devices.

The first step is to prepare the Ge surface for grafting. The Ge substrate has to be cleaned to remove oxide. Different cleaning methods, including soft methods such as water, were tested and compared to promote a better self-organization of the protecting layer. Both the surface state and the surface roughness were explored to determine the best routine to clean Ge before grafting. The surfaces were then functionalized by different ways to create either SAMs either a thin film depending on the anchoring system used. The spontaneous grafting of diazonium salts as well as the formation of SAMs of thiols were studied as well as the stability of the resulting organic layer. Fluorinated thiols and different alkylthiols were probed to determine the different parameters (chain length, π-stacking, anchoring group, absolute coverage) for designing the high-k molecules. In parallel, molecules presenting high k were also synthesized, grafted and evaluated.

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P032 – Hexagonal tungsten-trioxide: Preparation, characterization and modification

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Nanotechnology and nanostructured materials have been in the center of the attention in the past few decades. Nanotechnology is "the design, characterization, production, and application of structures, devices, and systems by controlled manipulation of size and shape at the nanometer scale (atomic, molecular, and macromolecular scale) that produces structures, devices, and systems with at least one novel/superior characteristic or property". The properties of these new materials are different from the properties of the bulk matter and that is the reason why they can be used widely.

Recently, much effort has been devoted to the synthesis of semiconductor nanowires, nanorods and nanobelts. Among metal oxides, WO_3 is a wide band gap semiconductor therefore it can be used in many applications like semiconductor gas devices, electrochromic devices or photocatalysis. WO_3 nanowires can be synthetized for example by heating a tungsten foil in argon gas or by electrochemically etching a tungsten tip.

In this work the hydrothermal method was used for preparing WO_3 nanowires. We used sodium-tungstate as precursor, sodium-sulphate as structure directing agent and hydrochloric acid to set the pH of the solution. The mixture was transferred into a Teflon lined stainless steel autoclave and it was kept at 180°C for 48 h.

The nanowires were decorated with metal nanoparticles by wet impregnation. The as-prepared sample was investigated by XRD, TEM, SEM, IR and UV-Vis spectroscopy

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P033 – Highly birefringent photonic crystal fiber by altering patterns and filling media of innermost air-holes

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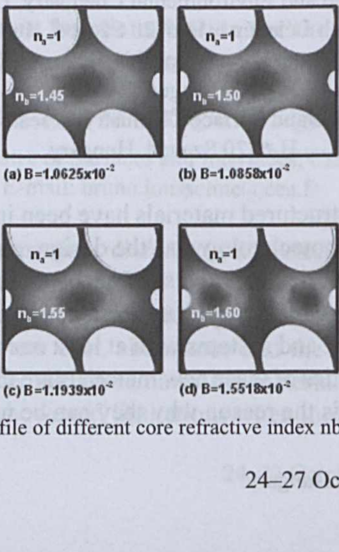
We numerically investigate a novel high birefringence and low confinement loss index-guiding photonic crystal fiber (PCF) using the finite element method. This PCF is composed of a solid silica core surrounded by six elliptical air-holes and a cladding



(a) $B=1.0625\times10^{-2}$ (b) $B=1.0858\times10^{-2}$

(c) $B=1.1939\times10^{-2}$ (d) $B=1.5518\times10^{-2}$

Figure 1. Field profile of different core refractive index nb of Type 1 structure

which consists of binary unit cells. The maximal modal birefringence and lowest confinement loss of proposed structures at the excitation wavelength of $\lambda = 1550$ nm can be easily achieved at a magnitude of the order of 10^{-2} and less than 0.39 dB/km because the modification gives rise to the strong confinement of guided modes. In addition, the effect of core index can influence the birefringence of PCFs due to the difference of refractive index between fiber core and innermost holes. The merits of our designed PCFs are that the birefringence and confinement loss can be easily achieved by altering the configuration of six innermost (closest to the core) air-holes and varying the core index, and are robust to against manufacturing inaccuracies.

P034 – Humidity-sensitive dielectric properties of titanate nanowires (TiONW)

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Elongated oxide nanostructures have gained much attention in the past decade due to their unique mechanical, optical, and electrical properties. Despite the vast amount of theoretical and experimental work on these materials, the mechanism of the water related electrical conduction in these systems has remained unsolved. Therefore the charge transport processes in hydrothermally synthesized trititanate nanowires (TiONW) at varying relative humidity (RH) have been investigated. Parameters characterizing these processes were extracted from dielectric spectroscopy (DRS) and ionic transient current (ITIC) measurements at room temperature. The dc conductivity varies exponentially with increasing RH. It is suggested to stem mainly from the exponentially increasing charge carrier concentration, while carrier mobility seems to have a much weaker influence on the long range charge transport. The changes in the constituent parameters of dc conductivity are thought to be due to the changes in the amount, surface structure and thermodynamic state of adsorbed water, which has been confirmed in the case of ionic mobility with moisture sorption and calorimetric (DSC) investigations. However, the microscopic origin of the exponentially increasing carrier concentration with RH still remains an open question.

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P035 – Hydrogen peroxide biosensor based on carbon nanotube/horseradish peroxidase bio-nanocomposite

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Keywords: horse radish peroxidase, carbon nanotube, fluorescence

Carbon nanotubes (CNTs) have unique properties, as good conductivity, high chemical stability and it is possible to bring them close to the redox centers of the proteins. Horseradish peroxidase (HRP) has long been a representative enzyme in understanding the biological behaviour of catalysed oxidation of the substrates H_2O_2, so it is the most commonly used enzyme in H_2O_2 detection.[1–3] The determination of H_2O_2 is of great interest because it is a product of reactions catalyzed by several oxidase enzymes in living cells and it is essential in environmental and pharmaceutical analyses.

The enzyme activity of HRP bound to carboxyl-functionalized multiple walled carbon nanotubes (MWNT-COOH) have been investigated. Binding procedure was carried out by N-Hydroxysuccinimide (NHS) and 1-[3-dimethylaminopropyl]-3-ethyl-carbodiimide (EDC) crosslinkers. We measured the fluorescence of tetra-guaiacol (which chemical is the product of guaiacol oxidation after addition of H_2O_2) as a function of time and we managed to determine the activity of the bio-nanocomposite. The LOD (limit of detection) for H_2O_2 was studied on carbon nanotube/horseradish peroxidase bio-nanocomposite. The optimized hydrogen peroxide biosensor we developed exhibited a detection limit of 4 μM H_2O_2/sec. This resolution was better than measured in solution by about a factor of two (it was 10 μM H_2O_2/sec in solution).

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P036 – Hydrogen production with Au or Pt modified TiO_2 photocatalysts as a function of noble metal nanoparticle size

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Keywords: size dependent activity, platinum, gold, TiO_2, H_2 production, photocatalysis

In the present work gold or platinum deposited *Aeroxide P25* TiO_2 photocatalysts were prepared with 1 wt% noble metal content. The aim of the experiments was to investigate the differences in the photocatalytic performance when these photocatalysts were deposited with differently sized Au or Pt nanoparticles.

Gold/platinum doped titanias have high efficiency for H_2 production when these catalyst suspensions are irradiated with UV light due to the low overpotential of hydrogen evolution. H_2 production is more effective when the suspension contains an easily oxidizable organic compound as a hole scavenger.

The noble metal deposition onto the titania surface was achieved by chemical reduction (*in situ* reduction onto the titania surface (CRIS) or sol-imregnation of the previously reduced nanoparticles to the aqueous suspensions of the photocatalysts (CRSIM). During the synthesis trisodium citrate was used as a stabilizing agent. Varying the citrate concentration differently sized noble metal particles were prepared. The reducing agent was sodium borohydride.

The samples were examined with transmission electron microscopy (TEM) to determine average noble metal particle size. TEM images revealed the presence of 2.5–5 nm platinum and 2.6–50 nm gold domains on the surface of the catalysts.

H_2 production measurements were carried out in the absence of dissolved O_2. Photocatalytic activity of the samples was examined in a special well-sealed reactor containing aqueous TiO_2 suspensions and irradiated with UV light ($\lambda_{max} = 365$ nm), using oxalic acid (50 mM) and methanol (50 mM) as model compounds. In these measurements, the H_2 production rates were dependent on the noble metal particle size. The optimal particle size was $\approx$3.2 nm for Pt and $\approx$5.7 nm for Au, at which the photocatalytic activity was the highest. Comparing the quantum yield of the catalysts for H_2 production and for the oxalic acid decomposition it turned out that hydrogen mostly evolves from the organic compound. Interestingly there is a high peak in hydrogen evolution in the first 40 minutes of the measurement using Pt-TiO_2. After this period, the H_2 evolution falls back but it stays at a constant rate in the rest of the experiment. This phenomenon was not observed with Au-TiO_2 where H_2 flow was almost constant for the whole experiment. Using methanol as a sacrificial reagent the H_2 production rate was notably higher with Pt-TiO_2 whilst it was almost one-fifth with Au-TiO_2 than in the cases using oxalic acid.

These experiments confirmed that suitable noble metal modified catalysts can be synthesized for efficient H_2 production. These catalysts are potentially able to utilize the UV component of solar irradiation to provide a relatively cost effective H_2 source.

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P037 – Hydrothermal synthesis and humidity sensing property of ZnO nanostructures, ZnO-In(OH)$_3$ and ZnO-In$_2$O$_3$ nanocomposites

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Keywords: ZnO, In(OH)$_3$, In$_2$O$_3$, hydrothermal method, nanocomposite

Prism-, and raspberry-like ZnO nanoparticles and ZnO-In(OH)$_3$ nanocomposites were prepared by template free hydrothermal method. The structure formation was controlled by temperature and addition rate of hydrolyzing agent. The ZnO-In$_2$O$_3$ nanocomposites were produced from the ZnO-In(OH)$_3$ samples by heat treatment at 500°C.

XRD investigations and scanning electron microscopy studies showed that pill-like In(OH)$_3$ with cubic crystal structure formed on the surface of ZnO nanoparticles resulting the increase of specific surface area of ZnO. TEM-EDX mapping images demonstrated that not only nanocomposite formation took place in the course of the synthesis, but zinc ions were also incorporated into the crystal lattice of In(OH)$_3$. SEM and crystallographic analyses of calcined samples revealed that spherical In$_2$O$_3$ nanoparticles with body-centered cubic and rhombohedral crystal structure – depending on the morphology of ZnO particles – were produced. The presence of indium had an influence on the optical properties (UV-Vis absorption and fluorescence) of the nanocomposites: band gap energy of ZnO-In(OH)$_3$ samples slightly increased, while the band gap energy of ZnO-In$_2$O$_3$ samples decreased with indium concentration compared to the pure ZnO. The raspberry-, and prism-like ZnO particles exhibited strong visible emission with a maximum at 585 and 595 nm, respectively, whose intensity significantly increased due to ZnO-In(OH)$_3$ nanocomposite formation. In case of the calcined ZnO and ZnO-In$_2$O$_3$ samples a shift towards the higher wavelengths and intensity increase of visible emission was observed. QCM measurements demonstrated that the morphology of ZnO and concentration of indium compounds had an influence on the water vapor sensing properties.

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P038 – Immobilization of zinc, nickel and copper in sediment using nanoscaled zero-valent iron particles

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Keywords: sediment, nanoscaled zero-valent iron particles, heavy metals, leaching tests

The aim of this study was to determine the possibility of using nanoscaled zero-valent iron particles (nZVI) for the immobilization of metals in contaminated sediment from the Great Backi Canal (Serbia). The assessment of the sediment quality based on the pseudo-total metal (Zn, Ni, Cu) content according to the corresponding Dutch standards and Canadian guidelines shows its severe contamination that requires disposal in special reservoirs and, if possible, remediation treatments. Immobilization treatments have been widely applied to treat soil, sludges and wastes with heavy metal contamination. The hazardous waste potential can be minimized by converting the contaminants into forms which are less soluble, less mobile or less toxic, or by encapsulating the waste within a solid of high structural integrity.Nanoscaled zero-valent iron particles have been demonstrated to be an efficient reductant to many pollutants, and have been extensively investigated for remediation of water contaminated by heavy metals. However, there are still some technical challenges associated with practical applications, such as the aggregation of nZVI particles. In order to determine the long-term behavior of sediment-nZVI mixtures, leaching tests were done in accordance with ANS diffusion test (ANS, 1986) in the period of 90 days, with DI water as the leachant. Treatment efficency was also evaluated by measuring the cumulative fractions of metals leached, effective diffusion coefficients – De and leachability indices – LX. Also, the standard Toxicity Characteristic Leaching Procedure (TCLP) and German standard leaching test (DIN 38414-4) were applied to evaluate the extraction potential of

Zn, Ni and Cu. In this study, leaching tests undertaken on sediment-nZVI mixtures showed that the concentrations of heavy metals in the leachates were largely inside the regulatory limits thus, and samples can be regarded as non-hazardous material. The efficiency of immobilization in the sediment-nZVI mixtures decreased in the order: **Cu > Zn > Ni**. The LX values were greater than 9, suggesting the sediment-nZVI mixtures are acceptable for controlled utilization. Based on effective diffusion coefficients – De metals showed low mobility or immobility (De in the range 10^{-10} to 10^{-14} cm^2s^{-1}) depending on the nZVI content. Based on the LX values, cumulative percentage of metals leached, diffusion coefficient and results of TCLP and DIN tests it appeared that treatment with nZVI was efficient in immobilizing metals.

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P039 – *In situ* synthesis of Maleic anhydride – Octene 1 – Vinyl Butyl/CdS and Maleic anhydride – Octene 1 – Vinyl Butyl/ZnS nanocomposites and their characterization with several investigation methods

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Keywords: nanocomposite, *in situ,* terpolymer

In this scientific work Maleic anhydride – Octene 1 – Vinyl Butyl/CdS and Maleic anhydride – Octene 1 – Vinyl Butyl/ZnS nanocomposites have been synthesized via *"in situ"* synthesis method. Maleic anhydride – Octene 1 – Vinyl Butyl terpolymer was used as the matrix in this method.

First of all maleic anhydride, octene 1, and vinyl butyl ether were polymerized to form a terpolymer as the result of radical terpolymerization process. Azobisisobutyronitrile (AIBN) was used as the initiator in this process. After 4 hours Maleic anhydride – Octene 1 – Vinyl Butyl terpolymer was obtained, washed, and dried. Obtained terpolymer was reacted with chlorides of cadmium and zinc in three – necked round bottom flask, in N,N – dimethylformamide solution to form Maleic anhydride – Octene 1 – Vinyl Butyl/CdS and Maleic anhydride – Octene 1 – Vinyl Butyl/ZnS nanocomposites. These nanocomposites are very useful in semiconductor technology and optoelectronics.

Several techniques were used for characterization of Maleic anhydride – Octene 1 – Vinyl Butyl/CdS and Maleic anhydride – Octene 1 – Vinyl Butyl/ZnS nanocomposites. Optical properties were characterized with SPECORD 250 PLUS, Thermical properties were characterized with DERIVATOGRAPH STA 449 F3 thermical analyzator.

Structural investigations were carried out by Energy – dispersive X-ray analysis method on EDX RÖNTEC Quantax analytical device, with X-ray Diffraction spectrometry method on Rigaku MiniFlex Desktop X-ray Diffractometer, and with Raman spectroscopy method on Thermo Scientific DXR Raman Microscope.

Surface topology of the Maleic anhydride – Octene 1 – Vinyl Butyl/CdS nanocomposite was described with Atomic force microscopy technique on NanoEducator – (NT – MDT) educational microscope.

Sizes of the CdS and ZnS nanocrystals were confirmed with Transmission electron microscopy method on TEM FEI TECNAİ G2 20 X – TWIN Microscope. Sizes of the nanocrystals were defined as less than 5 nm.

Acknowledgement: This work was supported by NAPEP FP7 project. Grant agreement number: 266600.

P040 – The influence of different co-activators on the photoluminescence properties of $SrAl_2O_4$ phosphors

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Inorganic phosphors have been extensively investigated for various applications in the optical and electronical fields. Within the different type phosphors the alkali earth aluminates have attracted great attention due to the very long persistent phosphorescence and high chemical stability. These alkali earth aluminates are mainly activated with divalent europium ions and co-doped with trivalent co-dopant ions, such as dysprosium. These $SrAl_2O_4$:Eu^{2+}, Dy^{3+} phosphors have good luminescent properties with long afterglow time which made them ideal material for many practical applications.

Traditionally the $SrAl_2O_4$: Eu^{2+}, Dy^{3+} phosphors are prepared at high temperatures with solid-state reaction method. In this case, the host material and the activators which replace some of the host ions are incorporated simultaneously during the calcination. In the preparation $Sr(CO_3)_2$, Al_2O_3, Eu_2O_3 and Dy_2O_3 along with some flux is mixed together and blended to get homogeneous mixture and fired at a suitable temperature.

Besides the solid-state synthesis, phosphors are also prepared by combustion method. The combustion method is a facile and very efficient method, which takes only a few minutes. In this method, all precursors are used as salts such as in their nitrate forms in our case. During the synthesis a proper amount of organic fuel is added to the aqueous solution of the nitrates and as a result of this exothermic redox reaction the doped strontium-aluminates formed in several minutes at relatively low temperature.

In this work $SrAl_2O_4$:Eu^{2+} phosphors were prepared by solid-state reaction and also with combustion method at 500°C. We used different rare-earths metals as co-dopants beside of the europium activator.

