

PANIC 2017

PhoBiA Annual Nanophotonics
International Conference

24-26 April 2017
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I. Committees





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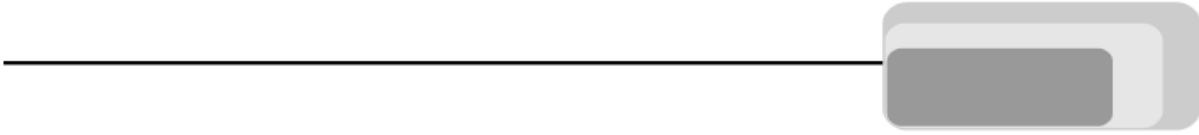


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Experimental Therapy**





III. Programme





Monday 24 April 2017

Session I

9:00 – 9:15 *Official opening ceremony*

9:15 – 10:30 **E. Zysman - Colman** - Invited lecture

10:30 – 10:45 **M. Duda** - Structural characterization of novel biofunctionalized coating for potential cardiovascular applications

10:45 – 11:00 **M. Pawliszewska** - Graphene and black phosphorus as saturable absorbers for ultrafast holmium-doped fiber lasers

11:00 – 11:15 **M. Waszkielewicz** - Strategies for gold nanoclusters photoluminescence enhancement

11:15 – 12:10 *Coffee break*

12:10 – 12:25 **F. Temel** - Detection of amino acid derivatives in aqueous media by chiral calix[4]arene coated QCM sensors

12:25 – 12:40 **N. Tarnowicz** - Phase transition of nematic liquid crystal induced by azobenzene photoisomerization sensitized by CdS nanoparticles

12:40 – 12:55 **M. Chrzanowski** - Synthesis of double shell type-II semiconductor nanocrystals for lasing applications

12:55 – 13:10 **M. Deiana** - Light-activated compounds as new tools to monitor and trigger bio-events

13:10 – 14:30 *Lunch time*

Session II

14:30 – 15:45 **T. Wójtowicz** - Invited lecture: Multidisciplinary research in the studies of the brain plasticity


15:45 – 16:25 *Coffee break*

16:25 – 16:40 **M. Chóluj** - The effect of spatial confinement on the two-photon absorption process

16:40 – 16:55 **B. Haspulat** - Photocatalytic activity of electrochemically synthesized Co doped polyaniline films

16:55 – 17:10 **M. Antoniak** - Hybrid nanoparticles for simultaneous and sequential two photon induced luminescence

19:00 – 24:00 *Conference dinner*



Tuesday 25 April 2017

Session III

9:00 – 10:15 **R. Metiver** - Invited Lecture

10:15 – 10:35 **M. Bański**

10:35 – 10:55 **M. Ziemińczuk**

10:55 – 11:15 **M. Rowińska-Żyrek**

11:15 – 11:35 **J. Olesiak-Bańska**

11:35 – 12:15 *Coffee break*

Session IV

12:15 – 13:30 **W. Fortuna**- Invited Lecture

13:30 – 13:45 **M. Tabakci** - Detection of p-nitrophenol by modified QCM sensor with bromopropyl functionalized calix[4]arene

12:30 – 12:45 **H. Deveci** - Epoxy composites including fly ash: mechanical, water sorption, adhesion, corrosion and thermal properties

14:00 – 15:30 *Lunch time*

15:30 – 17:30 *Poster session + Coffee break*

18:00 – 21:00 *Odra river cruise*



Wednesday **26 April 2017**

Session V

9:00 – 10:15 **E. Glowacki** - Invited Lecture: hydrogen-bonded organic semiconductors – from optoelectronics to bioelectronics

10:15 – 10:30 **J. K. Zaręba** - Spectrally-resolved third-harmonic generation in cobalt(II) tetraphenylmethane-based coordination polymer

10:30 – 10:45 **A. Olejniczak** - Surface charge minimization in AgInS₂ quantum dots – DFT calculations

10:45 – 11:00 **M. Kowalczyk** - Nonlinear absorption of Sn-doped Bi₂Te₂Se and its application to pulsed fiber lasers

11:00 – 11:40 *Coffee break*

Session VI

11:40 – 12:55 **A. Kiersnowski** - Invited Lecture: Where radiation meets soft matter: revealing the packing and phase composition of heterogeneous polymer systems for application in electronics

12:55 – 13:10 **J. Bednarska** - Theoretical modeling of the two-photon properties of difluoroborate compounds

13:10 – 13:25 **H. Woźnica** - Colloidal two-dimensional heterostructures

13:25 – 13:40 **A. Adamów** - The ASE enhancement in liquid crystals doped with perylene dye

13:40 – 15:00 *Lunch time*

15:00 – 15:15 **S. G. Mucha** - Unravelling the photophysical properties of light-activated compounds, based on azobenzene motif

15:15 – 15:30 **K. Popko** - Gold nanoparticles enhanced Gram-negative bacteria photoinactivation

15:30 – 15:45 **A. Lesiak** - General approach for thiol-capped CdS over coated semiconductor quantum dots

15:45 – 16:00 *Closing*





IV. Abstracts





Monday
24.04.2017



Structural characterization of novel biofunctionalized coating for potential cardiovascular applications

M. Duda¹, M. Wawrzyńska², W. Kałas³, H. Podbielska¹, M. Kopaczyńska¹

¹ Biomedical Optics Group, Department of Biomedical Engineering, Wrocław University of Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland

² Department of Medical Emergency, Faculty of Health Science, Wrocław Medical University, Parkowa 34, 51-616 Wrocław, Poland

³ Department of Experimental Oncology, Ludwik Hirszfeld Institute of Immunology and Experimental Therapy, Polish Academy of Sciences, Rudolfa Weigla 12, 53-114, Wrocław, Poland

Abstract

Atherosclerosis is currently one of the main diseases causing cardiovascular disorders resulting in blood vessel lumen narrowing. Percutaneous coronary intervention (PCI) is the direct solution to this complication and also, it is one of the most important procedures of modern interventional cardiology. PCI is performed with specialized intravascular implants, known as stents. Placing a foreign biomaterial into the human organism causes a certain response induced by the mechanism of vessel's wall healing process. Restenosis and thrombosis are two major, potentially lethal post-surgical complications, which cause secondary blood vessel occlusion [1]. The majority of scientific research trends addressing those two issues involve stent surface modifications, such as coating with biodegradable polymer with anti-proliferative factors incorporated into its structure.

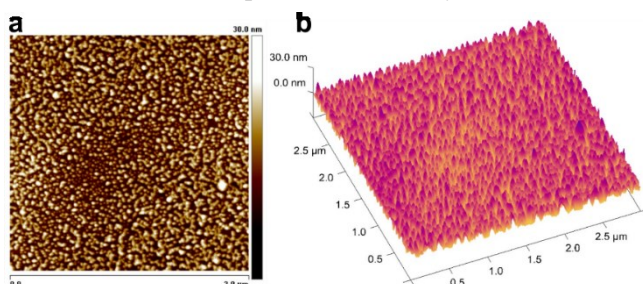


Fig.1. Atomic force microscopy (AFM) image of the biofunctionalized surface: a) topography, b) 3D projection.

The others focus on intravascular implants surface biofunctionalization, like immobilization of antibodies specific towards endothelial progenitor

cells (EPCs) that significantly facilitate the process of vessels endothelialization, hence the stents biocompatibility is significantly increased [2]. In this research, we present results of studies conducted on 316L stainless steel surface (standard cardiovascular material), that was functionalized with titanium based coating (Ti-BC), which underwent chemical modifications and was subsequently biofunctionalized with anti-CD133 antibodies, which exhibit excellent EPC-binding properties in cardiovascular applications [3]. Obtained samples were thoroughly examined with spectroscopic methods, such as Raman and FTIR spectroscopy. Additionally, microscopic assays, like AFM and confocal microscopy were employed to determine the surface roughness and the distribution of immobilized antibodies respectively. Furthermore, in vitro studies show that obtained biofunctionalized samples are much better at binding EPCs (HUVEC adhesion tests) in comparison to standard 316L surfaces and what's more, they display far weaker hemolytic properties. Concluding results suggest that developed coatings might constitute a good basis for future in vivo studies.

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Graphene and black phosphorus as saturable absorbers for ultrafast holmium-doped fiber lasers

M. Pawliszewska

Laser & Fiber Electronics Group, Faculty of Electronics, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland

Abstract

Numerous applications of lasers emitting ultrashort optical pulses beyond 2 μm include surgeries, spectroscopy or telecommunications [1]. This motivates the photonic community to further research pulsed laser sources based on holmium-doped crystals and fibers, which are capable of reaching wavelengths in the ~ 2080 nm range.

This work presents successful usage of novel two-dimensional materials: black phosphorus and graphene [2] for mode-locking all-fiber lasers utilizing holmium-doped active fibers as a gain medium. Experimental results confirm broadband optical properties of these materials. Two laser setups will be presented along with comparison of their performance. The generated optical solitons centered at 2070 – 2090 nm reach pulse duration and energy of ~ 800 fs and 2.2 nJ, respectively.

Methods of manufacturing saturable absorbers based on graphene/PMMA composite and black phosphorus solution will be shown, along with measurements of their nonlinear optical properties.

This work was supported by Polish Ministry of Science and Higher Education under the grant no. IP2015 073774, The National Science Center under the grant no. UMO-2014/13/D/ST7/02143, and statutory funds of Chair of EM Field Theory, Electronic Circuits and Optoelectronics.

References

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Strategies for gold nanoclusters photoluminescence enhancement

M. Waszkielewicz¹, J. Olesiak - Bańska¹, K. Matczyszyn¹, Clothilde Comby-Zerbino², Franck Bertorelle², Xavier Dagany², Philippe Dugourd², Rodolphe Antoine², M. Samoć¹

¹*Advanced Materials Engineering and Modelling Group, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland*

²*Institut Lumière Matière, UMR5306 Université Claude Bernard Lyon 1 - CNRS, Université de Lyon 69622 Villeurbanne cedex, France.*

Abstract

In the last decade thiolate gold nanoclusters have been extensively explored as they exhibit an attractive set of features like a precisely defined structure, a large Stokes shift (much larger than for standard organic dyes) and low toxicity [1]. Numerous papers have been published in the field of structural analysis and size-dependent optical properties [2], but one of the biggest challenges has been a relatively low photoluminescence quantum yield of the clusters. Much effort has been invested in understanding and enhancing fluorescence of the nanoclusters to make the most of the advantages of those structures.



Fig. 1. Emission of thiolate silver – gold nanoclusters

The investigations presented in this contribution have concerned strategies of photoluminescence enhancement of gold nanoclusters. Basic optical characterization (absorption, emission) has been made and the structure was defined with ESI-MS method. The transmission electron microscopy was used to observe changes in NCs organization. The impact of solvent, pH and doping with other noble metals on NCs fluorescence will be discussed as well as the relation between their structure and optical properties.

References

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Detection of amino acid derivatives in aqueous media by chiral calix[4]arene coated QCM sensors

F. Temel¹, E. Ozcelik¹, S. Erdemir², B. Tabakci², M. Tabakci¹

¹Chemical Engineering Department, Selçuk University, Konya, 42075, Turkey

²Chemistry Department, Selçuk University, Konya, 42075, Turkey

Abstract

Amino acids are the basic unit of proteins and important components for all chemical and biological systems. They combine to yield proteins, enzymes, structural elements and many other molecules with biological activity. Biosensors are devices which are used for controlling and sensing of biologic analytes due to their properties of biological sensing. In biosensor applications, there are several methods which are electrochemical, calorimetric, optical and acoustic systems [1-3]. Among them, Quartz Crystal Microbalance (QCM) is an acoustic

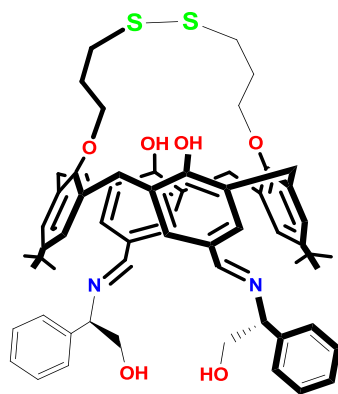


Fig. 1. Presentation of calix[4]arene derivative

microsensor which is simple, cost-effective, mass sensing device [4]. The QCM can be used in analytical chemistry, electrochemistry, and biochemistry applications. It's working principle depends on interaction between transducer surface and analyte interface. QCM sensors can convert mass accumulation due to interaction between analyte and sensing film layer to frequency shift. There are limited numbers studies about macromolecules as biochemical sensors even though there are many studies about polymeric materials. Among synthetic supramolecular compounds, calixarenes are widely used in host-guest chemistry for construction of various receptors for charged or neutral molecules (In Fig. 1).