The samples were characterized using XRD, TEM, SEM, EDX and PL measurements to compare the effect of varying the different parameters and co-dopant ions. In order to complement the XRD data we used Raman spectroscopy measurements. The interpretation of the spectra was complicated, because of the great number of modes, but this technique was used for phase identifications. We also investigate the decay behaviors of the differently synthesized and doped phosphor samples. The decay rates varied upon the synthesis methods and dopant ions which was attributed to the presence of various types of traps with different depths in the samples.

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P041 – Influence of preparation pH on the nanostructure of silicate based bioactive glasses

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Keywords: sol-gel, pH, nanostructured bioactive glasses

Sol-gel-derived bioactive glasses are known to have nanometer-scale textural porosity which increases the specific surface area by two orders of magnitude compared to melt-derived glasses in the same composition.[1,2] For this reason bioactive glasses in SiO_2, SiO_2-CaO, SiO_2-CaO-MgO, SiO_2-CaO-K_2O, SiO_2-CaO-MgO-K_2O systems, were prepared via sol-gel method. The samples were prepared at two pH values an acid one (~ 1.5) and a basic one (~ 8.5). The aim of this study is to evaluate the preparation pH effect to the physicochemical properties of the systems. Differential thermal analysis (DTA) and thermal gravimetric analysis (TGA) were used to understand how the pH influences the thermal events. The morphology and compositions were studied using X-ray diffraction (XRD) and scanning electron microscopy (SEM). The textural particularities of the investigated samples are proposed to be determined by performing N_2-adsorption measurements. The bioactive character of these materials with different pH was accessed in vitro by analyzing the ability for apatite formation onto the surface after being immersed in simulated body fluid (SBF) at 37°C.

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P042 – Influence of sintering temperature on the microstructure of nanocrystalline Ni-yttria stabilized zirconia cermets

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Keywords: SOFC, YSZ, nanocrystal, sintering, microstructure

Solid oxide fuel cell (SOFC) is an energy conversion device that produces electrical energy at high temperature by electrochemically combining fuel with oxidant gases across an ionic conducting oxide. SOFC provides many advantages, including high-energy efficiency, modularity, fuel adaptability and environmental friendship. The present work aims to elucidate the microstructure of nanocrystalline Ni-yttria stabilized zirconia (YSZ) cermets in order to fabricate nano-sized and porous cermets. The green NiO-YSZ bodies were sintered at 1300–1450°C in air. Subsequently, the sintered NiO-YSZ bodies were reduced at 1000°C in an inert gas atmosphere to fabricate nanocrystalline Ni-YSZ cermets. The sintered NiO-YSZ pellets consisted of NiO and YSZ phases, which crystallized in the cubic structure. The NiO and YSZ phases were homogeneously distributed for the sintered pellets. The microstructure of the nanocrystalline Ni-YSZ cermets depended strongly on the sintering temperature. The reduced Ni-YSZ pellets contained Ni and YSZ phases without any NiO phase. The grain size and density of the sintered and reduced pellets increased with sintering temperature. The porosity increased via the reduction treatment. In the present study, we systematically investigated the effect of sintering temperature on the microstructure of the nanocrystalline Ni-YSZ cermets.

P043 – Influence of the hydrophilic–lipophilic properties of surfactant mixtures on the droplet size and rheological behaviour of nanoemulsions

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Emulsions with droplet size in 10–50 nm range are often referred – without thermodynamic stability – as nanoemulsions. Against the kinetic stability of nanoemulsions the microemulsion are thermodynamically stable systems. Nanoemulsions are complex colloidal liquids because they have not only an aquatic and organic phase but contain also surfactants in both phase and the interface of phases. Nanoemulsions do not form spontaneously and their droplet size and stability depend upon the preparation pathway, the order of addition of the components, the nature of the liquid phases and chemical structure of applied surfactants. The main application of nanoemulsions is the preparation of nanoparticles where droplets act as nanoreactors. Moreover, nanoemulsions as a delivery tool can be contained oilfield chemicals may find applications in enhanced oil recovery (EOR) methods. Control of average droplet size in the mentioned applications is a key factor to obtain admissible nanoemulsion. Emulsification processes were performed with constant water/oil ratio and surfactant concentration. The hydrophilic-lypophilic balance (HLB) values of the surfactant mixtures were changed by mixing nonylphenol ethoxylate and sorbitan oleate. The average droplet size of nanoemulsions was measured by dynamic light (DLS) and small angle x-ray scattering (SAXS) techniques. We have used the Guinier-plot and Porod-presentation in the reciprocal space for droplet size and surface area determination at L/L surfaces. The inverse Fourier-transformation of the scattering functions allow us to present the pair-correlation functions of the complex fluid systems.

The viscosities of nanoemulsions were determined according to the flow curves taken on a rotational rheometer using temperature controlled double gap measuring system. The primary goal of the droplet size and rheological characterization was to reveal the correlation between the droplet size and viscosity of nanoemulsions and the HLB values of applied non-ionic surfactant mixtures.

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P044 – Interaction of porphyrin molecules with silver nanoparticles

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Keywords: silver nanoparticle, tetraphenylporhyrin, absorption spectrum

The optical properties and the photoactivity of the metallic and semiconductor nanoparticles are changing, if the particles are covered by dye molecules.

An aromatic dye molecule, tetraphenylporphyrin was studied as possible stabilizer and surface modificator in the synthesis of Ag nanoparticles. The characterization of this molecule was carried out by X-ray diffraction, FTIR, Raman and UV-Vis spectroscopies.

The nanoparticles were prepared in dimethyl formamide, as published earlier.[1] The composites were prepared with different nanoparticle – porphyrin concentration ratios. The stabilization effect and the interaction between the Ag nanoparticles and the tetraphenylporphyrin were studied by UV-Vis and Fluorescence spectroscopy.

The porphyrin molecules have a characteristic absorption spectrum. There is an intense absorption band between 390–425 nm, called B or Soret band. At a larger wavelength, there are two or four much weaker bands, called Q bands, situated between 480–700 nm. The number and intensity of these bands can give information about the porphyrin molecule: its substitutes and their position, whether or not it contains a metal ion.

Independent experiments showed that under our reaction conditions metaloporphyrins were not formed. Taking into account that the band intensities can change when the electron population of the energy levels is altered, the observed band intensity transformation in our experiment suggests that Ag nanoparticles might be accepting electrons from the tetraphenylporphyrin molecules during the interaction. The blue shift in the Q bands position could be related to the stronger probable interaction of the tetraphenylporphyrin through the metal "vacancy" of the molecule with the Ag atom in the nanoparticle surfaces.

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P045 – Investigation of sputtered nanocomposite Ti-based biocompatible coatings

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Keywords: TiC, nanocomposite, structure, biocompatibility, coating

Application oriented preparation of thin films or coatings needs reproducible technologies. As long as setting up a reproducible production characterised by a given set of preparation parameters is possible by an experimental trial and error technique, to understand the effect of these parameters on the properties of films is indispensable.

Modern methods of vacuum deposition provide great flexibility for manipulating material chemistry and structure, leading to films and coatings with special properties. These new special properties of nanocomposites are often unachievable in bulk materials.

A combination of metallic (Ti) and carbon phase can enhance certain physical properties of nanocomposite. Namely, hardness of the film can be improved by the introduction of boundaries or particles of hard phases for stopping deformation.

TiC exhibiting good corrosion resistance and high hardness, is widely used as a coating for cutting tools, wear parts and protective coatings. TiCN films are widely used for cutting tools, in parallel with relatively modern protective coatings mainly for their chemical stability and superior mechanical properties. TiCN coatings are also promising wear resistant films for applications at high temperature or highly corrosive environments.

In this work, the nanocomposite TiC and TiCN thin films have been developed as protective biocompatible coatings. The films were prepared by dc magnetron sputtering at 200°C in argon and nitrogen atmosphere. The structure of films was studied by transmission electron microscopy, atomic force microscopy and auger spectroscopy. The mechanical properties were measured by nanoindentation. MG 63 osteoblast like cells were applied for in-vitro tests of films.

P046 – Investigation of structure and thermal denaturation of protein-based drug nanohybrid systems

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Keywords: bovine serum albumin, protein denaturation, SAXS

According to develop new protein-based sustained release drug systems the study of interaction between protein and detergents are one of the most important research fields.

Sodium *n*-alkyl sulfates are most dominant classes of widely used anionic surfactants for example: in the field of medicine, pharmaceuticals, cosmetic and toiletry products, although this type of detergents perhaps has toxic effects.

In this work presented here, the interaction between bovine serum albumin (BSA) protein and surfactants with different alkyl chain length were studied in aqueous solution at pH = 3. The determination of specific surface charge of proteins is very important factor to identify the maximal amount of adsorbed other components like surfactants, biomolecules etc. The specific surface charge of macromolecule was determined with particle charge detector.

Moreover, the thermal denaturation characteristics of globular protein in the presence of increasing concentration of sodium *n*-alkyl sulfate (sodium *n*-octyl sulfate; sodium *n*-decyl sulfate; sodium *n*-dodecyl sulfate) has been determined by differential scanning calorimeter (DSC). The change in the enthalpy of phase transformation shows the effect of sorption on the albumin particles. Photoluminescence decay experiments show also the interaction between the albumin and surfactant molecule.

The change in particle size and the electrokinetic potential (ζ-potential) of globules or complexes were measured with dynamic light scattering (DLS) apparatus.

In order to characterize the structure of the prepared protein-detergent complexes small-angle X-ray scattering (SAXS) technique was also applied. Namely, we determined the gyration radius (R_g) and particle radius by Guinier representation and we compared these values to the result of the calculation of distance distribution function determined by inverse Fourier transformation of the scattering function. The weight and volume of macromolecules from SAXS results were determined as well. We found that the experimental SAXS results are in good agreement with the data of dynamic light scattering.

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P047 – Magic number of standing wave on the surface of a gold-shell nanorod

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Keywords: finite-element method, reactor, azide

We investigate the surface surface plasmon effects of a gold–shell nanorod by using the finite-element method in a three-dimensional model. The number of standing waves on the surface of a gold-shell nanorod and their optical properties are investigated. Results show that the near-field optical images show spatially oscillatory patterns (nodal fields) on the surface of gold-shell nanorod, and these phenomena are attributable to plasmon-mode wave functions. We interpret these phenomena in terms of the electric field nodes on the surface of the rod, and the results show good agreement with our experimental observation in the optical images.

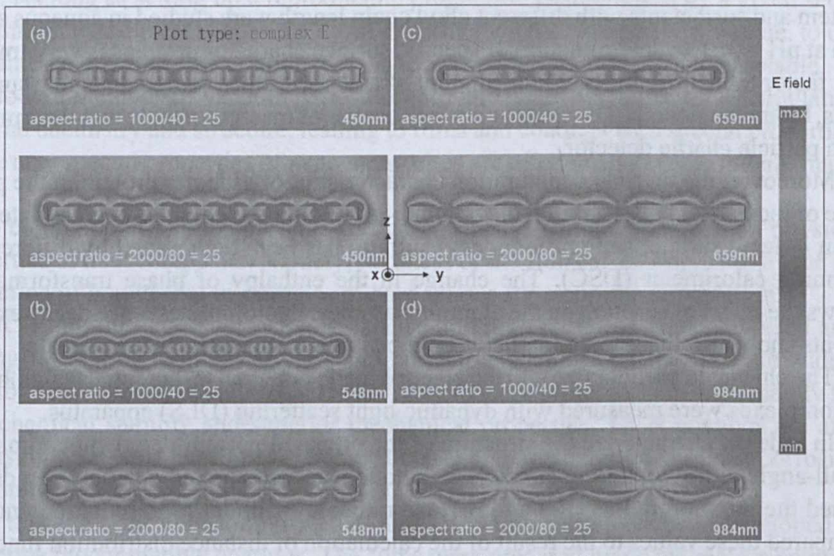

Figure 1. Standing wave numbers of a gold-shell nanorod

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P048 – Magnetic circular dichroism as probe of local magnetic moments in 1D iron-carbon nanotube hybrids

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Keywords: XMCD, filled carbon nanotubes, magnetic moments

Localized electronic and magnetic properties of iron inside metallic and semiconducting single-walled carbon nanotubes (SWCNT) was investigated by x-ray absorption spectroscopy (XAS) and magnetic circular dichroism (XMCD). Ferrocene (FeCp2) encapsulated in SWCNT was transformed into 1D Fe nanoclusters by means of nanochemical reactions. Differences in the interactions between the encapsulated material and the nanotubes were observed for the different metallicities of the tubes. The XMCD response is enhanced due to the formation of 1D Fe clusters. The orbital and spin magnetic moments of the 1D Fe clusters determined from the XMCD are found to be dependent both on the Fe cluster size and the metallicity of the tubes. The magnetic moments of these carbon nanotube hybrids measured by bulk superconducting quantum interference device (SQUID) evidence that the delocalized magnetisms contributes to the magnetic properties of these 1D nanostructures.

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P049 – Modification of acidic sites on the surface of titanate nanostructures

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One-dimensional titanate nanostructures, like nanotubes (TNT) and nanowires (TNW) have attracted great attention of scientific researches due to their unique and promising chemical and mechanical properties. The syntheses are based on an alkali hydrothermal process in 10 M NaOH aqueous solution under different circumstances.

TNTs and TNWs both have open ended one-dimensional morphology, TNTs possess multi-wall scroll-type structure, while TNWs presence in a layered morphology. Both materials can be described as having large external and internal surfaces and interlayer spaces. Their microstructure and negatively charged skeleton exhibit cation-exchange properties. With acidic post treatment of the pristine TNTs and TNWs sodium ions can be changed to protons or other cations.

Our aim was to characterize Lewis and Broensted acid sites and their structure modifier effect in the above mentioned one-dimensional titanate nanostructures with temperature programmed desorption and other material investigation techniques. The morphology of the as-synthesized nanostructures was observed by HRTEM, SEM measurements. We followed the Na^+/H^+ ratio in partially protonated TNTs and TNWs with EDS analysis. The specific surface area was determined from N_2 adsorption isotherms. The crystal structure of the materials was analyzed by X-ray diffractometry.

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P050 – Nanomodified PP-fibers for protection against environmental tobacco smoke

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Keywords: modified PP-fibers, surface modification, environmental tobacco smoke

Environmental tobacco smoke (ETS) exposure is one of the major problems of indoor air quality.[1] Development of nanotechnology allows to create functional textile materials with added-value (e.g. photocatalytic and biostatic) including a surface modification of single fiber.[2,3] The aim of presented study was to investigate the susceptibility of unmodified (PP) and nanomodified (PP/T) polypropylene fibers to sorption and photocatalityc decomposition of ETS-derived nicotine (basic marker of tobacco smoke exposure). PP/T fibers were modified with Titanium Dioxide doped by silver nanoparticles (TiO_2/Ag). Modern analytical techniques; gas chromatography, Raman spectroscopy, volumetric adsorption, scanning electron microscopy (SEM/EDS) as well as inductively coupled plasma mass spectrometry (ICP-MS) were applied for assessment of PP-TiO_2/Ag modification. Sorption testing was performed on the test stand as previously described [2] with the use of commercial cigarettes (0.8 mg of nicotine per cigarette). The fibers were exposed to sunlight directly after ETS sorption. The changes in nicotine concentrations after ETS sorption as the function of the sunlight exposure may be described by equation $c = c_o e^{-kP}$. Comparative studies have evidenced statistically significant faster decrease in nicotine concentration for modified PP fibers.

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P051 – Nanopore SERS substrate based on silver-coated anodic aluminum oxide

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Keywords: anodic aluminium oxide, surface-enhanced raman scattering, nanoplasmonics

Surface-enhanced Raman scattering (SERS) is one of the best powerful tools for biochemical applications because it enables ultrasensitive and real-time molecular monitoring. Most of SERS platforms are based on nanoparticles, nanowires and nanopores with novel metals. Anodic aluminum oxide (AAO) is a promising large-area and highly reproducible nanopore structure because it has a simple and cost-effective fabrication process, tunability of pore thickness and size, and large-area uniformity. Our study reports the fabrication of a SERS substrate based on silver-coated AAO and the characterizations of the SERS responses by controlling two parameters; AAO thickness and pore size. Optimized SERS signals of rhodamine 6G (R6G) were recorded. It was found that our SERS platform exhibits strong enhancement due to the localized surface plasmon resonance (LSPR) of silver-coated AAO.

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P052 – Nanoscale processes in thight reservoir rocks studied by photoacoustic spectroscopy

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Keywords: nanopore, reservoir rock, photoacoustic

The physical mechanisms behind fluid flow and gas storage in the nanopore size rock matrix is remarkably different from those in conventional natural gas reservoirs and consequently their measurement methods has to be different as well. In conventional measuring methods, transport mechanisms are tested by Darcy's law based measurements using pressure gradient generation and flow rate detection. However, transport processes of unconventional gas fields follow not simple Darcy's law, because of being driven by both pressure and concentration gradient and also by surface processes.

Our goal is producing more precise material parameters for unconventional well simulations and production prognosis. Therefore we develop a new type of test method based on photoacoustic spectroscopy. Photoacoustic detectors are very sensitive optical absorption based analysers. Due to their high sensitivity and selectivity, they are able to determine small gas concentrations and perform multicomponent analysis at the same time.

There are two permeation testing methods that can be adapted for mass transfer measurements through rock samples. The first one is based on establishing pressure and/or concentration gradient between two sides of planar samples and detection of equalization processes between the sides by recording as concentration changes in time. For nanopore size rocks in which various transport and surface processes are present simultaneously, there is a possibility to apply the so called immersion method, which can give more information about the fluid flow properties of the sample. This method starts by immersing the rock sample into the gas of interest for a long time till gas saturation is reached, then dropping the gas concentration suddenly around the sample and finally detecting gas desorption processes as a function of time. The gas depletion kinetics gives additional information about processes from smaller pores and nanopores.