Furthermore, they have a unique three-dimensional structure with almost unlimited derivatization possibilities. In our previous works, we have also synthesized some calixarene compounds and they has been investigated their sensing properties for volatile organic compounds. Thus we have prepared some chiral calixarene compounds and investigated their properties on detection of amino acid derivatives.

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Phase transition of nematic liquid crystal induced by azobenzene photoisomerization sensitized by CdS nanoparticles

N. Tarnowicz¹, M. Bański², A. Podhorodecki², K. Matczyszyn¹

¹Advanced Materials Engineering and Modelling Group, ²Department of Experimental Physics, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland

Abstract

Liquid crystalline phase is a unique state of matter which is located thermodynamically between two common states: solid and liquid, and combines their properties. Liquid crystals (LCs) exhibit orientational ordering, optical and electrical anisotropy characteristic to crystals and alike isotropic liquids are able to flow and can be described by physical parameters such as viscosity. [1, 2] LCs due to their unusual properties and ability to respond to external stimuli are widely used, e.g. as sensors, in displays and many optical elements. They are also a very important group of matrixes used in nanotechnology and photonics. [3]

Phase transitions of matter can cause dramatic changes of material properties and are essential part of studies in the field of materials engineering. [1, 2] Mesogens with photochromic groups or LCs doped with photochromic molecules are of special interest because of their ability to undergo phase transitions to isotropic liquids under irradiation. [4] Absorption of selected wavelength can cause photoisomerization of dopant molecule and its geometrical shape change. This results in most cases in distortion of LCs molecular ordering in the direct surroundings and leads to phase transition of LC. [5] This photo-induced phenomenon can be used in optical data storage, information processing or light-driven sensors and is totally reversible while not destroying the material itself. [4]

Within the scope of presented studies regular mixture of LC and photochromic molecules azobenzene type was additionally doped with CdS nanoparticles. The first aim of research was to determine if photoisomerisation of azobenzene derivative can be driven by wavelength absorbed by CdS instead of azobenzene – due to an energy transfer from nanoparticles. The second goal was to find out if CdS can photosensitize phase transition of liquid crystalline matrix of investigated system in the temperatures lower than its phase transition temperature.

References

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Synthesis of double shell type-II semiconductor nanocrystals for lasing applications

M. Chrzanowski, M. Bański, J. Misiewicz, A. Podhorodecki

Department of Experimental Physics, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław

Abstract

Core-shell semiconductor nanocrystals are of great interest due to their high capability for controlling radiative decay by application of wavefunction engineering, which aim is tuning the spatial confinement and overlap between charge carriers. Type-II NCs are promising tool for lasing applications, because of two main advantages. The first one is separation of charge carriers, which strongly reduces fast non-radiative Auger recombination decay associated with multiexcitonic nature of light amplification. The second one is enhanced exciton-exciton repulsion arising from imbalance of negative and positive charges, which allows optical amplification in single-exciton regime, enhancing potential of NCs as gain media with low threshold and continuous wave excitation.

We demonstrate the synthesis of ZnSe/CdS/ZnS semiconductor NCs utilizing wet chemistry methods. Core-shell structure was accomplished by slow growth of CdS shell on previously prepared ZnSe cores, resulting in type-II band alignment. Additional growth of outer ZnS shell enhances fluorescence quantum yield and photochemical stability. Both core size and shell thickness variation provide opportunity to reach spectral tuning of optical response in 500–580 nm range. NCs will be characterized using a transmission electron microscopy (TEM), X-ray diffraction (XRD) as well as absorption (ABS) and photoluminescence (PL) spectroscopy.

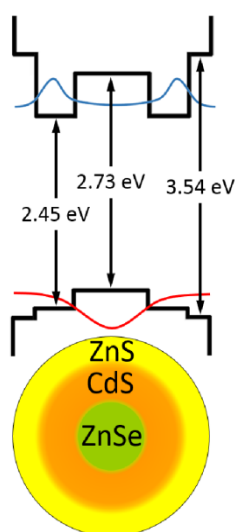


Fig. 1. Structure of ZnSe/CdS/ZnS type-II nanocrystal quantum dot and schematic representation of carriers localization in band potentials.

References

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Light-activated compounds as new tools to monitor and trigger bio-events

M. Deiana¹, Z. Pokladek², B. Mettra³, M. Ziemianek², L. Mazur¹, S. Mucha¹, K. Pawlik⁴,
P. Mlynarz², M. Buckle⁵, C. Monnereau³, C. Andraud³, M. Samoc¹, K. Matczyszyn¹

¹Advanced Materials Engineering and Modelling Group, Faculty of Chemistry, Wrocław University of Science and Technology, Wyb. Wyspiańskiego 27, 50-370 Wrocław, Poland

²Department of Bioorganic Chemistry, Faculty of Chemistry, Wrocław University of Science and Technology, Wyb. Wyspiańskiego 27, 50-370 Wrocław, Poland

³Laboratoire de Chimie, CNRS UMR 5182, Ecole Normale Supérieure de Lyon, Université Lyon 1, 69007 Lyon, France

⁴Ludwik Hirszfeld Institute of Immunology and Experimental Therapy, Polish Academy of Sciences, Rudolfa Weigla 12, 53-114 Wrocław, Poland

⁵LBPA, ENS Cachan, CNRS Université Paris-Saclay, 61 Avenue du Président Wilson, F-94235, Cachan, France

Abstract

Cellular events are mediated by complex processes involving networks of communicating bio-entities well-organized under precise temporally and spatially distributions. For instance, certain proteins may exert different functions in diverse biological *loci* depending on the particular growth stage of the cell. The spatiotemporal control of a biomolecule's pathway is lost when its activities are divided into components making this complexity difficult to reconstitute *in vitro*. Genetic approaches operating *in vivo* as "gene knockout(s)" often lack of temporal precision, since they irreversible interfere with the expression of biomolecules. Conversely, either optical probes or light-activated small molecules offer dynamic, reversible and tunable control of biomolecular functions in a time-scale comparable to that which occurs naturally. Hence, the use of molecules that upon binding to a specific target undergo intrinsic physicochemical changes detectable in real-time constitute an ideal mean to direct and manipulate a wide range of bio-events. In this context, two-photon fluorescent dyes and bistable molecular photoswitches are key components in the ongoing quest toward increasingly sophisticated, selective, sensitive, and versatile biological procedures. We outlines the properties of newly synthesized photonic materials and discuss their compatibility to biological systems in terms of structure-activity relationship (SAR). These results provide breakthroughs in the conception of innovative and smart composite vehicles, which may be potentially useful for future biological and/or photonic applications.



The effect of spatial confinement on the two-photon absorption process

M. Chołuj

*Department of Physical and Quantum Chemistry, Wrocław University of Science and Technology,
Wybrzeże Wyspiańskiego 27, PL-50370, Wrocław, Poland*

Abstract

The molecular systems under spatial confinement have been a topic of extensive research in the past few decades. The classic examples of this phenomenon are the inclusion compounds, artificial atoms and matter under high pressure. It is well established that the physical and chemical properties of the spatially limited atoms and molecules can differ significantly from those in the free space [1-4]. Therefore, such systems can contribute to development of various fields of science, including spectroscopy, photonics, nanotechnology, crystallography, astrophysics, etc.

In this study, we analyze the influence of spatial confinement on the two-photon absorption process. In doing so we consider the values of second-order transition moment. The external spatial confinement is assumed in the form of cylindrically symmetric harmonic oscillator potential, which mimics a nanotube-like confining cages [5].

References

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Photocatalytic activity of electrochemically synthesized Co doped polyaniline films

B. Haspulat, H. Kamış

Department of Chemical Engineering, Selçuk University, Konya, Turkey

Abstract

Organic dyes used in textile and food industries are their important sources of the environmental contaminations due to their non-bio degradability and high toxicity to aquatic creatures and carcinogenic effects on humans [1]. In order to reduce damage caused by organic dye pollution to environment and humans, the use of photocatalyst to degrade organic compounds in contaminated air or water or to convert them into harmless chemicals has been extensively studied. In this manner conductive polymers such as polyaniline(PANI) [1], polypyrrole [2], poly(3-hexylthiophene) [3] has been extensively used to degrade non-biodegradable organic dyes by photocatalytical routes.

In this study, PANI and Co doped PANI(PANI/Co) synthesized by using electrochemical cyclic voltammetry method on stainless steel(SS). The morphology and spectral analysis were investigated by scanning electron microscopy (SEM), FTIR spectra (FT-IR), UV–vis spectroscopy (UV–vis) analysis. The electrical conductivity of PANI/Co catalyst were measured on surface of ITO coated glass substrate by using four-point probe method. The electrochemical measurements were done by using cyclic voltammetry and electrochemical impedance spectra (EIS) in three electrode cell. The photocatalytic activity of PANI and PANI/Co films were investigated under UV and visible light irradiation by decolorization of methylene blue and rhodamine B dyes.

Acknowledgments

The authors are grateful for financial support by The Scientific and Technical Research Council of Turkey (Project no: 113Z656), Environmental Protection Foundation of Turkey and The Administrative Units of The Research Projects of Selçuk University (Project no: 16101013). This work produced from B. Haspulat's Ph.D. Thesis.

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Hybrid nanoparticles for simultaneous and sequential two photon induced luminescence

M. A. Antoniak, D. Wawrzyńczyk, J. K. Zaręba, M. Samoć, M. Nyk

*Advanced Materials Engineering and Modelling Group, Wrocław University of Science and Technology,
Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland*

Abstract

Lanthanide doped nanocrystals have recently gained interest, because of their ability to convert low-energy near-infrared radiation to high-energy visible light. Simultaneously, colloidal quantum dots are interesting candidates for bioimaging because of large one- and two-photon absorption cross-sections. However, in order to enhanced their optical properties and widen possible applications, promising approaches are given by the synthesis of hybrid nanoparticles. They can combine the features of those two (or even more) kind of nanocrystals into a single architecture.

This is why, we adapted and modified the synthesis proposed by Yan et al. [1], and successfully obtained nanostructures consisting of CdSe quantum dots conjugated to NaYF₄:Yb³⁺,Er³⁺ nanocrystals. Our material incorporates semiconducting and up-converting properties to the one nanoheterostructure. To connect these two different nanocrystals we have used disparate ligands: for CdSe it was oleylamine and for NaYF₄, it was oleic acid. Combining of different nanocrystals was caused by electrostatic discharge between charged particles.

Nonlinear optical properties of CdSe/NaYF₄:Yb³⁺,Er³⁺ were investigated with the two-photon excited emission method using a femtosecond laser system tunable in the range from 925 nm to 1350 nm. This technique was used for determination of values of the two-photon absorption cross sections σ_2 , as we reported previously [2]. The σ_2 values were calculated based on comparison of the fluorescence signals, obtained upon two-photon excitation, of meso-tetraphenylporphyrin in CCl₄ and CdSe/NaYF₄:Yb³⁺,Er³⁺ dispersed in chloroform. Those multifunctional nanostructures can combine high two-photon absorption cross-sections with intense up-conversion emission. The total two-photon cross section of a single hybrid nanoparticle was determined to be about 190×10^6 GM at 1150 nm. The unique optical properties of CdSe/NaYF₄:Yb³⁺,Er³⁺ could be potentially useful as nonlinear optical labels.