Different types of rock samples with known mechanical properties were tested. It was justified that depletion kinetics correlated well with mineral composition of rock samples. Our results evidence that the developed measuring system can be used for studying diffusion processes in nanopores.

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P053 – Nanostructured liquid crystals with thiophene unit: Synthesis, properties and applications

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Keywords: liquid-crystals, nanomaterials, self-organization, thiophene, nematic, smectic A phase

Liquid crystals (LC) became one of the essential nanomaterials of the modern era. They are used in advanced technological sources well-known as LCD displays.[1] Since in most applications an ordering of the conjugated systems leads to improved properties,[2] the induction of liquid-crystallinity in p-conjugated materials is one of the promising approaches to control the self-organization processes. This concept was successfully applied in a synthesis of a new series of rod-like mesogens containing thiophene moiety.[3] All the compounds possess substituted 2-aminothiophene unit as a main element in the structure attached to a stilbene moiety with a terminal alkyloxy chain (OR^1, OR^2 where $R^1 = C_nH_{2n+1}$, $R^2 = C_mH_{2m+1}$; n, m ranging from 6 to 12). In general, the versatility of thiophene chemistry and the p-donating character of thiophene provides the basis for the synthesis of most conjugated p-systems.[4] The monitoring of the properties of the p-conjugated mesogens with functionalized 2-aminothiophene core in dependence on the alkyloxy chain length allowed us establishing valuable structure-property relationship. It is well known that liquid-crystalline system properties are dependent on the size of nanoparticle and inter-particle spacing. Compounds with medium sized alkyloxy chains and higher symmetry exhibit both, nematic and smectic A phase, while shortening of alkyloxy chain and/or symmetry breaking favours only the nematic phase. Such mesogens, that are 4.0–4.2 nm of size in SmA phase, exhibit fluorescence related to the presence of stilbene unit in the molecular structure. The electrochemical band gap for these mesogens was found to be ca. 3.0 eV. Explored liquid crystals could be in the scope of interest in the development of novel electro- and photo-functional metamaterials. Further investigations of 2-aminothiophene containing mesogens creating an external liquid-crystalline coating on metal surfaces[5] are also under progress.

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P054 – Nasal delivery of meloxicam nanoparticles

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Keywords: meloxicam, nanoparticle, intranasal delivery

Novel formulations and sites of drug administration for systemic delivery offer opportunities to develop innovative pharmaceutical compositions. The nasal pathway represents an alternative route for non-invasive systemic administration of drugs, although the nasal epithelium forms a restricting barrier.[1] Nanonization of drugs increases their solubility and permeability through mucosal barriers. Previously we have investigated the preparation process of meloxicam (MEL) nanoparticles by co-grinding with polyvinylpyrrolidone.[2] The influence of different parameters on the particle size was studied, the optimization of the process was performed, and the physico-chemical properties of MEL nanoparticles were characterised. We also established and characterised an in vitro cell culture model of the nasal epithelial barrier to test the toxicity and permeability of innovative nasal formulation.[3] The aim of the present study was to investigate a pharmaceutical composition containing MEL nanoparticles for nasal delivery by *in vitro* and *in vivo* methods. Nanonization increased the solubility of MEL, and the extent of dissolution; complete dissolution of MEL was observed within 15 min. Real-time monitoring of cell viability by cell microelectronic sensing technique indicated no sign of disruption of the integrity of human RPMI2650 nasal epithelial cell layers. The lack of change in cell index suggests that MEL nanoparticles are not toxic and cross the cell layers via the transcellular pathway. The flux of MEL through the epithelial cell layers was significantly slower than in the case of the Franz cell diffusion model, reflecting the complexity of the nasal epithelial barrier. Pharmaceutical compositions containing MEL in nanonized form were tested on Sprague-Dawley rats. The *in vivo* data showed a favourable pharmacokinetical profile of MEL nanoparticles after intranasal administration.

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P055 – Neurotoxicity of combined intratracheal metal nanoparticle exposure in rats

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Keywords: manganese, iron, chromium, rat, nanoparticle, electrophysiology

Manufacturing of metals usually requires high temperature operations, such as welding, during which metal fumes are released into the air resulting in significant inhalational occupational exposure. Many of the particles derived from the welding process are nanoparticles (NPs). The most common elements in steel that welders are primarily exposed to by inhalation are iron (Fe), manganese (Mn) and chromium (Cr). Such airborne particles have major adverse health effects, causing among others neurological disorders. The neurotoxicity of Mn has been described extensively but the role that other agents peculiar to welding may play in the causation of neurological disorders are still unknown.

For modelling welding-related metal NP exposure, young adult male Wistar rats were intratracheally instilled with a suspension of the double and triple combinations of MnO_2, Fe_3O_4 or $Cr(OH)_3$ NPs (2 mg/kg b. w. respectively). Treatment was performed in brief diethyl ether anaesthesia, once a day, 5 times per week, for 4 weeks. At the end of the treatment period, motor behavioural test (open field, OF) and electrophysiological recording was conducted. In the latter, spontaneous electrical activity (electrocorticogram, ECoG) and sensory evoked potentials (EPs) were recorded from the somatosensory (SS), visual (VIS) and auditory (AUD) cortical areas. The body weight of animals was regularly measured. Following electrophysiological recording, the animals were sacrificed and dissected. Metal level was determined from blood, brain and lung samples by ICP-MS.

Body weight gain of the animals was significantly reduced by Fe+Cr *(FC)*, Mn+Cr *(MC)* and the three-metal *(FMC)* combinations. As for the organ weights, the most prominent alteration was the increase of the lungs' relative weight (related to brain weight or 1/100 body weight). In the OF test, local activity and immobility were increased and vertical activity was decreased by *FC, MC* and *FMC*. In the ECoG, application of Cr-containing combinations caused a significant shift to higher frequencies. The EPs showed significantly increased latency on the action of *FC* and *MC,* and slightly also of *FMC*. Mn content of the brain, lungs, and also blood was significantly increased by each of the metal combinations; Cr levels were, however, not increased in brain, only in blood and lung samples. The effect of Fe was only seen on increased lung Fe levels. The correlation between brain Mn levels and SS and VIS ECoG index and SS and VIS latency was significant in *MC* group.

The interactions of the three metals studied were dissimilar on various parameters. The effect of Mn on body weight gain, and on electrophysiological and some behavioural parameters, were counteracted by Fe, but Cr was apparently not involved in such interaction. In the tissue metal levels, Fe acted on Cr but not on Mn. All that indicated that measured internal dose is not the sole determinant of the functional alterations and so, not an ideal biomarker of effect.

P056 – Noble metal deposited TiO_2/WO_3 composite photocatalysts for oxalic acid degradation and hydrogen production: The role of the localization of the gold or platinum nanoparticle

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Keywords: titanium dioxide, tungsten trioxide, hydrogen production, platinum, gold, composite photocatalysts

The synthesis of nanomaterials capable of photocatalytic hydrogen production is nowadays a major research field in materials science. Several semiconductor oxides and composites coupled with noble metal nanoparticles are intensively studied to achieve higher hydrogen production yield. In the case of the composites, the main role of the individual components combined with the proper noble metal particles is not clarified yet in the literature.

Consequently, titania/tungsten (VI) oxide/noble metal (gold and platinum) composites were obtained by the means of selective noble metal photodeposition on the desired oxide surface (either on TiO_2 or on WO_3). The noble metal particles' localization was proved by SEM-EDX, while their size with DRS and TEM. The influence of the noble metal nanoparticles' position was investigated successfully on the light absorption properties, photocatalytic activity towards oxalic acid and photocatalytic hydrogen production.

Major differences were observed in the photocatalytic performance of the catalysts in which only the position of the noble metal was changed. Consequently, highly active composites were obtained, that surpassed the reference catalysts' (TiO_2(Au), TiO_2(Pt), WO_3(Au), WO_3(Pt)) oxalic acid degradation yield and were also quite active for photocatalytic hydrogen production.

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P057 – A novel design of a plasmonic nanoantenna

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Keywords: plasmonics, core-shell dipole antenna

We numerically investigated a core-shell dipole antenna which is composed of two identical castle-like contour nanometal with a dielectric medium filled inside the hollow by using the 3D FEM. Simulation results show that the resonant wavelength of the

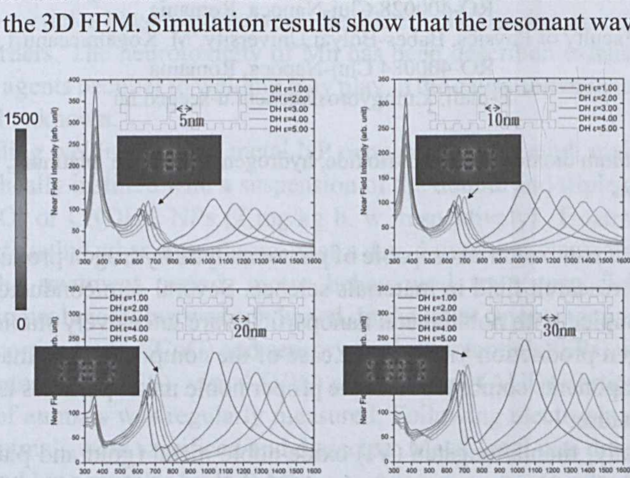

Figure 1. Field patterns and field intensity vs. wavelengths at different gap width of designed plasmonic nanoantenna

proposed nanoantenna may be tuned over a broad spectral (ranging in ultraviolet-visible, visible light and infrared light) by considering the contour of a castle-like core-shell antenna and introducing the design parameters (gap width, media filled inside the hollows and contour thickness). The antenna resonance generates a peak in scattering spectra, while the cavity resonances lead to multiple peaks in the scattering spectra. The cavity resonant frequency can be tuned by varying the value of the dielectric constant. The local field enhancement inside the hollows (cavity) is maximized when the gap width, castle-like core-shape (grating effects) and DHs when the cavity and antenna resonant frequencies coincide with each other.

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P058 – On-line investigation of climate relevant carbonaceous nanoparticles by photoacoustic spectroscopy

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Keywords: source apportionment, photoacoustic, optical absorption, Ångström exponent

Reducing uncertainties in current estimates of climate forcing is one of the most relevant issues in climate science today. The ambient aerosol is responsible for the vast majority of the uncertainties in the global radiative forcing calculations. According to one of the most reliable current estimates the net cooling effect refers to the direct and indirect effect of aerosol may exceed more than the half of two third warming effect caused by the greenhouse gases (Penner et al. 2001). However, the uncertainties quoted for the aerosol contribution are as large as or larger than the mean value of the estimates themselves. These uncertainties are mainly governed by the carbonaceous fraction of the ambient dust, especially by the recently discovered light absorbing carbonaceous matter so-called in collective terminology as Brown Carbon (BrC). Despites of its importance the spectral characteristic of carbonaceous nanoparticles typically appeared in the ambient are none or poorly characterized in the literature, in part since the lack of the reliable instrument.[2] The only method that could measure directly the optical absorption of ambient aerosol with high reliability is the photocoustic spectroscopy.[3] Although the PAS (Photoacoustic Spectroscopy) has favorable characteristics for absorption measurement, the PA based instrument for ambient aerosol investigation is not widespread yet.

In this study we present the absorption feature of the artificially generated, model, as well as re-dispersed ambient carbonaceous nanoparticles in the climate relevant

UV-VIS-NIR spectral region using our novel multi-wavelength photoacoustic instrument.[1] We experimentally demonstrated that although the absorption of the carbonaceous nanoparticles is not a conservative indicator of the chemical composition, the absorption feature of that including relevant information for source apportionment. We experimentally introduced here first that the wavelength dependency of the absorption is a chemical selective parameter. Finally, we demonstrated the correlation between the on-line measured optical and size spectra of the ambient carbonaceous nanoparticles.

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P059 – Optimization of adsorption conditions of thiamethoxam on CNTs by statistical design of experiments (DoE)

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Keywords: adsorption, thiamethoxam, statistical design of experiments (DoE)

In recent years there has been increasing public concerns for the disposal of large amounts of wastewater containing potentially toxic organic compounds. Taking into account the consequences of these substances on the environment, the polluted water requires the appropriate treatment prior to disposal.[1] It has been shown that carbon nanotubes due to their unique physico-chemical properties possess great removal capacity for many toxins.[2] The aim of this work was to optimize the conditions of thiamethoxam adsorption on ccHNO_3-treated multi-walled carbon nanotubes (MWCNTs) from aqueous solutions using the statistical design of experiments (DoE). The as-grown MWCNTs were synthesized by catalytic chemical vapor deposition method in the flow of ethylene/nitrogen mixture over 5%Fe-Co/Al_2O_3 catalyst. Prior to the adsorption process, the tubes were purified and functionalized by ccHNO_3 in order to remove the catalyst remains and increase the number of potential active sites for thiamethoxam bonding. The adsorption conditions optimization was performed in 16 runs arranged in a fractional factorial design. This arrangement enables the rapid testing of 5 factors affecting the amount of adsorbed thiamethoxam: initial solution concentration, pH, temperature, contact time and MWCNTs dosage. In addition to the impact of these main factors to the adsorbed amounts of thiamethoxam, the applied design considers also the two-factor interactions. The results of the optimization indicate the greatest impact of thiamethoxam initial concentration, solution pH and contact time and their mutual interactions. The uptake of insecticide is favored in the conditions of higher initial solution concentrations, pH values and contact time as well as lower temperature and MWCNTs amount. The Langmuir and Freundlich models are employed to analyze the adsorption occurred in the experiment. The experimental data could be well fitted only by Freundlich isotherm which indicates inhomogeneous energy distribution on the surface of MWCNTs. It is probably a consequence of the presence of different functional groups attached to the tubes during the acid treatment.

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P060 – Photocurrents generated by photosynthetic reaction center protein/bio-nanocomposite systems

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Keywords: reaction center protein, carbon nanotube, ITO

A large number of studies have shown recently that photosynthetic reaction center proteins (RC) purified from purple bacterium *Rhodobacter sphaeroides* R-26 bind successfully to nanostructures while retaining their functional activity.[1,2] The major goal of current research is to find the best systems and conditions for efficient photoelectric energy conversion and for the stability of these bio-nanocomposites. In our studies, RC protein was bound to amine- and carboxyl-functionalized multiwalled carbon nanotubes (MWNTs) immobilized onto the surface of ITO by using specific silane. The binding of RC to MWCNTs results in an accumulation of positive and negative charges followed by slow reorganization of the protein structure after excitation.[3] Both structural (SEM) and functional (absorption change and conductivity) techniques have shown that RCs can be bound effectively to amine- and carboxyl-functionalized CNTs. The photocurrent generated by the composite material is measured in an electrochemical cell designed especially for this purpose. The special electronic properties of the CNT/protein complexes open the possibility for several applications, e.g. in microelectronics, analytics or energy conversion and storage.

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P061 – Photoluminescence effect in double-walled carbon nanotubes

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Keywords: photoluminescence, DWCNT, carbon chains

The photoluminescence (PL) effect in Carbon Nanotubes has drawn the attention of many scientists to this subject for more than a decade now due to its possible applications, e.g. in biomedical environments such as markers.[1] Single-Walled Carbon Nanotubes (SWCNT) that were mostly used in these experiments are very sensitive to the degree of bundling which is necessary for the nanotubes to show PL, also the chemical environment plays an important role. Double-Walled Carbon Nanotubes (DWCNT) are expected to withstand these external factors since the outer tube would act as a shield for the luminescent inner tube but there has been a long controversy whether DWCNT can exhibit PL or not. The protecting outer tube is believed to cause nonradiative relaxation of the inner tube and therefore prohibit PL.

In this work, we show PL measurements of DWCNT produced with the Chemical Vapour Deposition (CVD) method. The as-produced samples were annealed in high vacuum at high temperatures which leads to the formation of linear carbon chains inside the inner tube of the DWCNT following.[2] The properties of the samples were investigated with Raman Spectroscopy, Optical Absorption Spectroscopy and measurements of the Photoluminescence. The carbon chains cause an increase of the PL signal similar to the PL enhancement of SWCNT filled with ferrocene.[3] The degree of enhancement of the PL shows a direct connection to the growth yield of the carbon chains which can be seen in Raman measurements. These findings contribute an important keystone to elucidate on the capability of DWCNT regarding their effective PL quantum yield.

Acknowledgement: Funding by the FWF is greatly acknowledged.

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P062 – Photoluminescence of $Ca_{3-3x/2}(VO_4)_2$:xEu ($0.01 \le x \le 0.09$) red-phosphors prepared by solution combustion method

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Keywords: phosphor, $Ca_{3-3x/2}(VO_4)_2$:xEu, photoluminescence, nanopowders

A red emitting nano-sized phosphor, $Ca_{3-3x/2}(VO_4)_2$:xEu ($0.01 \le x \le 0.09$), was successfully synthesized by the solution combustion method. The characteristic photoluminescence peaks of the $Ca_{3-3x/2}(VO_4)_2$:xEu phosphors caused by the $^5D_1 \rightarrow {}^7F_1$, $^5D_1 \rightarrow {}^7F_2$, $^5D_0 \rightarrow {}^7F_1$, $^5D_0 \rightarrow {}^7F_2$, $^5D_0 \rightarrow {}^7F_3$, and $^5D_0 \rightarrow {}^7F_4$ transitions of Eu^{3+} were observed at 537, 556, 592, 613, 654, and 701 nm, respectively. The photoluminescence intensity depended strongly on the Eu^{3+} content. The $Ca_{2.925}(VO_4)_2$:0.05Eu phosphors showed the strongest emission intensity and the highest ratio of the $^5D_0 \rightarrow {}^7F_2$ (red color) to the $^5D_0 \rightarrow {}^7F_1$ (orange color), indicating the strongest and the purest red light emission. In this study, we discussed the crystal structure, microstructure, and photoluminescence properties of the $Ca_{3-3x/2}(VO_4)_2$:xEu, depending on the Eu^{3+} content.