References

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Tuesday
25.04.2017

Detection of *p*-nitrophenol by modified QCM sensor with bromopropyl functionalized calix[4]arene

M. Tabakci, F. Temel, E. Ozcelik, M. Akpınar, I. Senkul

Chemical Engineering Department, Selçuk University, Konya, 42075, Turkey

Abstract

Arising of new products and services increases gradually due to many developing in industry. This advancement causes not only producing useful technology but also more usage of chemical. Most of chemical contamination originated organic compounds plays important role with respect to environmental healthy [1]. For this reason, concentration of contaminated chemicals are limited with legal obligations. In organic pollutants, phenolic compounds constitute the 11th of the 126 chemicals, which have been designated as priority pollutants [2]. Among phenolic species, *p*-nitrophenol is widely used in pharmaceuticals, petrochemicals, and other chemical

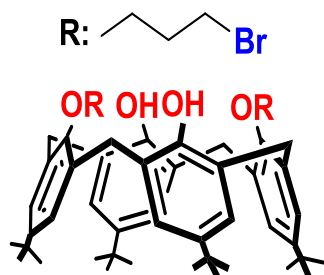


Fig. 1. Bromopropyl Calix[4]arene Derivative

manufacturing processes. Removal organic contaminations such as phenolic hydrocarbons in industrial wastewater is considerable difficult process. For this purpose, many treatment technologies such as chemical oxidation, solvent extraction and adsorption were performed. Adsorption properties of organic contaminations can be monitored and controlled by sensor technologies such as QCM (Quartz Crystal Microbalance) technique. QCM technique is defined as response according to mass change on quartz crystal. QCM compose of a piezoelectric quartz crystal which has sensitive and selective coating that serves as adsorption surface. Developments in sensor

technology has led up the preparing of new synthetic adsorbent materials such as calix[n]arenes (especially, n= 4, 6 and 8). Calix[n]arenes are cyclic oligomer consist of phenol units and are very well known as attractive excellent ionophores because they provide a unique three-dimensional structure with almost unlimited derivatization possibilities [3]. In this study, it was prepared bromopropyl functionalized calix[4]arene (Fig. 1) to use as coating material in QCM system. Thus, it was obtained a calixarene-modified QCM sensor, and then it was used for the detection of *p*-nitrophenol in aqueous solution.

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Epoxy composites including fly ash: mechanical, water sorption, adhesion, corrosion and thermal properties

G. Guzel Kaya, E. Yilmaz, H. Tutar Demir, H. Deveci

*Department of Chemical Engineering, Faculty of Engineering,
University of Selcuk, Campus, 42031 Konya, Turkey, hdeveci@selcuk.edu.tr*

Abstract

Polymer composite materials are one of the emerging fields in composite science that have attracted researchers in the academic and industrial areas. Polymer composites have many application areas such as buildings, automotive, aerospace, and packing industries [1]. Traditional polymers are filled with organic or inorganic oxide powders to enhance the mechanical, electrical, thermal and rheological properties. Epoxy resins have gained an important place among polymeric materials for many environmental applications due to their excellent chemical and heat resistance, high strength and modulus and good adhesion to various substrates. Industrial wastes such as red mud, cordierite and fly ash are one of the most appropriate and low-cost materials as a filler. Fly ash, a waste by-product of coal combustion in thermal power plants, generates in large amounts poses disposal problems [2]. Fly ash depending on source of coal consists of silica, alumina, iron, calcium, magnesium oxides with trace amount of elements [3]. This study focused on the physico-mechanical and thermal properties of the epoxy composites filled with fly ash. Composite materials including epoxy resin (NPEF 170) as matrix, fly ash and modified fly ash with tetramethylammonium chloride (TMAC) as fillers, polyethylene glycol (PEG) as plasticizer and Epamine PC 17 as curing agent were prepared. Mechanical, thermal analysis, hardness, adhesion, corrosion and water sorption tests were carried out to determine the properties of composite materials. The results of all analyses and tests were compared with neat epoxy.

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Wednesday
26.04.2017

Invited lecture

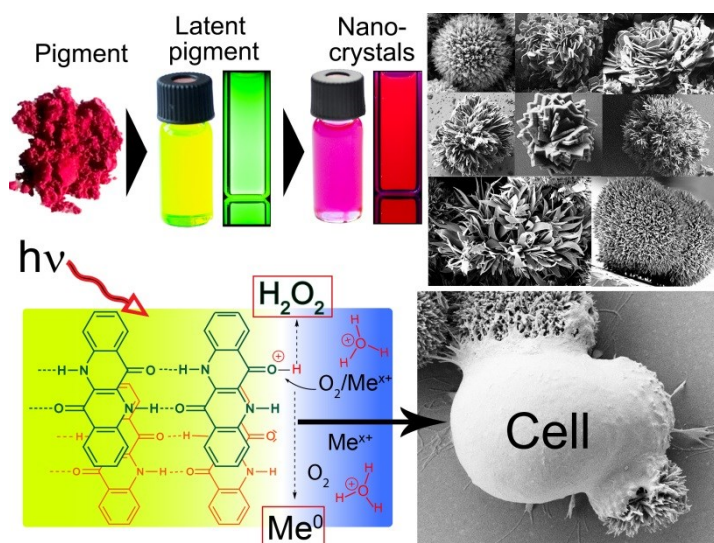
Hydrogen-bonded organic semiconductors – from optoelectronics to bioelectronics

E. D. Glowacki

Laboratory of Organic Electronics, Linköping University, Sweden

Abstract

Organic pigments have been ubiquitous throughout history and are widely produced today industrially as colorants in everyday products as various as cosmetics and printing inks. Largely regarded by chemists as “yesterday’s research” there are many attractive properties of these materials that should be rediscovered in the context of modern technologies. I will cover what are some critical features of these materials and what they have to offer to semiconductor-based devices, especially in the context of applying semiconductors at the interface of biology. I will discuss methods to transform commercial pigments into nano and micro-structured semiconducting crystals, and will highlight two emerging applications: catalysis and cellular interfacing.



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Spectrally-resolved third-harmonic generation in cobalt(II) tetraphenylmethane-based coordination polymer

J. K. Zaręba¹, J. Janczak², M. Nyk¹, M. Samoć¹

¹*Advanced Materials Engineering and Modelling Group, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland*

²*Institute of Low Temperatures and Structure Research, Polish Academy of Sciences, 2 Okólna St., P.O.Box 1410, 50-950 Wrocław, Poland*

Abstract

Metal-organic frameworks (MOFs) and coordination polymers (CPs) are classes of materials which are obtained by reaction of polytopic organic ligands with metal ions. The most important feature of those materials is precisely defined crystal structure (in which coordination bonds can extend in one, two or three dimensions), in contrast to most of organic polymers, which are usually non or only partially crystalline. Large number of possible ligands and wide choice of binding metal ions gives the possibility for the synthesis of various materials with “preprogrammed” magnetic and optical properties.

Our group has recently become interested in nonlinear optical (NLO) properties of such systems, since interplay of energy levels of organic molecules with those of metal ions can elicit not only intense metal-to-ligand or ligand-to-metal charge-transfer bands (MLCT and LMCT, respectively) but can also possibly enhance NLO properties through, for example, electron pushing or withdrawing effect. A more detailed discussion of various contributing phenomena can be found elsewhere soon. [1]

Until recently, characterization of NLO phenomena in those materials has been limited mostly to single-wavelength second-harmonic generation (SHG) studies. Thus, we have provided the proof of concept of spectrally-resolved SHG (SR-SHG) powder tests on polycrystalline cobalt(II) CPs as a method that provides more information than that available from single-wavelength measurements.[2] With this method, we were able to reveal distinct maxima and minima in SHG action spectra, in particular when a CP of interest possesses absorption bands in the Vis-NIR region. We have also demonstrated that comparative analysis of solid state absorption spectra with SHG action spectra can explain, at which wavelengths the SHG response is suppressed, due to material’s absorption of fundamental or harmonic radiation.

In this communication we will report our latest findings on spectrally resolved third-harmonic generation (SR-THG) measurements of a tetraphenylmethane-based CP. With the use of analogous methodology as previous for SR-SHG, we will try to rationalize in detail the observed THG action spectra by absorption effects of either the pumping radiation or its third harmonic. The report is supplemented with structural and physico-chemical analysis of properties of the obtained CP.

We acknowledge financial support from the Polish National Science Centre under “Maestro” DEC-2013/10/A/ST4/00114 grant and the Faculty of Chemistry, Wrocław University of Science and Technology.

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Surface charge minimization in AgInS₂ quantum dots – DFT calculations

A. Olejniczak, B. Cichy, W. Stręk

Department of Spectroscopy of Excited States, Division of Optical Spectroscopy, Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Okólna 2, 50-422 Wrocław, Poland

Abstract

Over the last years ternary A^IB^{III}X^{VI}₂ quantum dots (QDs) (where A = Cu, Ag; B = Al, In, Ga; X = S, Se) have been found as a promising candidates for cadmium-free, red-shifted bio-probes [1]. Especially AgInS₂ (AIS) QDs have found significant attention due to their reduced toxicity (compared to e.g. CdSe QDs), relatively high quantum yield (ca. 22%) and long fluorescence lifetimes (ca. 100 ns) being very useful for the fluorescence lifetime imaging measurements [2]. Although, number of interesting applications of the QDs have already been reported [1,2], accurate description of complex kinetics of excited states relaxation in such systems is still far from understanding [2,3].

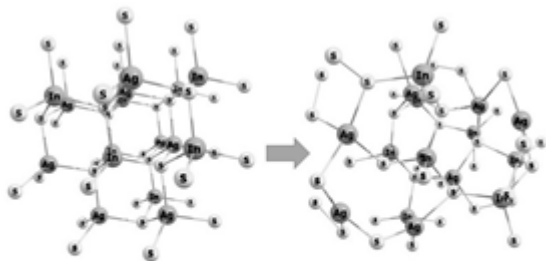


Fig. 1. Surface charge state minimization in pristine AgInS₂ cluster after structural optimization.

We present the results of density functional theory (DFT) calculations of several pristine and Zn-doped AIS clusters. We show the structural reconstruction, formation of surface defect states and the absorption spectra of AIS clusters as well as the influence of Zn ions.

Our results show an essential influence of the surface and surface defects on the mechanisms of relaxation of fundamental excitations. Accurate knowledge about processes of relaxation of fundamental excitations in QDs will contribute to

their more effective control and to the limitation of unfavourable nonradiative processes.

Acknowledgements: Numerical computations performed in this work were supported by PL-Grid Infrastructure.

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Nonlinear absorption of Sn-doped $\text{Bi}_2\text{Te}_2\text{Se}$ and its application to pulsed fiber lasers

M. Kowalczyk

Laser & Fiber Electronics Group, Faculty of Electronics, Wrocław University of Science and Technology, Wybrzeże S. Wyspiańskiego 27, 50-370 Wrocław, Poland

Abstract

Due to their nonlinear optical properties, saturable absorbers based on low-dimensional nanomaterials have been extensively developed for pulse generation in lasers operating in infrared range. Here we demonstrate a novel material, $\text{Bi}_2\text{Te}_2\text{Se}:\text{Sn}$, which can be used as an universal saturable absorber for various spectral regimes. The material was mechanically exfoliated from a bulk crystal and attached to the surface of the side-polished fiber. Optical properties of the fabricated device have been characterized and it has been subsequently employed in ytterbium- and erbium-doped all-fiber resonators. This enabled us to obtain pulse generation in passively Q-switched regime at 1 μm and 1.56 μm . The oscillators emitted stable, linearly polarized radiation with the single pulse energy as high as 343 nJ.

This work was supported by the National Science Centre (NCN, Poland, grant no. 2014/13/B/ST7/01699) and by the Faculty of Electronics, Wrocław University of Science and Technology (grant no. 0402/0190/16).

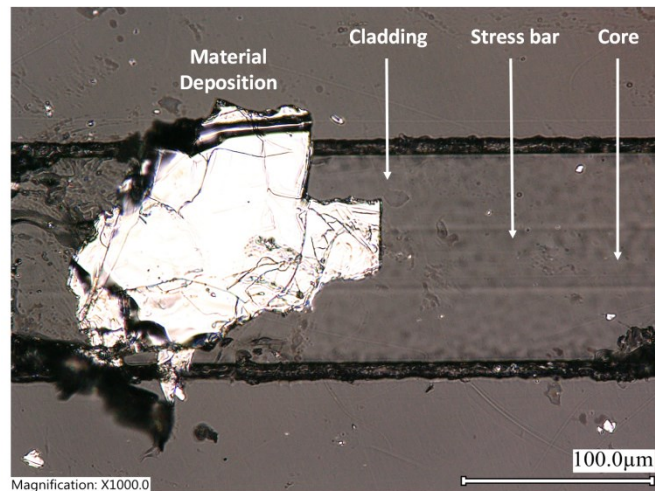


Fig. 1. Microscope image of Sn-doped $\text{Bi}_2\text{Te}_2\text{Se}$ deposited onto a 1.56 μm side-polished fiber.