P063 – Plasmonic coupling of lysozime- and amino acid-gold nanodispersions

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Keywords: lysozyme, fluorescence, gold nanoparticle

Lysozyme stabilized gold nanodispersions were investigated. Gold nanoparticles can influence the fluorescence properties of lysozyme because of plasmonic coupling effect. The lysozyme-Au nanocomposite has a remarkable optical properties as well as a high stability. The prepared samples are stable in 1 M NaCl solution. The emission peak of lysozyme solution is around 350 nm, but by creating lysozyme-gold nanoparticle a new emission peak appears around 660 nm and the emission peak of the lysozymes shifts to 366 nm. The emission spectra of the lysozyme-Au nanoparticle can be simply altered with modifying the amount of lysozyme. The appearance of a new emission peak can be attributed to an effect so called metal enhanced fluorescence, where the metal nanoparticle interacts with the chromophore group of the molecule. In our system the lysozyme acts as the reducing agent at pH = 12. According to the TEM images and DLS measurements average diameter of the gold nanoparticles are below 10 nm.

The emission of the lysozyme originates from the tryptophan amino acid. Functionalized Au nanoparticles were reacted with tryptophan to determine the origin of the 660 nm emission peak. In order to investigate the interaction between tryptophan and lysozyme DSC and IR measurements were carried out. Au rods can also influence the emission spectra of dye molecules and amino acids through a plasmonic coupling. In the case of tryptophan (emission peak at 350 nm) and phenylalanine (emission peak at 280 nm) the addition of Au rods their emission intensity increased due to their coupling with the Au rods.

Experiments with tryptophan and phenylalanine showed that there is no shifting in the emission spectra, only the intensity changed.

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P064 – Plasmonic resonances on cysteine-functionalized noble metal nanoparticle aggregates

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Keywords: nanoparticle aggregates, coupled plasmonic resonances, illumination direction, array effect

The absorptance spectra of spherical gold and silver nanoparticles (NPs) functionalized by *L*-cysteine amino-acid (Cys) were measured by UV-visible spectroscopy, and computed numerically by finite element method. The experimentally observed sensitivity of the split spectra to the pH of aqueous dispersions and to bio-molecule concentration proved that it is possible to develop NP-Cys aggregate-based bio-sensors.[1] The systematic variation of the aggregate geometry characterized by N number and d diameter of NPs, g gap between the NPs, and t thickness of *L*-cysteine shell uncovered the relationship between the spectra and the parameters of linear and wavy bio-conjugates. The tuning of the illumination directions specified by the angle of incidence and by the **E**-field oscillation direction in p-polarized light with respect to the aggregates proved that fine spectral engineering is possible by applying proper illumination conditions. The inspection of the normalized **E**-field distribution around the aggregates has shown that fundamentally different multipolar modes can be excited due to coupled plasmonic resonances on NPs in spectral intervals of the primary and secondary peaks. The high intensity localized **E**-fields are useful to reach high sensitivity in bio-detection of bio-molecules preferring to attach at specific locations in noble metal particle-aggregates.[2] Interestingly, the degree of aggregation and the corresponding splitting is very different at analogous e.g. ~4.9 pH value in dispersions of Au-Cys and Ag-Cys bio-conjugates. Very short linear chain-like aggregates may account for the spectra with two commensurate maxima observed on Au-Cys bio-conjugates, which maxima are less sensitive to the orientation and weakly affected by coupling on arrays. Wavy or very long linear aggregates result in two-times larger split according the highest secondary peaks experimentally observed on Ag-Cys conjugates. It was demonstrated that the wavy Ag-Cys aggregates exhibit the largest primary peak, which becomes rapidly dominant by increasing the angle of incidence. The inter-aggregate near-field coupling occurring between closely packed long linear aggregates contributes to the inter-particle and array coupling phenomena, and manifests itself in broadening of the spectra.

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P065 – Polymerizable carbon nanodots hybrid optical functional organic-inorganic gel glasses

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Keywords: polymerizable nanomaterials, hybrid copolymeric gel glass, optical limiting, luminescence

Stably embedding nanomaterials in solid-state architectures and retaining their intrinsic properties are huge challenges.[1–3] Here, we report the design and versatile preparation of various silane pre–functionalized carbon nanodots, their macrostructure and organic–inorganic nanohybrid gel glass monoliths with excellent optical performance, in which the polymerizable carbon dots are covalent bonded to organic–inorganic modified silica networks by self- or co-polymerization with various silanes. So, molecular level and arbitrarily doping (0–100% scale) of carbon nanodots in solid gel matrix could be achieved, and these properties of prepared gel glass could be modulated accordingly. Agglomeration and phase separation are completely prevented and resultant gel glasses offer sustained optical performance. All of these materials are highly luminescent (quantum yields = 47% and 88%, respectively) with broadband optical limiting properties (532 and 1064 nm). The glasses are optically (>28 months), thermally (>700ºC), and mechanically (could be cut, polished and further processed) stable as well as highly transmissive (90%) in the visible and near IR region. This novel one-step approach is promising to be a versatile tool to design and prepare new optical materials as well as nanocomposite and hybrid organic-inorganic copolymeric materials.[4]

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P066 – The potential of organometallic polymeric carriers for paclitaxel delivery to tumor cells

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Keywords: nanopolymer, cytotoxicity, breast cancer cell line, paclitaxel

Nanocarriers which can encapsulate biologically active agents are intensively investigated and used in drug applications. They can lower the effective dose, reduce side effects, defend molecules from enzymes, control the release of drugs, and specifically target active pharmacons. Nanoparticles may help in the transport of hydrophobic molecules, efflux transporter ligand drugs, and biopharmacons. Redox responsive delivery vehicles, a group in nanocarriers, have a potential to release their contents into the intracellular compartments with local redox gradient. Poly(ferrocenyl silanes) (PFS) are redox responsive polymers. The backbone contains ferrocene and silicon units, and forms micelles which are suitable for molecular delivery.[1]

Our aim was to determine the toxicity profile of PFS micelles on cultured human cells and test their suitability for formulation of paclitaxel, a highly lipophilic antineoplastic drug. Human cell lines, Caco-2 intestinal epithelial, MCF-7 and T-47D breast cancer, A-549 lung epithelial cells were used in the experiments. Four PFS (Jf024B, Jf025B, Jf031C, Jf047B) samples and one paclitaxel containing PFS (Jf047B) were investigated. Cellular toxicity and inhibition of proliferation were measured by MTT dye conversion, lactate dehydrogenase release, and real-time cell microelectroninc sensing (xCELLigence, Roche).

The toxicity of each PFS sample was determined on human Caco-2 intestinal epithelial cells, a model for intestinal drug adsorption. The polymers did not cause damage to Caco-2 cells below 10–300 µg/ml concentrations. The absence of serum in the culture medium increased the toxic effect on epithelial cells. Paclitaxel was formulated in Jf047B polymer. We could demonstrate on breast cancer cells that the toxicity of paclitaxel was enhanced by PFS at a concentration which alone did not induce changes in cell viability.

These results indicate that poly(ferrocenyl silanes) may be suitable for the formulation of paclitaxel used in cancer chemotherapy. Further studies are needed to determine the mechanism of the enhanced efficacy of the drug-polymer micelles on tumor cells.

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P067 – Preparation albumin/polyelectrolite core-shell nanoparticles for controlled drug release

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Keywords: albumin, kynurenic acid, interferon-α, core-shell nanoparticle, sustained release

Nowadays the formulation of sustained release dosage forms is very important in the case of sensitive active agents such as proteins. These materials have short half life time and the gastric fluid can injury the protein active agents therefore the absorption route is the injection. But the injections have some disadvantages such as frequent applications therefore the compliance can decrease.[1] The compliance can increase with application of a sustained release injection.

Our aim was the formulation and investigation of sustained release core-shell nanoparticles[2,3] containing albumin (BSA and HSA), which can be applied in injection formulation. The core was the precipitated albumin, and the layers contained chitosan and polystyrene sulfonate (PSS). The albumin was chosen as core because this protein has a very good binding effect, therefore the other active agents (e. g. interferon-a, kynurenic acid) can bind to albumin. The first step was the precipitating the albumin with Na_2SO_4 and the next steps were the preparation of layers (PSS/chitosan/PSS) during continuous mixing. We have also applied kynurenic acid in this system. During our preexperiment the SPR technique was used in order to investigate the binding effect between the albumin and the kynurenic acid. On the basis of these results the nanoparticles containing kynurenic acid was prepared. The samples were examined with dynamic light scattering, differential scanning calorimeter and transmission electron microscope. *In vitro* release studies were executed under physiological conditions.

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P068 – Preparation and characterization of PE/NR-CuS, PbS, CdS, ZnS nanocomposites on the basis of nitrile rubber/polyethylene polymer composites

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Keywords: oxidative, chlorophosphorylation, PbS

In recent times the obtain of polymer nanocomposite play very great importance part of chemical and physical field. Copper sulfide (CuS) has been found to have very useful electrical and optical properties and have attracted great interest for their potential use in energy applications, such as applications in achievement of solar cells and in photo chemical conversion of solar energy as solar absorber coating , as selective radiation filter son architectural windows for solar control in warm climates, and as electro conductive coatings deposited on organic polymers . In addition , lead sulfide (PbS) has been utilized as photoresistance, diode lasers, humidity and temperature sensors, decorative and solar control coatings.

In this study, we have presented a chemical method to elaborate the PbS, CuS, CdS, ZnS nanocrystals embedded in a polymer matrix. The purpose of the presented work is the preparation of semiconductor nanoparticles in polymer matrix.

In the present work for preparation polymer nanocomposites as initial polymer were used BNR-26 mark of nitrile-butadiene rubber and polyethylene (PE).This polymer mixture was synthesized from oxidative chlorophosphorylation reaction by participation of phosphorus thrichloride (PCl3).The reaction was carried out in the mixture of benzene-chloroform at 60ºC temperature for ~30min. On the second stage polymer layers were obtained by the "flow" method from the formed polymer solution which was taken reaction condition. For formation of CuS, PbS, CdS, ZnS nanoparticles have been applied by the method of "layer by layer". The sorption of compatible metal ions have been carried out from the 10^{-3}M in water solutions of $Pb(NO_3)_2$; $ZnSO_4 \times 7H_2O$; $CdCl_2 \times 2.5H_2O$; $CuSO_4 \times 5H_2O$ salts. Then polymer layers which processing of metal salt solutions have been washed by distillation water and have been added 10^{-2}M $Na_2S \times 9H_2O$ in water solution. This process was laminated a few times and different dimension composite particles were formed . CuS and PbS nanocrystals have been characterized by X-ray diffraction (XRD) and UV-VIS absorption. The apsorbtion and transmition spectrumes of CuS nanoparticles have been characterized by SPECORD 250 UV-Vis spectrometr in (190–1100) nm area and analysed of the optical band gap of the films indicate an indirect gap of 2.5 eV for CuS nanoparticles. Measured size of CuS nanoparticles is approximately 5.5 nm. X-ray diffraction (XRD) study confirmed the formation of cubic phase of PbS nanocrystals into the polymer matrix. The average PbS nanoparticle size was found 8 nm.

P069 – Preparation and characterization of MWCNT-ionic conducting polymer nanocomposites

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Keywords: nanocomposite, conducting polymer, carbon nanotube

The knowledge of physical and chemical properties of organic semiconducting materials drive the development of low-cost optoelectronic applications such as organic light-emitting devices (OLEDs), solar cells, field-effect transistors, and photosensing devices, and nonvolatile memory devices.[1] The well-defined ionic polyacetylenes were prepared through the activated polymerization of ethynylpyridine(EP)s with alkyl halides, methanesulfonic acids, halogens, or halogenic acids. These ionic polyacetylene derivatives contain pyridinium ring substituents associated with halide, methanesulfonate or trifluoromethanesulfonate counter ions. We had also prepared various pyridine-based conjugated polymers having different functionalities and characterized the polymer properties.[2] The performance of CNT/polymer nanocomposites depends largely on the dispersion of CNTs in the matrix and interfacial interactions between the CNT and the polymer and diverse chemical and physical methodologies have been developed to synthesize the CNTs/conducting polymer nanocomposites.

Here, we report on the facile synthesis of conducting polymer-coated MWCNT using the uncatalyzed polymerization of 2-EP in the presence of surface functionalized MWCNT. The physical and morphological properties of the MWCNT-P2EP nanocomposites were studied. The polymerization of 2-EP on the surface of MWCNTs took place spontaneously without any additional initiator or catalyst. As the polymerization proceeded, the color of the reaction mixture changed from the initial light brown into dark brown and the reaction solution became more viscous. In XPS of MWCNT–P2EP hybrids, the N1s signal corresponding to the pyridine group was observed at 400 eV while no nitrogen was found for pristine MWCNTs and MWCNT–COOH. Further evidence for the presence of P2EP chains grafted on MCWNTs was provided by TGA analysis. HRTEM and FESEM analyses revealed the core-shell type of the composite morphology.

The cyclic voltammogram of MWCNT-P2EP nanocomposites exhibited irreversible electrochemical behavior between the oxidation and reduction peaks. The kinetics of the redox process of composite was very close to a diffusion-controlled process from the experiment plotting the oxidation current density of this composite versus the scan rate.

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P070 – Preparation and characterization of nanoparticles for drug delivery to brain

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Keywords: targeted drug delivery, blood-brain barrier, polymer micelles, preformulation, physicochemical characterization

Associative colloids are bilayered vesicles which are able to encapsulate pharmacons (hydrophylic/amphiphlic/lipophilic) and serve as potential drug carriers. These nanoparticles are formed from the self-assembly of non-ionic amphiphiles in aqueous media. Targeting can be achieved by labeling their wall with ligands of blood-brain-barrier (BBB) transporters. The objective of the development study is to test if nanoparticles can be used for targeted delivery of hydrophilic molecules to the CNS. Vesicles with an average hydrodynamical size of 200 nm were prepared by different production methods and formulation compositions from biocompatible /and biodegradable/ materials.[1]

The formulations were designed by varying the preparation methods and the concentration ratios of the components as independent variables. Average hydrodynamical size, zeta potential and drug content of the vesicles were evaluated. *In vivo* experiments included kinetic studies by eXplore Optix in mice.

The structure of the vesicles and the structural changes due to the ingredients, the production methods and targeting ligands were analyzed using thermoanalytical and spectroscopy methods. DSC was used to study the relationship between the changes in the independent variables and the thermal events of the nanovesicles. Raman spectroscopy was used to investigate and confirm the possible interactions between the components.

It was demonstrated that appropriate choice of the independent variables could lead to molecularly dispersed drug in the vesicles. Significant variations in the product structure, physicochemical parameters and drug liberation were demonstrated.

Using the Evans blue-Albumin containing labeled vesicles accumulation of the test molecule could be observed in the brain as compared to other organs in contrast to non-targeted vesicles. Our results indicate that vesicles labeled with glucose analogues can be used for targeting hydrophilic molecules across the BBB.

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P071 – Preparation of polarized electrode of an electric double layer capacitor using a spray pyrolysis technique

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Keywords: electric double layer capacitor, polarized electrode, spray pyrolysis technique

Recently, solar energy and wind energy as a renewable energy has been used in energy supplying systems. However, output powers of these energy are unstable under surrounding environment and weather condition. Therefore, electrical energy generated by these energy sources is accumulated in energy storage devices. Electric double layer capacitor (EDLC) was attracted attention as the energy storage device. EDLC is a type of physical battery without a chemical change. Therefore it has a long cycle life and it does not deteriorate theoretically. In this research, preparation method of polarized electrode was carried out using a spray pyrolysis technique. A spray pyrolysis technique is the process of depositing. The solid phase is precipitated from the liquid phase on the heated substrate, which is one of the chemical methods for preparing thin films. This method is based on the principle of the atomizer, when the spray towards the substrate or space that is overheating of a material solution, the chemical reaction and thermal decomposition of the solute and evaporation of the solvent occurs, thin film is formed. The experiment was performed using a pulse spray coating systems manufactured by Nordson. Polarized electrodes were prepared as substrate collector electrode made of aluminum by varying the conditions spray coating such as the number of times applied with a coating solvent mixed with activated carbon, conductive material, and the PTFE. Ketjenblack used as a conductive material. As various analyzes, such as electrode structure investigated by X-ray diffraction (XRD) analysis and surface morphology by scanning electron microscope (SEM) were performed. Polarized electrodes were compared with the same electrode fabricated by hot press method. As the result, Polarized electrodes prepared by spray pyrolysis method have been able to confirm by SEM that the conductive material has been evenly spread extensively than those prepared by hot press method.

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P072 – Preparation of polymeric membranes using functionalised MWCNTs as fillers for desalination processes

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Keywords: flow, reactor, mixed matrix membrane, polyimide, CNT

The polymeric membranes have a high application capacity in separation processes. The separation is based on a solution-diffusion mechanism. This phenomenon involves interactions between the permeating molecule and the polymeric membrane. The prepared membrane shows an asymmetric structure with dense like layer at up surface of membrane and sponge like structure in cross section. The characteristic parameters of a membrane are essentially two: flux and rejection. The carbon nanotubes (CNTs) could be used in the preparation of Mixed Matrix Membrane (MMM). The aim of this research is to prepare and characterise hybrid membranes containing several percentages of CNTs. The membrane preparation technique used is dry-wet nonsolvent induced phase separation (NIPS). A high chemical affinity is needed to obtain a good dispersion of CNTs in the casting solvent and, later, in the polymeric matrix. Synthesis of Multi Walled Carbon Nanotubes is performed by Catalytic Chemical Vapour Deposition (CCVD) of ethylene on Co, Fe supported on NaY zeolite. The as-made product has to be purified by HF before its application in a polymeric membrane to eliminate the presence of impurities (calcined catalyst) in the sample. Moreover, a functionalisation by a mixture of nitric and sulphuric acid was carried out after the purification step. The polymer chosen for the preparation of the membrane is a commercial polyimide by Lenzing commercialised P84. Preparation technique used to form the membranes is the phase inversion method induced by non-solvent. The imide bonds of the membranes are converted to amide bonds by means of the cross-linker DAMP (1,5-Diamino-2-methylpentane). Polymeric and hybrid membranes were characterised by SEM, FT-IR analysis, flux and rejection measures of different salts. SEM images highlight an asymmetric structure. The cross-linking reaction and the presence of CNTs modify the membrane structure. Flux and rejection test of the polymeric and hybrid membranes have been carried out. In this case, it can be noted that the hybrid membranes maintain the same performances after the rejection of salts. This result is very interesting for application in desalination processes. In fact, this application is often limited by polarisation and fouling phenomenon determining a reduction of performances of the membrane. Mechanical tests demonstrated that the Young modulus, the breaking stress and the breaking elongation are not affected by the percentage of CNTs in the membrane. Rejection tests are carried out using sodium and magnesium chlorides to simulate the performances in the sea water. PI membranes crosslinked with DAMP show more rejection of salts (NaCl and $MgCl_2$) compared with uncrosslinked PI membranes. Those tests demonstrated that the performances of polyimide membranes are not only affected by molecular sieve effect, but the mutual interaction between the electrolytes present in solution and the charged groups in the membrane. Functionalised CNTs, thanks to the presence of acidic ionisable groups, can increase the total charge. The optimal percentage of CNTs in the membrane is linked to their distribution.

P073 – Preparation, structures and properties of poly(*p*-phenylene benzobisoxazole) nanocomposites reinforced with graphene

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Keywords: PBO, graphene, nanocomposite, fiber, structure, property

Poly(*p*-phenylene benzobisoxazole) (PBO) has been known as a rod-like heterocyclic polymer with extended chain conformation. PBO fibers prepared from the polymer have attracted great interest from industrial and academic points of view, because of their superior tensile strength and modulus, cut and abrasion resistance, and flame retardancy.[1]

On the other hand, nano-sized materials such as silicates, carbon nanotube, carbon black, silica, POSS, metal fibres and powders have been considered typical reinforcing fillers for polymeric composites with improved physical properties. Among the reinforcing nano-materials, graphene sheets have recently been found to exhibit unique structure and physical properties.[2] Structurally, graphene sheets are mono-layers of carbon atoms arranged in 2-dimensional honeycomb lattice and they are easily stacked each other due to the van der Waals interaction. Graphene sheets exhibit excellent mechanical strength (Young's modulus of ~1 TPa), electrical conductivity of ~10^4 S/cm, and thermal stability. Accordingly, considerable research effort has been recently devoted to processing and characterization of nanocomposites with graphene sheets to improve mechanical, thermal, electrical, and gas barrier properties of polymers.

In the present study, we have prepared a series of PBO/graphene nanocomposites by using in-situ polymerization of 4,6-diamino resorcinol dihydrochloride (DAR) and terephthaloyl chloride (TPC) in the presence of graphene sheets and following solution casting. For the purpose, graphene sheets are also prepared via acid-treatment and rapid thermal expansion of natural graphite flakes. Structure, morphology, thermal stability, tensile mechanical properties, and electrical properties of the nanocomposites with different graphene contents are investigated with the aid of XRD, SEM, TEM, POM, TGA,UTM, and multi-ohmmeters. In addition, PBO/graphene nanocomposite fibres are also manufactured by in-situ dry-jet wet spinning of the polymerization products. Influences of graphene content on structures and physical properties of the PBO/graphene nanocomposite fibres are systematically investigated.

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P074 – Purification of phenol and *E. coli* contaminated water by visible light activated titanias

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Keywords: photocatalysis, visible light, *Escherichia coli,* titanium dioxide, spin trapping

This study compared the photocatalytic activities of various titania (TiO_2) photocatalysts for phenol degradation and *E. coli* inactivation under visible light illumination (conventional energy saving 24 W compact fluorescence lamps). Commercially available bare (Aeroxide P25, Aldrich anatase and rutile), doped titanias (Kronos VLP7000 and Sumitomo TP-S201) and our novel TiO_2 photocatalysts such as nitrogen, iron doped titanias, modified P25 containing silver, gold or sulphur and nitrogen were compared.

Undoped Aldrich rutile had the highest efficiency for inactivation of *E. coli* bacteria and also had high activity for phenol degradation. Four doped titanias had higher efficiency for phenol degradation than Aeroxide P25 but much lower (if any) activity for bacteria inactivation, including Kronos VLP7000, which revealed extremely high efficiency for phenol decomposition.

To obtain further insight into these unexpected results and examine the underlying formation of reactive oxygen species (ROS), we used electron spin resonance (ESR) spectroscopy and spin trapping. The ESR results pointed out that titanias that generated OH• radicals were active for deactivation of *E. coli* bacteria, and those which were unable to produce OH• radicals did not show significant bactericidal action.

The observed extremely high efficiency of Kronos VLP7000 for phenol decomposition is most likely due to the generation of singlet oxygen in relatively high concentration and its high specific surface area.

Acknowledgements: This work was partially financed by the European Union through the Hungary-Serbia IPA Cross-border Co-operation Program, HU-SRB/0901/121/116. This work was also co-financed by the grant from the Hungarian National Office of Research and Technology (OTKA CK 80193) and the Swiss Contribution (SH/7/2/20). KM thanks the financial support of the Hungarian Research Foundation (OTKA PD78378) and the János Bolyai Research Scholarship of the Hungarian Academy of Sciences.

P075 – Raman fingerprint of *stage I – stage VI* graphite intercalation compounds from theory and experiment

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We present a systematic experimental and theoretical study in graphite intercalation compounds (GIC). We determine the intrinsic G-line and double-resonant Raman processes from *stage I* to *stage VI* GIC with spectral and spatial resolution by using an in situ multi-frequency Raman analysis. The results in *stage I* KC_8, CaC_6, and LiC_6 highlight the contribution from the optical Raman modes to the electron-phonon coupling mechanism in superconducting materials. Our findings from a controlled de-intercalation processes, confirm the intrinsic Raman fingerprint in *stage II* to *VI* in potassium graphite intercalation compounds. The line-shape and position for *stage II* GIC revealed a slightly asymmetric Fano-line at 1610 cm^{-1}. The results from *stage III* to *VI* allowed a completely new insight into the nature of the split G- and 2D-band in GIC as a novel tool for studying mono- and few-layer graphene. We performed ab-initio calculations of the electronic structure, phonon dispersion and full cell-optimization of KC_{36}, and KC_{72} in order to explain the observed Raman response in GIC. The qualitative agreement between the experimental Raman analysis, the theoretical *ab initio* calculations, the nearest layer and non-adiabatic models; give solid evidence about nature of the G-line and the 2D-line Raman response in GIC which will serve for further studies on graphene based materials.

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P076 – Raman mapping in surface analysis of PP-fibers modified with TiO_2

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Keywords: Raman mapping, modified PP-fibers, surface analysis

Vibrational spectroscopy methods: FT-IR ATR spectroscopy and dispersive Raman spectroscopy offer the possibility of direct, non-destructive analysis with advantages over other methods for many diverse materials, hence they are satisfactorily applied in different fields of science and technology, as e.g. chemistry of polymers, surface analysis, biological structure analysis, materials science, etc.[1] Raman spectroscopy connected with mapping system seems to be useful also for the examination of nano-modified surfaces, eg. textile fibre with added-value components. The aim of presented study was focused on analysis of titania modifier and modified PP-fibers identification. The dispersive Raman with Leica microscope (In Via Spectrometer, Renishaw, excitation source $\lambda = 785$ nm) was applied for surface analysis of fibers under the study. Raman spectra of studied modified PP-fibers showed the presence of band at 143 cm^{-1} that is characteristic for TiO_2 anatase form.[2,3] Fiber surface and fiber cross-sections were analyzed using Renishaw WIRE 2.0 Raman mapping system, i.e. series of Raman spectra detected step by step on every 0.1 mm of the studied surface on defined region (e.g. line, rectangle). Raman micro-maps performed on fiber surface and cross-section allowed to illustrate the TiO_2 presence and distribution on studied areas as well as the thickness of the TiO_2 layer.

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P077 – Reactivity indexes in nitrogen-doped fullerenes

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Keywords: fullerenes, nitrogen, density functional theory

Carbon-cage structures such as fullerenes have extensively stimulated a variety of scientific studies on their structure and reactivity. They have been considered as building blocks for novel and interesting materials. Fullerene doping can be performed out of the cage (exo), inside (endo) and instead of carbon atoms. The electronic properties of these materials depend strongly on their size and structure. Another reason to study these mixed systems is to understand fundamental aspects of chemistry such as the nature of the chemical bond in these clusters and the effect of doping and substituting other atoms different from carbon in the more stable carbon clusters. Among the interesting properties for this kind of materials, there is the possible use as high-density gas storage containers,[1,2] new optical devices,[3] effective gas separation materials,[4] and chemical sensors.[5]

Recently,[6] there has been proposed a new structure, nanostructured polymeric nitrogen, where a polymeric nitrogen chain is encapsulated in a carbon nanotube. This opened a new path towards stabilizing polynitrogen or polymeric nitrogen at ambient conditions. In this work, the Density Functional Theory (DFT) results obtained from our study of nitrogen containing fullerenes $N_n@C_{70}$ (where n = 2–10) are shown. The lowest energy structures and reactivity indexes were computed, in order to explain the reactivity that could be shown by these materials and the possibility to find interesting behavior in fullerenes.

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P078 – Self-assambled nanoplasmonic gold particle on graphene via reduction process

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Keywords: plasmonic, grapheme

Research on plasmonic, a relatively new branch of optics, has received an increasing level of international attention over the last decade. This interest is mainly driven by the fact that surface plasmons, travelling along the interface between a metal and a dielectric, allow confining optical energy to volumes that are significantly smaller than those accessible with conventional dielectric waveguiding structures such as optical fibers. Graphene is also a hot issue of research.

Recently, property of device including graphene is considered more important than graphene. In this study, realize self-assembled plasmonic nanoparticles on graphene via reduction process. This fabrication method is relatively simple and can be fabricated at low temperatures. In this result, amplify light by plasmonic effects implemented on graphene is expected to be utilized in optical electronic organic devices and optical biosensor.

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P079 – SEM-FIB investigation of composition dependent sintering behaviour of $Cu_xNi_{(1-x)}$ printed structures

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Keywords: focused ion beam, printed structures, CuNi alloy

CuNi alloys have advantageous mechanical, catalytic, anticorrosion, thermoelectrical and electrical properties. CuNi alloys containing ca. 40 wt.% nickel have a low temperature coefficient of resistivity (TCR), i.e. their electrical resistivity is almost temperature independent, and due to their considerable strain sensitivity (piezoresistivity) they are commonly used for resistive applications, e.g. for strain gauges. However, in contrast to silver, dispersions from CuNi alloys suitable for maskless printing purposes are not commercially available up to now.

In the present study characterization of $Cu_xNi_{(1-x)}$ $(x = 0 - 1)$ printed layers is presented by means of FIB-SEM. Suspensions made from chemically prepared $Cu_xNi_{(1-x)}$ $(x = 0 - 1)$ nanoparticles with different morphologies dispersed in ethylene glycol were tested in Aerosol Jet® printing. Van der Pauw test microstructures were deposited onto silicone substrate, followed by sintering at 300–800°C under reducing atmosphere (H_2). Microscopical studies (SEM-FIB) of printed and sintered CuNi structures showed that the sintering properties of nanoparticles were dependent on their chemical composition and morphology.

Conductivity reached maximum values for the structures sintered at 700 and 800°C, where the calculated resistivity data were around 1000 nΩm, which is only 2 times higher than that of the reference commercial CuNi alloy.

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P080 – Single Au or Cu atom impurity effect on thermal stabilities of Cu_{55} or Au_{55} clusters with icosahedron geometry

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Keywords: molecular dynamics, cluster, surface, nanoparticles, phase transition, alloy, catalysis

Thermal stabilities of Cu or Au icosahedral clusters with single Au or Cu impurity are studied by employing molecular dynamics simulations. The simulations show atom movements' differences of these clusters by selective doping on heating, and their effects on the local arrangement of atom packing. The structures of Au_1Cu_{54} clusters are more stable than those of $Au_{54}Cu_1$ clusters. When the Au_1Cu_{54} clusters are in molten states, the copper atoms are full of the inner parts of these clusters, and the one Au atom is in the outer part. At high temperature, each of the $Au_{54}Cu_1$ clusters is composed of two clusters.

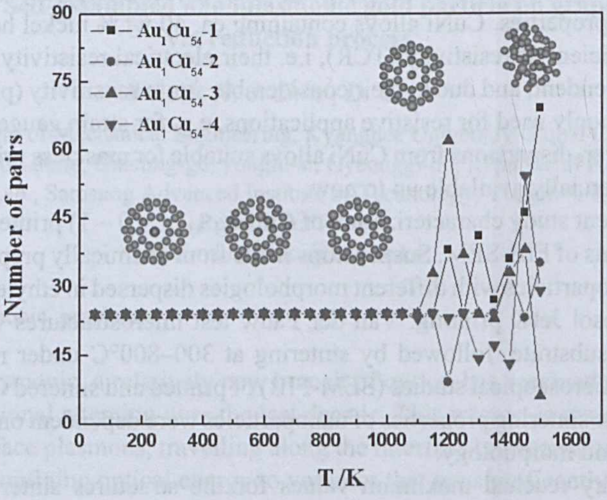

Figure 1.

P081 – Sorption properties of mechanical modified titanate nanowires and nanotubes

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Today, by the results of nanotechnology, materials properties can be manipulated on the nanometer range by different synthesis methods. Titan-dioxide has difficult production process but beneficial properties, that's why long has been the focus of research. By the preparation process of Horváth et al. TiO_2 nanowires ($Na_xH_yTi_3O_7$) have been made from nanotubes. The typical length was around 5 mm with 50–100 nm width.

As the mechanical stability of the nanowires was studied, we found that by using different milling energies different titanate structures are obtained. For grinding a planetary ball mill type Fritsch Pulverisette-6 was used with different materials milling drum. For accurate monitoring the cumulative energies of milling were precalculated by a milling map.

We found that by high energy milling the fibrous morphology deteriorated quickly into nanosized particles, whereas by increasing the milling time crystallization was observed so the presence of anatase and rutil was detected.

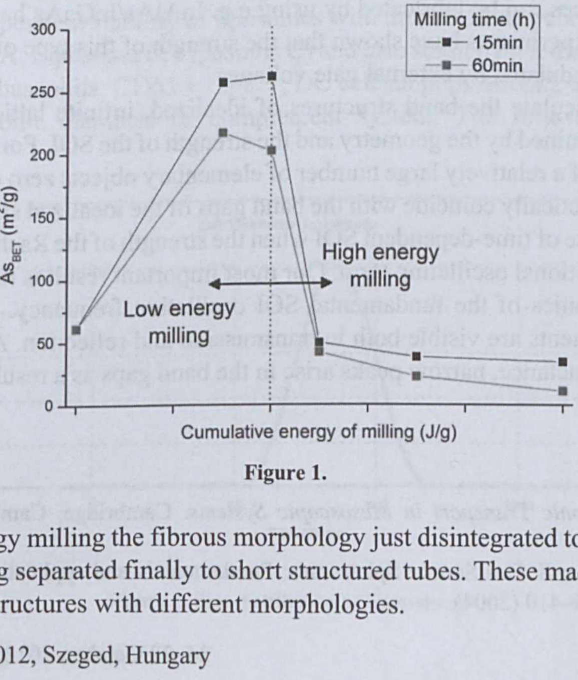

Figure 1.

By low energy milling the fibrous morphology just disintegrated to group of tubes first, then to long separated finally to short structured tubes. These made it possible to create titanate structures with different morphologies.

For detailed characterization X-ray diffraction, electronmicroscopic technics and specific surface area were measured.

Acknowledgement: The financial support of the TÁMOP-4.2.2.A-11/1/KONV-2012-0047, TÁMOP-4.2.2.A-11/1/KONV-2012-0060 and FP7 INCO "NAPEP" 266600 projects is acknowledged.

P082 – Spin-dependent interference in lateral superlattices: Conductance properties

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Keywords: nanoscale superlattice, Rashba-type spin-orbit interaction, conductance

Spin resolved currents and conductance properties of nanometer sized systems have been investigated since the end of the 20th century. Mesoscopic (nanoscale) objects consist of a large number of atoms but their behavior is considerably influenced by quantum interference effects.