Invited lecture

Where radiation meets soft matter: revealing the packing and phase composition of heterogeneous polymer systems for application in electronics

A. Kiersnowski

Faculty of Chemistry, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego, Wrocław, 50-370 Poland

Heterogeneity is an inherent property of numerous complex organic materials such as semicrystalline polymers, blends or composites. Depending on its nature, heterogeneity can have a different meaning indicating, for instance a certain nanostructure or, in the case of crystalline materials, occurrence of crystals differing in morphological features such as sizes or intrinsic topologies. The most usual approach to study structure and morphology of heterogeneous materials involves application of microscopic imaging that has the power to provide direct information about the analyzed systems. Despite doubtless advantages, microscopy is inappropriate when solving quantitative problems of, for instance, crystal imperfections, polymorphism or crystallinity degree. Because of the limited volume probed in a single analysis, information acquired with use of a microscope has also limited value in terms of statistical representation. From this point of view, spectroscopic or scattering techniques can be considered a negative of microscopy: the structural information is provided indirectly while the volume probed in the analysis is large enough to consider the experimental results representative at the macroscopic scale.^{1,2}

Here, the application of X-ray scattering techniques and nuclear magnetic and infrared spectroscopy is discussed with respect to interesting classes of materials: semiconducting (such as poly(alkylthiophenes) – P3ATs) and piezoelectric (as e.g. poly(vinylidene fluoride) – PVDF) polymers as well as their blends and nanocomposites. The contribution is aimed at showcasing the way to determine the parameters having crucial influence on electronic performance of the materials: crystallinity, crystal polymorphism, as well as structural coherence of crystals and their orientational structure in bulk and thin films.³⁻⁵

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Theoretical modeling of the two-photon properties of difluoroborate compounds

J. Bednarska

Department of Physical and Quantum Chemistry, Wrocław University of Science and Technology, Wyb. Wyspiańskiego 27, PL-50370, Wrocław, Poland

Abstract

Over the past decades we have witnessed a growing interest in the molecular design and the synthesis of two-photon probes with an eye towards the applications in bioimaging. Among the plethora of potential candidates characterized by the high values of fluorescence quantum yield

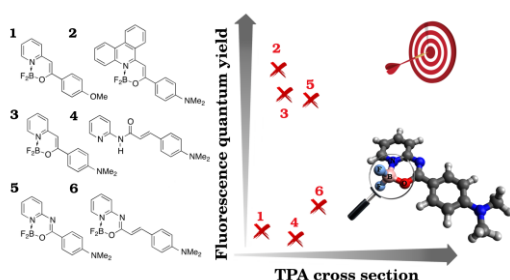


Fig. 1 The structures of investigated difluoroborate compounds (left), the scheme demonstrating a relation between experimental values of ϕ and σ_2 (right)

(ϕ), absorption/emission wavelengths at biological transparency window, photostability and biocompatibility a much smaller subset was successfully used in the two-photon microscopy due to the insufficient values of two-photon absorption cross section (σ_2). The maximization of two-photon absorption cross section can be accomplished by, e.g. the elongation of π -conjugated pathway or by including the strong electron-accepting/-donating moieties, however, it does not always coincide with the growth of fluorescence quantum yield [1]. Thus,

the insight into the design strategies for different molecular systems by using the experimental and theoretical methods is of pivotal importance. In this work, we perform the theoretical analysis of two-photon activity for the set of difluoroborate compounds (depicted in Fig. 1), which have been recently of high interest [2]. The structure-property relation has been examined in detail by employing systematic structural modifications and unravelled with the aid of quantum-chemical calculations combined with a few-state model [3].

Acknowledgements

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Colloidal two-dimensional heterostructures

H. Woźnica, M. Bański, A. Podhorodecki

Department of Experimental Physics, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland

Abstract

Wet chemistry methods of nanomaterials synthesis allow to obtain nanocrystals of different sizes and shapes, ranging from quantum dots (QDs) and rods (QRs) to two-dimensional nanostructures such as nanosheets and nanoplatelets (QPs). The latter exhibit extremely narrow features in terms of photoluminescence with the full width at half maximum reaching several nanometres [1]. This is possible, because the synthesis conditions allow to control the thickness of nanoplates with a monolayer precision. Since it is the thickness that is responsible for quantum confinement in semiconductor nanoplates, they show no inhomogeneous broadening which is present in typical sphere-shaped QDs and which emerges from their size distribution.

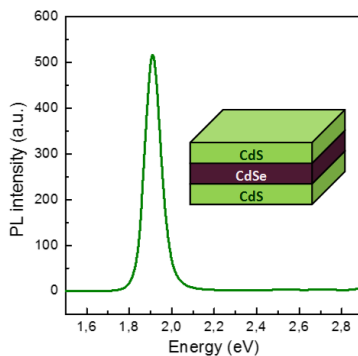


Fig. 1. Photoluminescence spectrum of CdSe-CdS core-shell nanoplatelets.

In our recent work, we focus on developing facile synthesis and optical investigation of multilayer core-shell CdSe-CdS or CdSe-CdZnS nanoplatelets, that are composed of two-dimensional seeds with thickness of a few atomic layers and additional shell layers grown on them. The shell is crucial for applying nanoplatelets in

any device, as it secures the surface and makes further tuning and engineering of the ligands and molecules attached to the nanoparticle possible without any damage to the optical properties.