Our quantum mechanical model describes a two-dimensional lateral superlattice, where Rashba-type spin-orbit interaction (SOI) influences the flow of charge carriers. Such superlattices can be fabricated by using e.g. InAlAs/InGaAs based heterostructures. Recent experiments have shown that the strength of this type of spin-orbit coupling can be modulated by external gate voltages.

First we calculate the band structures of idealized, infinite lattices. The energy bands are determined by the geometry and the strength of the SOI. For a finite network which consist of a relatively large number of elementary objects zero conductance energy ranges practically coincide with the band gaps of the idealized structure. We also consider the case of time-dependent SOI when the strength of the Rashba-type interaction has an additional oscillating term. Our most important result is the appearance of the high harmonics of the fundamental SOI oscillation frequency. These high frequency components are visible both in transmission and reflection. Additionally, focusing on conductance, narrow peaks arise in the band gaps as a result of the oscillating SOI.

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P083 – Stability and immune – Modulatory effects of liposomes with various compositions

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Keywords: nanomedicine, liposome, dinamice, light scattering, basotest

Introduction: The nanomedicine is the application of nano-scale materials in the medical procedures. The nanomaterials opened a new horizon in the personalized medicine. They have very different physico-chemical properties (structure, shape, size, etc.). These parameters basically determine their impacts on biological systems. Liposomes are widely used as drug delivery vehicles, so their stability, temperature dependence and direct effects on human immune system are essential.

Aim: The main purpose of our study is the investigation of the stability, temperature dependence and activation effects of liposomes of various compositon on the innate immune system.

Material and methods: We investigated the size distribution, homogenity and termperature dependent stability of liposomes with three different chemical composition (Liposome A, Liposome B, Liposome C) and also studied their direct effect on the cell activation (basophils: CD63 + / IgE +, DC cell subpopulations), as well as on the activation of some elements of complement system. The following tests were

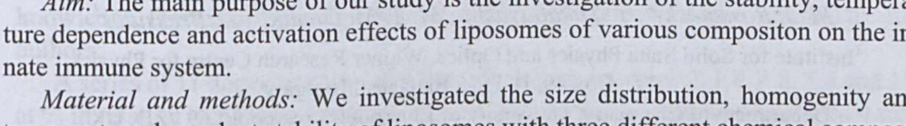

Figure 1. Size distribution of liposome A

perfomed: Basotest (BD), DC Identification Kit (BD), SC5b-C9 (Quidel) and for size measurement Dinamic Light Scattering method was used.

Results: The size distribution range was good (Fig. 1) and the sizes were between 46–103 nm in the case of different liposomes.

The complement activation parameters did not show any differences none of the examined liposome composition compared with control samples. In basophil activation we saw a light increase of CD63 expression. All of the liposomes caused an enhanced expression of surface CD11c and CD123 antigens on dendritic cells.

Discussion: The size, homogenity, aggregation status, zeta potential is important physico-chemical parameter that determines the biological behavior of nanomaterials, and ultimately toxicity. In our work we demonstrated that liposomes have a role in the activation process of basophils as well as DC subpopulations as part of allergic reactions.

Reference

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P084 – Static and dynamic Jahn–Teller effect in solid fullerides

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Keywords: alkali fullerides, superconductivity, Jahn–Teller distortion

We have investigated the Jahn–Teller effect in various fulleride compounds. The Jah–Teller effect is a molecular phenomenon which can be observed in magnetic and non-magnetic insulator fullerides with different crystal structures, thus these systems serve an ideal model system to probe. Using different spectroscopic methods the contribution of the crystal field and Jahn–Teller effect on the detected distortion can be separated. We also discuss the influence of the Jahn–Teller effect on superconductivity as well as on magnetism manifesting the Mott–Jahn–Teller ground state.

P085 – Structural properties and photoluminescence of nanocrystalline gahnite doped with titanium

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Keywords: Ti-doped zinc aluminate, sol-gel processing, X-ray powder diffraction, Rietveld refinement, transmission electron microscopy, luminescence

Zinc aluminate, $ZnAl_2O_4$ (gahnite), has been widely known as a mineral and also as a ceramic and catalytic material.[1,2] It is also a semiconductor, as well as a suitable host material for transition metal cations and rare earth cations providing luminescence, which makes it applicable for various optoelectronic devices.[3] To the best of our knowledge, there is no literature data on studies of Ti-doped gahnite reported by other authors.

A series of Ti-doped gahnite samples with doping levels of 0, 1.8, 3.8, 5.4 and 11.6 at % in relation to Al were prepared by a sol-gel technique followed by thermal treatment. The samples were characterized by X-ray powder diffraction (XRPD), transmission electron microscopy (TEM), electron paramagnetic spectroscopy (EPR), UV-vis reflectance spectroscopy and photoluminescence (PL) measurements. Diffraction patterns showed that samples possessed a spinel-type structure. Diffraction lines were broadened which suggested that samples were nanocrystalline. EPR spectroscopy indicated that titanium was present as Ti^{4+} ion in the doped samples, while results of UV-vis reflectance spectroscopy evidenced that Ti^{4+} was situated on octahedral cation site in the gahnite structure. The structure of all prepared samples was refined by the Rietveld method, simultaneously with the size-strain analysis. TEM investigations showed that samples contained evenly shaped particles of about 20 nm in size. Ti-doped gahnite samples showed a strong UV absorption, and blue photoluminescence under UV excitation. The PL intensity was strongly dependent on Ti-doping level.

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P086 – Structure and properties of poly(*p*-phenylene benzobisoxazole) nanocomposites with single-wall carbon nanotubes functionalized under ozone gas flow

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Keywords: PBO, multi-wall nanotube, ozone treatment, nanocomposite, fiber, compressive strength

Poly(*p*-phenylene benzobisoxazole) (PBO) fibers have attracted great interest since they have superior tensile strength and modulus, cut and abrasion resistance, and flame retardancy.[1] But there exists a problem of relatively low axial compressive strength compared with carbon and glass fibers,[1,2] which limits the use of PBO fibers in composites.

Since the discovery of carbon nanotubes (CNT), polymer/CNT nanocomposites have been interested in the field of improving properties of polymers.

In the present study, we have prepared a series of PBO/Single-wall carbon nanotubes (SWNT) nanocomposites through in-situ polymerization of 4,6-diamino resorcinol dihydrochloride (DAR) and terephthaloyl chloride (TPC) in poly(phosphoric acid) (PPA) and presence of SWNT. For the purpose of introducing lateral interactions between PBO and SWNT, SWNT was functionalized under ozone gas flow before in-situ polymerization. It was confirmed that oxidative groups such as –OH and –COOH were introduced to SWNT by analysing with Raman spectroscopy and X-ray Photoelectron Spectroscopy. Moreover, in order to obtain uniform SWNT dispersion, it was sonicated in 98% phosphoric acid (71% based on P_2O_5 concentration) which has much lower viscosity than PPA, followed by dissolving additional P_2O_5 in order to adjust the P_2O_5 concentration of PPA to the level of 83-85% which was used as medium for polymerization.

PBO/SWNT nanocomposite fibers were prepared by spinning as-polymerized solution at liquid crystalline state. The morphology, mechanical and thermal properties of the PBO/SWNT fibers were systematically investigated. Compressive properties of the fibers were measured through Elastica loop test and recoil test.

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P087 – Structure of nanocomposites on the basis polypropylene and zirconium dioxide nanoparticles

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In the article, was synthesized of the new nanocomposite material based on isotactic polypropylene with a particle size of 0.5–1.0 mm and nanopowders with spherical nanoparticles ZrO_2 size 21 nm. Nanoparticles ZrO_2 stabilized with 3% yttrium oxide Y_2O_3. Synthesis of nanocomposite material carried out in the polymer solution at the temperature 120ºC. ZrO_2 powder in the initial state does not stick together and not agglomerated. Found that the direct introduction of nano powder particles at the first stage of mixing the components form a fractal structure in the form of dendrites. This is explained by the fact that during the mechanical mixing of polymer with nanopowders in the presence of the particles are non-linear self-organization processes of nanoparticles, which lead to the emergence of a complex fractal structure of the ordered distribution of particles in a matrix of polypropylene. To ensure the stability of sediment dispersion of zirconium oxide in the polymer system was carried out wetting powders in a small amount of toluene. Then the mixture of zirconium nanopowder with toluene was introduced into the polymerization system. This procedure provided a uniform and stable distribution of the powder filler in the initial polymerization system and in the final material. Then has been obtained nanocomposite films by hot pressing method at the melting temperature of the polymer at a pressure of 10 MPa. Thus were synthesized nanocomposites with a filler of ZrO_2 0.1, 0.5, 1, 2, 5, 7, 10% masses content. It was determined a limit to fill nanopowders in the polymer and show that it is 10% filler zirconium dioxide.

The electron-microscopic study was carried out (Merlin Carl Zeiss) nanocomposites based on PP + ZrO_2 with a beam energy of 3.0–20 keV for study the distribution of nanoparticles in the volume of polymer. It is found that at a beam energy of up to 3 keV nanoparticles in the polymer can be seen it is not clear, but with increasing energy of the electron beam above 4 kV distribution of nanoparticles are seen clearly. Electron microscopic study showed that ZrO_2 nanoparticles are not distributed on the surface, they were distributed in the volume of the polymer.

Has been studied IR spectra of polypropylene(PP) and nanocomposites (PP + ZrO_2) on base polypropylene and nanoparticles zirconium dioxide with different masses contents of ZrO_2. IR study of nanocomposites shows for the content 0.5–1% ZrO2 in the polymer the intensity of the absorption bands at 2839 sm^{-1}, 1376 sm^{-1} and 1459 sm^{-1} increase. Absorption band at 1376 sm^{-1} corresponds to the symmetric deformation vibrations CH_3 groups, 1459 sm^{-1}-antisymmetric deformation vibrations CH_3 groups, 2839 sm^{-1}-stretching vibrations of CH_2 groups. In the case of concentration of zirconium dioxide nanoparticles more than 1% the intensity of bands at 2839 sm^{-1}, 1459 sm^{-1} and 1376 sm^{-1} decrease. Thus, the comparison of IR spectra of PP and PP + ZrO_2 nanocomposition showed that the introduction nanoparticles into polymer matrix change the physical structure of the polymer.

P088 – Studies on the interaction of mycotoxins and macrocycles by molecular modelling

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Keywords: sensors, mycotoxins, macrocycles, docking

The goal of our work is to develop a selective sensor to detect the gene wrecking and carcinogenic mycotoxin molecules.[1,2] Hence our research group applies functionalized gold nanoparticles and thin films to measure these analytes. In this investigation modified thiolated macrocycle molecules (mainly cyclodextrins) were applied to functionalise the gold surfaces on the nanoparticles.

The cyclodextrins containes α-D-glucopyranoside unites, which connect to a ring with 1,4 glycosidic bonds. The best known three cyclodextrins are the α-, β- and γ-cyclodextrin, these form six, seven and eight glucopyranose molecules, respectively. In the inner cavity, there are hydrogen atoms and the oxygens of the 1,4 glycosidic bonds. The hydroxyl groups are placed on the flange of the hoop. So, the inner cavity of the cyclodextins is hydrophobic, and the outer surface is hydrophilic. This property makes cyclodextrin molecules able to form inclusion complexes with hydrophobic molecules like the aflatoxins. The hydrophobic character and the hydrogen donor hydroxyl groups warrants the relatively strong binding. The modification of cyclodextrins with the suitable chemical groups gives the selectivity of the sensors.

To choose of the appropriate modified cyclodextrin molecules and predict the binding affinities to mycotoxins, we investigated the complexes with molecular modelling.

To improve our fundamental understanding of the nanomaterials functionalized with macrocycle molecules, we use the tools of the molecular docking, molecular mechanics (MM) and molecular dynamics (MD), semiempirical quantum chemistry and the density functional theory (DFT) methods.

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P089 – Study on deterioration factors of cylindrical electric double-layer capacitor cell

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Keywords: electric double layer capacitor, deterioration

Human civilization has continued to develop consumimg fossil fuels and other petroleum and coal. Fossil fuel releases carbon dioxide when consuming, however, this carbon dioxide causes global warming and fossil fuel will be surely depleted. Then, development of alternative energy sources is urgently needed. Recently, power generation that uses renewable energies, for example solar energy and wind energy are paid to attention. These energy are sustainable and low environmental power source, however, these energy receive influence of environment and climate easily and these output power are unstable. In order to supply the power stablely, high efficiency power storage device are required. An electric double layer capacitor (EDLC) contains nanocarbon is used as power storage device. The EDLC is physical cell that has not chemical change. Therefore, cycle life of the EDLC becomes theoretically infinity. However, the performances deterioration such as increasing of internal resistance and decreasing of capacitance are reported under high temperature environment and overvoltage. The purpose of this study is to clarify deterioration factor of EDLC. A cylindrical EDLC (rated voltage 2.5 V and capacitance: 350 F) was used as measurement sample. The constant charge and discharge current of 1 A was applied at 2.5 V, 2.7 V, 3.0 V, 3.2 V charging voltage. It was confirmed the cycle lifes were shortened when charging voltage were increased. After the experimant, five kinds of EDLC including new sample was dismantled, and the property of the structural nanomaterials were evaluated. Polarized electrode made of nanocarbon were analysed from surface observation and elemental detecting. Surface conditions were observed using scanning electron microscope (S-5500, Hitachi). As the result of the surface observation, fusion of conductive materials derived from acetylene gas were not be confirmed in new sample. But, these phenomena in the deterioratied samples in overvoltage were confirmed and the attachment was confirmed in neighborhood of activated nanocarbon after the test at 3.2 V. Element on the activated nanocarbon were analysed useing X-ray photoelectron spectroscopy (S-3300, Shimadzu). As the result of elemental analysis, same element were detected in all samples. However, The amount of surface functional groups were confirmed in each sample. Electrolyte were also analysed from the measurement of moisture contents.

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P090 – Study on electronic type separated carbon nanotube thin films

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Keywords: carbon nanotubes, thin film, transparent conductors

Carbon-based systems are still the most promising materials for the substitution of indium tin oxide (ITO) for the use as transparent conducting layers. The separation of nanotubes by electronic type seemed to be a huge step toward the realization of this goal. We have performed wide range optical studies together with transport measurements on separated carbon nanotube thin films. The effect of p-type doping with nitric acid was also investigated. Our results show that doping is more effective in increasing the optimal conductivity and transparency (in the visible range) than separation. Mixed doped nanotubes seem the best candidates for wavelengths important for solar cell applications, but separated tubes can be applied for other, specialized purposes as e.g. in the infrared spectral range.

P091 – Superconductivity of carbon nanotubes in a longitudinal magnetic field

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Keywords: nanotube, magnetic field, superconductivity, thermodynamic potential, energy gap, magnetization

The discovery of new forms of two-dimensional structures, first, nanotubes and then grapheme, substantially increased interest in studies of superconductivity in such systems. This grown interest is related to an appearance in literature of reports on an observation of superconductivity of a carbon nanotubes beam.[1] In our work the microscopic theory of superconductivity of carbon nanotubes in a longitudinal magnetic field was built and developed where a quantum cylinder – electronic gas on cylindrical surface is used as a model of nanotubes. Using the Hamiltonian the BCS, method (u-v) conversion of Fermi operators and Bogolyubov's variation principle, we calculated thermodynamic potential and received equation for the energy gap.[2] These results allow us to study the dependence of critical temperature upon the surface electron concentration and the radius of nanotubes, with or without presence of a magnetic field.[3] The heat capacity jump of electronic gas of nanotubes in superconducting and normal state with critical temperature was calculated.[4] The dependence of the difference of thermodynamic potentials and the difference between magnetic moments of nanotubes in superconducting and in normal condition upon the induction of a magnetic field were investigated. The results describing the dependence of the width of an energy gap upon temperature and Aharonov–Bohm's parameter value, as well as the dependence of the critical temperature upon Aharonov–Bohm's parameter value were introduced.

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P092 – Synthesis and characterization of SBA16-Fe_xCo_{1-x} magnetic nanocomposites

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Concept. Nanostructures differ from micro-structures and macro-structures by more than just scaling in size, as the surface-to-volume ratio increases significantly for nano-objects, often leading to novel and unexpected physical and chemical properties. Besides, if the nano-objects are distributed in a solid matrix, the resulting nano-composite material displays a behaviour that depends on both the nanophase and the matrix properties. To deeply understand the physical and chemical properties of a nano-composite material, characterization techniques are particularly beneficial if they are able to reveal the richness of microstructure in three dimensions rather than just providing 2D projection views.

We present here the morpho-structural study of magnetic nanocomposites constituted by SBA-16 mesoporous silica in which Fe_xCo_{1-x} nanoparticles have been dispersed by impregnation method.[2] Structure and morphology of these materials have been investigated by XRD, TEM and Electron Tomography techniques, the latter providing a 3D reconstruction of the matrix-nanophase assembly. Finally, the magnetic properties of the materials have been studied.

Motivations and Objectives. Conventional TEM analysis is a premier method to perform characterization of particles shape and to determine their mean size and distri-

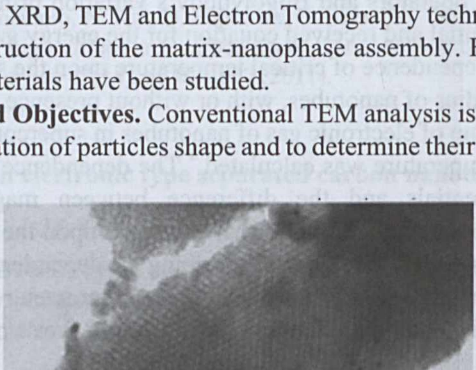

Figure 1.

bution in a matrix. However, analysis of 3D particle shape from 2D projection is indirect, as well as by conventional TEM is not trivial to determine if the nanoparticles are distributed over the entire volume of the matrix or only in its most external part. Moreover, one of the key parameters that have to be finely determined in order to correctly fit the collective magnetic response of our SBA-16/Fe_xCo_{1-x} materials is the mean distance among the iron-cobalt alloy particles in the hosting mesoporous silica matrix. The Electron Tomography analysis[1] performed on one of our materials was in fact useful to address the key-points reported above.

Results and Discussion. All the characterization techniques indicated that the ordered structure of the mesoporous silica is conserved after both the impregnation and the thermal treatments needed to give rise to the alloy nanoparticles formation and growth. Figure (a) shows a conventional TEM image of a sample FeCo/SBA-16 (Thermal Treatment performed at T = 800°C), where the ordered structure of the matrix can be observed together with the alloy nanoparticles. In that case, a mean size of 5.5 nm was measured for the nanoparticles, that were embedded in ordered silica having pores with cubic symmetry and corresponding d-spacing of 13.7 nm. The mean pore size was measured to be 3.6 nm. Figure (b) shows a view obtained from the the 3D reconstruction of the nanocomposite structure and performed by Electron Tomography. It allowed to observe that: a) the FeCo nanoparticles were distributed over the entire volume of the hosting ordered silica matrix but in random positions; b) that the mean distance (in the space) between two first neighbour particles was equal to XX nm. All these data were used to correctly understand the magnetic behaviour measured for such nanocomposite material.

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P093 – Synthesis and investigate of maleic anhydride-oktene-1/CdS nanocomposites

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Keywords: copolymer, matrix, nanoscale, CdS

In the large field of nanotechnology, polymer matrix based nanocomposites have become a prominent area of current research and development. Nanocomposites of inorganic materials in polymer matrices have attracted a great deal of attention because of their wide applications as biosensors, optical devices, micromechanical devices, semiconductor materials and advanced catalytic membranes. Among the many applications of nanocomposites can note in particular the semiconductor materials. Semiconductor nanocrystals have attracted impressive attention because of their novel optical and electronic properties. In recent development of semiconductor nanocrystals has been intensively pursued because of their size dependent characteristics, and their novel electronic, magnetic, optical, chemical, and mechanical properties that cannot be obtained in their bulk counterparts. For example Cadmium sulfide (CdS) is one of the most important chalcogenide semiconductor materials because of its direct band gap (2.42 eV at 300 K), which leads to many valuable properties such as photoluminescence, electroluminescence, and photocatalytic effects.

Nanocomposites are synthesized by different ways according to application areas. The sol-gel methods, self-assembly synthesis, kriochemistry synthesis, synthesis of a consistent, high-pressure synthesis, *in situ* method, etc. can be mentioned.

For this synthesis of CdS nanocomposites in the practice of *"in situ"* method, and maleic anhydride-oktene-1 copolymer matrix have been used.

In the first stage of the process of synthesis of maleic anhydride-otene-1 was a coplymer. The process for conducting maleic anhydride, octene-1 and initiator (2-2'-Azoisobutyronitrile) have been solved in ether and was heated in glycerine bath for 4 hours. Then copolymer was precipitated from solution with isopropanol and washed and was dried. In the second stage maleic Anhydride-Octene-1 copolymer has been solved in N,N-dimethylformamide and $(CH_3COO)_2Cd{\cdot}2H_2O$ were added to the solution and was heated in a water bath for 5 hours and then thiocarbamide (CH_4N_2S) were added to the flask with syringe .The reaction continued for another 2 hour, and a yellow clear solution was obtained, which indicated the formation of CdS nanoparticls.Experiments were carried out at 90ºC and mixing.

In the last stages the different properties of the copolymer have been investigated by UV-vis spectrophotometer and X-ray diffraction. UV-vis spectrophotometric measurement showed high transparency (in the wavelength range 200–1100 nm) of the solutions with a direct allowed band gap which is 3.94 eV. Also element content of maleic anhydride-octene-1/CdS nanocomposites has been investigated with Philips PW1606 X-ray fluorescence spectrometer. Reconstitution method was used in the study of element content.

Continue to explore other properties of the nanocomposites. Can be applied in various areas of the nanocomposites for instance it can be application in manufacture light emitting diode (LED), semiconductor materials, infrared photodetector, photocatalysis, photoluminesce, etc.

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P094 – Synthesis and luminescence of nano-sized $Sr_{2.91}V_2O_8$:$Eu_{0.06}$ phosphors by solution combustion method

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Keywords: nanopowders, microstructure, photoluminescence, LED, $Sr_{2.91}V_2O_8$:$Eu_{0.06}$

$Eu3_{+}^{-}$ doped $Sr_3V_2O_8$ phosphors have attracted interests due to their potential application in lamps, display source, and white LEDs. In this work, we studied the microstructure and photoluminescence (PL) characteristics of the $Sr_{2.91}V_2O_8$:$Eu_{0.06}$ phosphors synthesized by the solution combustion method, using various fuels such as aspartic acid, glycine, urea, and citric acid. X-ray diffraction results showed that the fabricated phosphors had a single phase with the palmierite-type structure. The fabricated $Sr_{2.91}V_2O_8$:$Eu_{0.06}$ phosphors showed nanocrystalline and high-quality powder characteristics, showing spherical and smooth morphology. The PL emission spectra of all the $Sr_{2.91}V_2O_8$:$Eu_{0.06}$ phosphors showed the green broad emission band centered at 510 nm and the red sharp emission peak at 614 nm, which were caused by the charge transfer transition of VO_4^{3-} group and the f-f level transition of Eu^{3+} ion, respectively. The type of the fuels used significantly affected the microstructure and PL characteristics of the $Sr_{2.91}V_2O_8$:$Eu_{0.06}$ phosphors.

P095 – Synthesis of aerogel nanocomposite catalysts for the production of carbon nanotubes

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Highly porous FeMo-SiO_2 nanocomposite aerogel catalysts were prepared by a sol-gel procedure with co-gelation of the precursors of the dispersed and of the matrix phases following a 2-step procedure[1,2] using absolute ethanol as mutual solvent. In the first step a solution of tetraethoxysilane ($Si(OC_2H_5)_4$, TEOS) and metal precursors $Fe(NO_3)_3 \cdot 9H_2O$ and either $(NH_4)_6Mo_7O_{24} \cdot 4H_2O$ or MoO_3 are prehydrolyzed by adding a hydrolyzing acidic solution of nitric acid. In the second step, a gelifying basic solution containing urea (NH_2CONH_2) is added to the pre-hydrolyzed sol to promote a fast and homogeneous gelation, which occurs in less than 2 days. The use of different complexant agents as DMF and EDTA were investigated in order to promote the Mo precursors dispersion.

In order to obtain aerogels with highly extended and open porosity (up to 98%), low densities and high inner surface areas, the wet gel undergoes supercritical drying in an autoclave (Parr, 300 cm^3) which avoid the capillary forces at the liquid/vapor interface responsible for shrinkage and cracking of the original porous structure. The detailed characterization of aerogel catalysts was carried out using a multitechnique approach involving X-ray diffraction (XRD), nitrogen physisorption at 77 K, transmission electron microscopy (TEM) and thermal analysis (TGA/DTA). All the structural characterization techniques indicate that the aerogel catalysts are mesoporous and the nanocrystals are well dispersed within the matrix.

These highly porous nanocomposites possess several properties which are expected to be crucial for hi-tech applications: in particular the high surface area allows loading and immobilization of nanoparticles within the pore network, giving rise to innovative catalytic properties. In particular, these nanocomposites were tested as catalysts in the production of Multi Wall Carbon Nanotubes (MWCNTs) by Catalytic Chemical Vapour Deposition (CCVD). Carbon nanotubes (CNT) offer great potential as components in a variety of devices, due to their peculiar thermal, electronic (metallic or semiconducting), mechanical (being the most flexible and strongest fibres) and chemical properties. Catalytic chemical vapour deposition (CCVD), which is widely acknowledged as the most effective approach for the large-scale production of CNTs[3–5] via the catalytic decomposition of hydrocarbons, or other suitable precursors, on metal nanoparticles, offers the advantage of controlling the features of the CNTs by a proper design of the catalysts. The CNT growth is strictly related to the presence of metal catalyst nanoparticles that can be generated in situ or distributed inside a suitable support.

The catalytic tests were carried out using aerogel nanocomposites constituted of FeMo dispersed in a silica matrix. The catalytic tests were performed at different temperature between 650°C and 800°C using acetylene (C_2H_2) as carbon source and the products have been investigated mainly by transmission electron microscopy (TEM), X-ray diffraction (XRD) and thermal analysis (TGA/DTA). Although the FeMo-SiO_2 aerogel nanocomposite does not contain alloy nanoparticles but at the best the two separate metals, it still showed an interesting catalytic activity.

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P096 – Synthesis of aluminosilicate nanotube from rice husk ash and its characterization

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Keywords: aluminosilicate nanotube, rice husk ash, recycle

Rice husk is an agricultural by-product abundantly available in rice-producing countries that on average accounts for 20% of the paddy produced, on weight basis. An increasing application of rice husk is used as fuel in the power plant, due to its high calorific value of approximate 13 to 16 MJ/kg.[1] In this combustion, rice husk (RHA) is produced and it causes environmental problems related to disposal. Therefore, finding an appropriate utilization of the RHA are desirable to solve this problem.

Aluminosilicate nanotube (imogolite) has a high surface area over 250 m^2/g, and is often found naturally in soil origination from volcanic material such as pumice and volcanic ash.[2] The chemical composition of the aluminosilicate nanotube is $(OH)_3Al_2O_3SiOH$, with 1 and 2 nm in inner and outer diameters, respectively, and several hundreds of nanometer in length.[3] There are micropores within nanotubes and mesopores among nanotubes, so the aluminosilicate nanotube is a promising adsorbent, catalyst and catalyst support.[4] However, the amount of naturally occurring aluminosilicate nanotube is very small, so it is hoped that large-scale synthesis can be carried out.

In this study, RHA was obtained from rice husk power plant in Myanmar, and was characterized by several instruments. The RHA contained 91.65 wt% of silica composed of a mixed phase of cristobalite, tridymite and amorphous silica. Using this silica component as raw material, we successfully synthesized aluminosilicate nanotube. The synthesized nanotube had a BET surface area of 282.0 m^2/g, and a web-like structure formed by fibrous buldles.

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P097 – Synthesis, investigation and fields of application of silicon nanocomposites containing rare earth metals

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Keywords: nanocomposite, rare earth metals, photoconverter

Silicon nanocomposites with rare earth elements (RE) are very promising material in optoelectronics. It is known that the presence of rare earth elements causes the appearance of photoluminescent properties in silicon nanomaterial (nc-Si). In particular the introduction of erbium in nc-Si photoluminescent peak is observed at 1.54 µm,[1] ytterbium – 1 µm,[2] terbium – 545 nm.[3] The matrix of nc-Si was usually dielectric (SiO_2). This work is devoted to study the influence of RE impurities on properties of nanocrystalline silicon with semiconductor matrix (α-Si).

Silicon nanocomposites with rare earth metals were synthesized by electron-beam evaporation. The structure of nanocomposites was studied by atomic-force microscopy. The size of nanocrystallites was about 10–20 nm. Also chemical composition of obtained material was examined. The distribution of rare earth elements was uniform in film thickness, but it was characterized by a presence of maximum peak at the interface film-substrate. In the work the electrical and optical properties of nanocomposites Si:RE were investigated. It was found that some RE dopants cause the increase of electroconductivity by 1–2 orders of magnitude. In addition, silicon nanocomposites with Eu or Y were characterized by high sensitivity to visible radiation. The ratio of dark to light resistance was achieved to 2 orders of magnitude, making this material very promising to use in thin-film photoresistors. After deposition of nanocomposites Si:RE on silicon substrate, the heterojunction was formed at the interface film-substrate, for which the sensitivity to visible radiation was observed too (1–2 mA/lmV). Also, it was shown the presence of photovoltaic effect in such structures, so they can be the basis of cheap thin-film solar cells, using the relevant design solutions.

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P098 – Synthesis, structural characterization and magnetic properties of highly porous $ZnFe_2O_4$-Sio_2 nanocomposite aerogels

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In this work, we present the synthesis and the structural and magnetic characterization of highly porous nanocomposite aerogel constituted of zinc ferrite nanoparticles dispersed into a highly porous amorphous silica matrix. The synthesis of this nanocomposite makes use of a sol-gel procedure with co-gelation of the precursors of the dispersed and of the matrix phases following a 2-step procedure[1,2] using absolute ethanol as mutual solvent. In the first step a solution of tetraethoxysilane ($Si(OC_2H_5)_4$, TEOS) and metal salts ($Fe(NO_3)_3 \cdot 9H_2O$ and $Zn(NO_3)_2 \cdot 6H_2O$) are prehydrolyzed by adding a hydrolyzing acidic solution of nitric acid. In the second step, a gelifying basic solution containing urea (NH2CONH2) is added to the pre-hydrolyzed sol to promote a fast and homogeneous gelation, which occurs in less than 2 days. In order to obtain aerogels with highly extended and open porosity (up to 98%), low densities and high inner surface areas, the wet gel undergoes supercritical drying in an autoclave (Parr, 300 cm^3) to avoid the capillary forces at the liquid/vapor interface responsible for shrinkage and cracking of the original porous structure.

Metal spinel ferrites (MFe_2O_4, M being a divalent cation) are of great interest in materials chemistry due to their good thermal and chemical stability combined to the possibility to finely tune the magnetic and catalytic behavior as a function of the divalent ion. In addition, innovative properties such as superparamagnetism and enhanced catalytic performance can be observed in nanosized ferrites. In this work, $ZnFe_2O_4$-SiO_2 highly porous nanocomposites are prepared with the scope of obtaining well-dispersed nanocrystals supported on an extended and open porous silica matrix for perspective catalytic applications.

The detailed characterization of $ZnFe_2O_4$-SiO_2 nanocomposite aerogel was carried out using a multitechnique approach involving X-ray diffraction (XRD), nitrogen physisorption at 77 K, transmission electron microscopy (TEM), thermal analysis (TGA/DTA), SQUID magnetometry and Mössbauer spectroscopy. The results refer to a nanocomposite aerogel having a nominal ratio of 10 wt% of ferrite in the final nanocomposite ($ZnFe_2O_4/ZnFe_2O_4 + SiO_2$).

The XRD pattern of the nanocomposite aerogel shows the presence of a single nanocrystalline phase which can be ascribed to the zinc ferrite superimposed to an amorphous halo due to the silica matrix. Also, structural characterization points out that the formation of nanocrystalline $ZnFe_2O_4$ starts at 750°C and at 900°C an increase in the amount and size of the ferrite phase is observed.

TEM investigation indicates that the matrix has a necklace mesoporous texture. The zinc ferrite nanoparticles are homogeneously distributed within the matrix and the average size is about 11 nm.

ZFC/FC curves, hysteresis loops and Mössbauer spectra of the nanocomposites show a superparamagnetic behavior.

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P099 – Tailoring the functionality of single-walled carbon nanotubes by metallocene filling

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Keywords: single-walled carbon nanotube, metallocene, Raman spectroscopy, electronic properties

Single-walled carbon nanotubes (SWCNTs) have attracted an attention of many researches because of their unique 1D electronic properties that can be tailored in an ambipolar manner by donor and acceptor molecules. One very effective way of modifying the electronic structure and the chemical environment in a controlled way is via advanced filling reactions.[1–3]

In this work we performed the filling of the single-walled carbon nanotube channels with mean diameter of 1.7 nm with ferrocene, nickelocene and cobaltocene molecules and carried out furnace annealing of these samples at different temperatures in vacuum to transform filled SWCNTs to double-walled carbon nanotubes (DWCNTs). The temperature dependence of inner tube growth and the electronic properties of obtained nanostructures were investigated by the Raman spectroscopy, the ultraviolet photoelectron spectroscopy (UPS) and the X-ray photoelectron spectroscopy (XPS).

We show that the temperature of beginning of inner tube formation depends on the chemical nature of metal atom in metallocene. This temperature increases in line Ni-Co-Fe. The investigation of samples by multifrequency Raman spectroscopy allowed performing a precise analysis of growth of inner tubes of different chiralities and diameters ranging from 0.7 nm to 1.4 nm. According to XPS data, the filling of carbon nanotubes with metallocenes leads to donor doping, because the maximum of the C 1s spectra of filled SWCNTs are upshifted as compared with the spectra of pristine ones. In contrast, in samples after conversion of SWCNTs to DWCNTs the acceptor doping was observed. This data are in accordance with the UPS data that clearly show the shift of π^*-peak of valence band in spectra of filled and converted tubes.

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P100 – A temperature dependent study of the growth yield of linear carbon chains inside double walled carbon nanotubes

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Keywords: carbon chains, double walled carbon nanotubes, Raman spectroscopy, annealing

Linear carbon chains (LC-chains), as carbon allotrope, get increasing attention due to their unique properties as true one-dimensional (1D) carbon nanostructure. Encapsulating the LC-chains into CNTs is an effective method to protect them from being damaged and decomposed.[1–3] Here, we have successfully synthesized double walled carbon nanotubes (DWCNTs) by high vacuum alcohol chemical vapor deposition, which contain a high yield of thin inner tubes (around 0.7 nm in diameter). These nanostructures can act as nanoreactors for the preparation of inner linear carbon chains (LC-chains). In a second step, we applied a heat treatment of the purified DWCNTs under high vacuum at temperatures from 1000 to 1550°C in order to study the formation and yield of LC-chains inside the tubes. According to the results from Raman spectroscopy, we found that LC-chains can be formed even at temperatures as low as 1000°C, and the optimum temperature is 1460°C. This study has important implications to understand the growth and identification of LC-chains.[4]

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P101 – Theranostic hyaluronic acid nanoparticles for cancer and Alzheimer's disease

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Keywords: hyaluronic acid, theranostics, cancer

Hyaluronic acid (HA), a natural polysaccharide in the body, has received increasing attention as the anticancer drug carrier because HA specifically binds to the receptor (CD44) which is over-expressed on the cancer cell.[1] In recent years, our group has developed poly(ethylene glycol)-conjugated hyaluronic acid nanoparticles (P-HA-NPs) for tumor targeting.[2,3] We have demonstrated that systemic administration of P-HA-NPs results in selective accumulation of the nanoparticles in tumor tissue through the enhanced permeation and retention effect and strong receptor binding to the CD44. Colon cancer is the second leading cause of cancer-related death in the United States. In this study, we established a versatile theranostic system for early tumor detection and targeted tumor therapy by using P-HA-NPs. After intravenous injection of Cy5.5-P-HA-NPs into the tumor-bearing mice, small-sized colon tumors as well as liver-implanted colon tumors were effectively visualized using the a near-infrared fluorescence (NIRF) imaging technique. For targeted therapy, the anticancer drug, irinotecan (IRT), was physically encapsulated into the hydrophobic cores of P-HA-NPs. Owing to their tumor targetability, IRT-P-HA-NPs exhibited an excellent antitumor activity. Interestingly, the therapeutic responses could be simultaneously monitored by Cy5.5-P-HA-NPs. These results implied that P-HA-NPs are useful theranostic nanoparticles for the early detection, targeted therapy, and therapeutic monitoring of colon cancer.

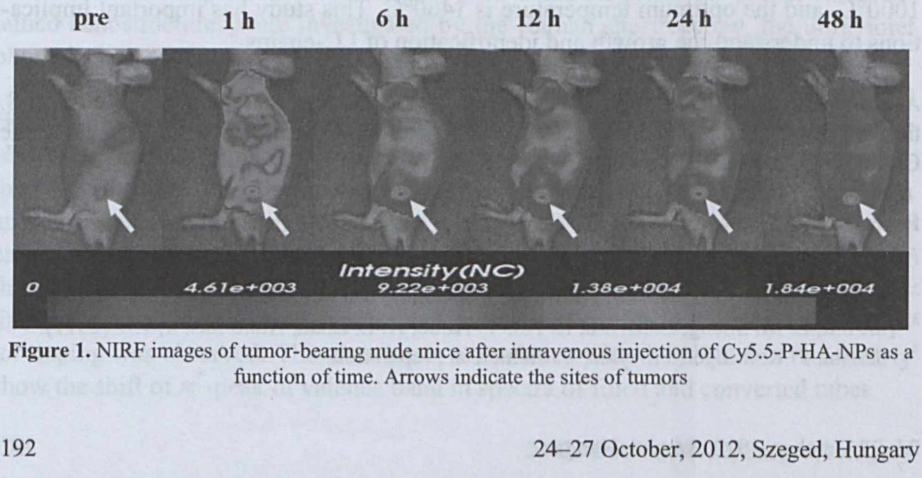

Figure 1. NIRF images of tumor-bearing nude mice after intravenous injection of Cy5.5-P-HA-NPs as a function of time. Arrows indicate the sites of tumors

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P102 – Thermal stability test of one-dimensional $CePO_4$ nanostructures for a potential solid oxide fuel cell application

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Nowadays global warming and air pollution have become urgent problems mostly caused by our prodigal industrial and transport technology. Currently fuel cells are the most promising candidates which could provide a quite elegant solution for these problems.

Solid oxide fuel cells are a class of fuel cell in which a solid oxide or ceramic material is used as the electrolyte. This type of fuel cell has the advantages of high efficiency, fuel flexibility, long-term stability, low emissions, and relatively low cost. Nevertheless their typical operating temperature can reach the 500–1000°C which raises some mechanical and chemical compatibility issues.

In the recent years much attention has been focused on the preparation of rare-earth phosphate nanomaterials. Their unique electronic configuration makes them promising candidates for the application in optoelectronics, catalysis, biological fluorescent labeling and fuel cells. However only few studies have been published on the structural stability of $CePO_4$ nanowires and sea urchin-like nanostructures against elevated temperatures and pressures. One-dimensional $CePO_4$ nanostructures can be prepared by various synthetic procedures such as template based, microemulsion, sonochemical, microwave assisted or hydrothermal methods.

Recently a simple, template-free, room temperature synthesis has been developed by our research group for the preparation of ultra-long cerium-phosphate nanowires and sea urchin-like nanostructures in hexagonal phase.

In this study thin membranes were prepared from $CePO_4$ nanostructures by applying different temperatures and pressures. The structural stability and crystallinity of the nanostructures were examined by transmission electron microscopy, X-ray diffraction and Raman spectroscopy. The microstructure and the porosity of the membranes were examined by scanning electron microscopy and nitrogen adsorption surface area analyzer.

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P103 – Thin films of copper phthalocyanine – 2D conductive polymer

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Keywords: 2D polymer, organic semiconductor, thin films

Metal polyphthalocyanines (PPCs) are a unique class of organic semiconductors, possessing 2D electronic conjugation. This makes them of especial interest for science and technology.[1–3] PPCs have been discovered more than 50 years ago,[4] but their application has been hindered by the lack of processability: they are practically insoluble in all solvents and cannot be melted or evaporated.[1] For these reasons it is impossible to process PPCs by conventional methods: spin-coating, sputtering, thermal evaporation. However, in order to access the promising applications of PPCs, it is highly desirable to obtain these materials in a form of thin films on any arbitrary wafer (especially dielectric).

In this work we investigate the experimental approach to the synthesis of CuPPC thin films, which enables us to obtain this 2D polymer directly in a CVD set-up. We prove that in this way the conductive PPC films of high uniformity and high polymerization degree can be obtained. We use infrared spectroscopy, transmission electron microscopy, XRD, UV-visible absorption and sheet resistance measurements to prove the structure and investigate the properties of the films.

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P104 – Time-resolved GISAXS study of formation of a silver nanoparticle crystal with FCC symmetry

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Keywords: solvent-assisted self-assembling, silver nanoparticles, face-centered cubic symmetry, GISAXS

Here we report on time-resolved study of self-assembling of silver colloidal nanoparticles performed at micro-GISAXS beamline at PETRA III. The 2D GISAXS pattern of dried nanoparticle droplet is shown on the Fig. 1a. The displayed map refers to face-centered cubic lattice with (*111*) preferred orientation (ABC stacking). The lattice constant of nanocrystal was determined to $a = 11.9$ nm. The interparticle distance in hexagonally ordered layers is then 8.4 nm and inter-layer distance between adjacent layers is 6.9 nm. The temporal series of GISAXS patterns was analyzed following the paracrystal model to get a time-resolved picture of the nanocrystal formation. Paracrystal model is widely used for characterization of short range ordered structures.The important application of it is to evaluate distortion parameter along particular direction in nanoparticle crystal.Here we examined peak widths of three particular Bragg peaks (*111*), (*222*), (*333*) formed at detector scan which provide us information about the quality of layering. The temporal evolution of the distortion parameter along (*111*) direction is shown on the Fig. 1b. After some 100 s we observe short period of sudden improvement in the quality of layering (black arrow in the Fig. 1b). Here, the majority of the organic solvent is already evaporated and the volume for the nanoparticle re-arrangement is strongly reduced but still large enough to allow the nanoparticles to keep their full hydrodynamic size and to organize themselves into a well ordered 3D structure. Finally, the rest of the solvent giving mobility to the nano-

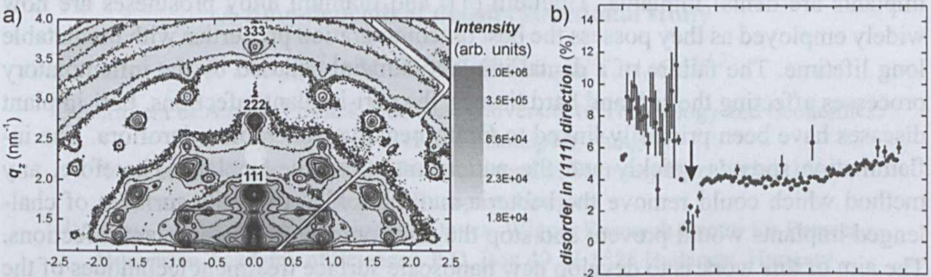

Figure 1

particles via their surfactant shell is evaporated and the conditions for the 3D nanocrystal formation are worsened (180–400 s). Here we observe a partial increase of the disorder parameter that levels off at a saturated value of 4%.

P105 – TiO_2-Ag/Au/polymer nanohybrid coatings targeting prevention of peri-implant infections of dental implants

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Biointegration of alloplastic materials is one of the most important targets and research fields of medical, dental and biological sciences. The most frequently used medical implants are dental implants. Titanium (Ti) and titanium alloy prostheses are now widely employed as they possess the best osseointegration properties with predictable long lifetime. The failure of a dental implant is mainly caused by the inflammatory processes affecting the soft and hard tissues, the peri-implant infections. Peri-implant diseases have been primarily linked to Gram-negative anaerobic microflora. The inflammation spreads quickly and the patient may lose the implant. Therefore, any method which could remove the bacteria and the toxins from the surfaces of challenged implants would prevent and stop the development of peri-implant infections. The aim of this work is to develop new nanoscale surface treatment techniques of the surface of titanium dental implants to prevent peri-implant infections.

Titanium sample discs 1.5 mm thick and 9 mm in diameter were cut from commercially pure (CP4) titanium rods (Denti® System Ltd. Hungary), used for the fabrication of dental implants. The surfaces of the control (untreated) discs were sandblasted and acid etched as in case of the osseointegrating part of the implant. The following spray coatings were developed preparing copolymer based nanohybrid layers titanium discs: i) 60% TiO_2/40% copolymer film (poly-ethylacrylate and poly-methylmethacrylate); ii) 60% $AgTiO_2$/40% plextol ([Ag] = 0.5 m/m%); iii) 60% $AgDSTiO_2$/40% copolymer. The latter coating contained dodecyl-sulphate (DS) which gave the hydrophobic feature of the surface. The same experiments were made using TiO_2 Ag/Au noble metal alloys. The roughness (Ra) of the samples were analyzed with atomic force microscopy (AFM, PSIA XE-100 instrument; PSIA Inc., South Korea). To test the antibacterial activity of the coatings against the growth of bacterial colonies a Micro BCA Protein Assay Kit (Pierce Biotechnology, Rockford, IL) was used. The quantity of Porphyromonas gingivalis bacterial protein was measured after 4 days of incubation.

The AFM measurements indicated a roughness value of $R_a = 544 \pm 47$ nm (mean ± SEM) for the control samples. After 4 days of incubation with *P. gingivalis,* the protein content measurement showed a significant decrease in the amount of bacteria on the $AgDSTiO_2$ treated Ti discs as compared to the control ones (78% vs. 100%). This composite has an antibacterial activity against the growth of *P. gingivalis* bacterial colonies.

The developed $AgDSTiO_2$ or Ag/Au TiO_2 copolymer based nanohybrid layers present a new possibility in the treatment and prevention of peri-implant infections. In order to establish which is the more predominant effect between the hydrophobic feature and the Ag nanoparticles further studies are needed.

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P106 – Tuning the optical gap of small diamondoid cages by sulfurization: A time-dependent density functional study

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Keywords: diamondoids, biomarker, absorbant, optical gap

Diamondoids are small diamond nanocrystals with perfect hydrogenated surfaces. The optical gap of nanometer sized diamond cages, i.e., diamondoids lies in the ultraviolet spectral region. This gap can be tuned by reducing the size of nanoparticles, that is called the quantum confinement effect, or by attaching to the surface a carefully chosen absorbants. This is now a major focus of nanoscale research in the applications of biomarkers, photovoltaics and photocatalysis. Here we show by hybrid functional based time-dependent density functional calculations that by varying the number of

C=S double bonds at the surface of diamondoids, the absorption onset can be tuned toward the infrared spectral region. Our finding has an important implication for *in vivo* biological applications where toxic and unstable dye molecules may be substituted by the luminescent sulfurized diamondoids.[1]

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P107 – Ultrashort pulse characterization utilizing highly nonlinear ZnO nanostructures

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Keywords: ZnO nanorods, pulse characterization, second harmonic generation

ZnO is a material that possesses second order nonlinear optical coefficients exceeding conventional materials like BBO by a factor of 5 or more.[1,2] Beside specific advantages with respect to phase matching and enhancement effects, the excellent stability, damage threshold and optical transparency of this material enable new applications in laser physics, photovoltaics or optical sensors. In particular, ZnO was identified as a promising candidate for two-dimensional frequency conversion of Ti:sapphire lasers which extends the classical approaches of pulse diagnostics significantly.[3] Recently, we published preliminary results on second harmonic generation (SHG) in certain types of nanorods.[4] In this work we report on studies of SHG in ZnO nanowires of improved structure and its application to the characterization of sub-20-fs pulses. The nanostructures were prepared either by chemical bath or vapour-liquid-solid (VLS) methods. In these experiments, angular and polarization dependent SHG was detected. Optimized nanomaterials were used to perform second order interferometric autocorrelation with enhanced efficiency. It is concluded that tailored nanomaterials might be key components of novel types of sensitive pulse characterization systems that operate over a remarkably broad spectral range and represent a cost effective alternative to conventional thin film materials. The authors acknowledge financial support from a LaserLab Europe project (NEXT).

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P108 – Zinc containing bioglass-derived porous scaffolds for tissue engineering

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Keywords: synthesis and characterization of nanostructures and nanocomposites

In tissue engineering an ideal scaffold needs to create optimal conditions for cell survival, proliferation and therefore tissue formation. Since cells are usually organized into three-dimensional (3-D) tissues, scaffolds can act as highly porous template to accommodate cells and guide their growth and differentiation into tissue in three dimensions.[1] One of the many methods used to produce these kind of porous bioglass scaffolds is replication technique. An ideal scaffold should be a macroporous bioglass having an interconnected morphology of micropores and mesopores. In order to obtain sol-gel derived macroporous bioglasses, polyurethane sponge was used as pore former that functioned as a sacrificial agent during samples sintering. Another important requirement for bioglasses to be used as scaffolds is to have osteoinductive properties. The bone stimulating properties of bioglasses can be improved by incorporating of bone stimulating ions, such as zinc, into their chemical composition. The aim of the present study was to produce sol-gel derived macroporous zinc containing bioglasses based on SiO_2-CaO-ZnO-P_2O_5 system, by a combination of polyurethane sponge as template and evaporation induced self-assembly process and to investigate their characteristics. Samples with three different SiO_2/ZnO ratios were prepared through the sol-gel route. The obtained sols were coated on polyurethane and dried several times followed by a heat treatment at 900ºC for 2 h (1ºC/min) to drive off the porogen. For the characterization of the samples we used scanning electron microscopy (SEM), Brunauer-Emmett-Teller (BET) analyses for specific surface area, Barrett-Joyner-Halenda (BJH) method for pore size distributions, X-ray diffraction (XRD) as well as

Fourier transform infrared spectroscopy. The effect of the zinc content on bioglass properties, mainly on their porosity, was correlated with the *in vitro* bioactivity of the obtained samples that was evaluated in simulated body fluid.

Acknowledgement: R. V. the author wishes to thank for the support provided from programs co-financed by Contract POSDRU 88/1.5/S/56949.

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[1] Q. Chen, D. Mohn, W. J. Stark, *J. Am. Ceram. Soc.* **94**, 4184 (2011).

P109 – Hierarchical hollow mesoporous carbon as a highly efficient anode electrode in Li-ion battery

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Keywords: hierarchical structure, hollow mesoporous carbon, anode electrode, Li-ion battery

New energy technologies are critical for the energy future that seeks the goal of sustainable energy development. Rechargeable lithium-ion batteries are becoming a key-enabling technology and have potential applications in electric and hybrid vehicles due to their high energy density, high voltage, and long lifespan. However, their rate capability which is dominated by the diffusion rate of lithium-ions and the electron transport in electrode materials, needs to be improved greatly. Recently, much attention has been paid to high surface area porous carbons with various nanostructures due to the expected reduced diffusion length of lithium-ions and rapid charge transfer.[1,2] Hollow Core-Mesoporous Shell Carbon (HCMSC) spheres with hierarchical nanostructure were prepared and explored as anode in Li-ion battery.[3] Compared with commercial graphite, ordered mesoporous carbon (CMK-3), the HCMSC not only demonstrates higher Li-storage capacity, but also better cycling performance and rate capability. HCMSC possesses unique structural characteristics such as large surface area and mesopore volume, particularly the multimodal porositiy composed of well-developed 3D interconnected mesopores embedded in the mesopore shells, facilitating fast mass transport and charge transfer. The enhancement in anode performance especially in the cycling performance and rate capability is mainly attributable to the superb structural characteristics of the HCMSC particularly the macropore core encapsulated in well-developed 3D interconnected mesoporous shell, which act as efficient Li-storage and buffer reservoirs to reduce volume change during the charge-discharge cycling especially at high rates.

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