Acknowledgements

The authors acknowledge the National Science Centre for their financial support within the Sonata 8 project no. UMO-2014/15/D/ST5/02744

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The ASE enhancement in liquid crystals doped with perylene dye

A. Adamów¹, E. Chrzumnicka², T. Martynski², J. Myśliwiec¹

¹ The Advanced Materials Engineering and Modelling Group (W3/K1), Wrocław University of Science and Technology, Wybrzeże Stanisława Wyspiańskiego 27, 50-370 Wrocław, Polska

² Department of Optical Spectroscopy, Faculty of Technical Physics, Poznań University of Technology, Nieszawska 13a, 60-965 Poznań, Polska

Abstract

Recently, a lot of research groups have shown an increased interest in organic materials which have potential in optoelectronic applications [1]. Dyes based on the perylene condensed ring hydrocarbon became very valuable mostly because of their excellent optical properties [2] and they give the opportunity to contribute in the host-guest systems [3]. Basically, in such systems the liquid crystals can serve as matrices for perylene dyes because of the compatibility with these materials [4].

In this work, results of amplified spontaneous emission (ASE) coming from the dye-doped liquid crystal (LC) cell are reported by the excitation of nanosecond pulse laser (Nd:YAG). The hybrid system contained the nematic LC matrix characterized by the negative dielectric anisotropy and luminescent dye based on the perylene, which chemical structure is shown in



Fig. 1. We report on the ASE characteristics in function of different excitation pulse energy densities and electric field applied into the sample. Likewise the photodegradation of investigated material has been set and reported.

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Unravelling the photophysical properties of light-activated compounds, based on azobenzene motif

S. G. Mucha¹, M. Deiana¹, L. M. Mazur¹, Z. Pokladek^{1,2}, K. Matczyszyn¹, M. Samoć¹

¹Advanced Materials Engineering and Modelling Group, Wrocław University of Science and Technology, Wyb. Wyspiańskiego 27, 50-370 Wrocław, Poland

²Department of Bioorganic Chemistry, Wrocław University of Science and Technology, Wyb. Wyspiańskiego 27, 50-370 Wrocław, Poland

Abstract

Azobenzene derivatives may exist in the *trans* and *cis* conformation, which are featured by different symmetry, dipole moment and water affinity. Moreover, the photophysical properties of these light-activated compounds are dependent on the substituent moieties linked with the azo motif.[1,2,3] We synthesized molecular photoswitches coupling azobenzene with two tyrosine

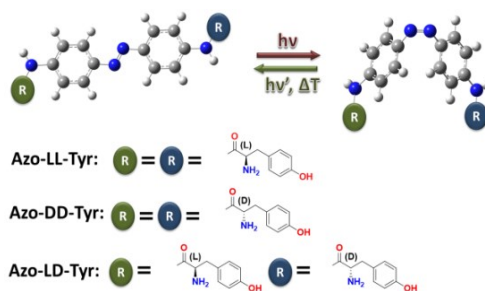


Fig. 1. Structure and isomerization pathway of azobenzene derivatives.

units bearing different spatial configuration. The fluorescence parameters were determined using steady-state and time-resolved fluorescence measurements. The obtained results shown an increase of PLQY and decay life-time when compared to unsubstituted azobenzene. The determined photoluminescence quantum yield and average lifetime were found to be $\Phi_f \approx 0.05\%$ and $\langle \tau \rangle \approx 4.00$ ns, respectively. By exploiting these data we estimated the radiative (k_r) and non-radiative (k_{nr}) kinetic rate constants. These information may be useful in materials science for design new composite systems with improved physicochemical responses.

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Gold nanoparticles enhanced Gram-negative bacteria photoinactivation

K. Popko¹, I. Maliszewska¹, K. Matczyszyn² O. Rac-Rumijowska³

¹*Division of Medicinal Chemistry and Microbiology, Faculty of Chemistry, Wrocław University of Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland*

²*Advanced Materials Engineering and Modelling Group, Faculty of Chemistry, Wrocław University of Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland*

³*Department of Microsystems and Photonics, Faculty of Microsystem Electronics and Photonics, Wrocław University of Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland*

Abstract

It goes without saying, that antibiotic resistance is recently a rising problem in healthcare systems. Therefore, prospecting for innovative methods of bacteria inactivation are on track. In this paper, evaluation of the two collective Gram-negative bacteria strains' (*P. aeruginosa* ATCC10145 and *E. coli* PCM2057) efficient photoinactivation has been made. Bacteria cells were treated by Methylene Blue (MB) photosensitizer (approved for clinical use in the European Union) with the absorption band ranging between 550 and 700 nm [1]. In the next step they were irradiated by OLED (532nm). Many sources suggest that gold nanoparticles (Au-NPs) combined with photosensitizers can enhance photodynamic antimicrobial photo-therapy [2,3]. Therefore, the influence of Au-NPs on photoinactivation process was also investigated. Au-NPs combined with MB impact on the cells, revealed their high destructive potential. The duration of light exposure for each sample was equal to 5 and 15 minutes. Obtained mortality rates for both investigated strains were above 99% when 10mW light power was applied.

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General approach for thiol-capped CdS over coated semiconductor quantum dots

A. Lesiak^{1,2}, M. Chrzanowski², M. Bański², J. Cabaj¹, A. Podhorodecki²

¹Department of Medicinal Chemistry and Microbiology,

Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław

²Department of Experimental Physics, Wrocław University of Science and Technology,
Wybrzeże Wyspiańskiego 27, 50-370 Wrocław

Abstract

Semiconducting quantum dots (QDs) are inorganic fluorophores, which have the potential to revolutionize biological imaging¹⁻⁴. This is mainly due to a presence of quantum confinement effect in this type of material. In consequence of this effect, QDs demonstrate an unique optical properties, such as sharp and tunable emission spectra, high emission quantum yield, and broad absorption band. Moreover, they also indicate no photobleaching and recently no emission blinking either⁵.

However, due to organometallic synthesis of QDs, where the hydrophobic surfactants are used to stabilize the QDs, the QDs are initially soluble in non-polar media⁶. Thus, from the bio-application point of view⁷ it is crucial to achieve the hydrophilic surface with bio-compatible chemical groups.

Ligand exchange is one of method to achieve this goal⁸. Especially, when used sulfur contain compounds. Moreover, thiol forms an important class of capping molecules⁹.

In the present study, we described functionalization of semiconductor CdS- and PbS-based nanocrystals by two different ligands: 3-mercaptopropionic acid and d-penicillamine (Fig.1). We had successfully produced disperse in water QDs with a good stability in a wide range of pH and time.

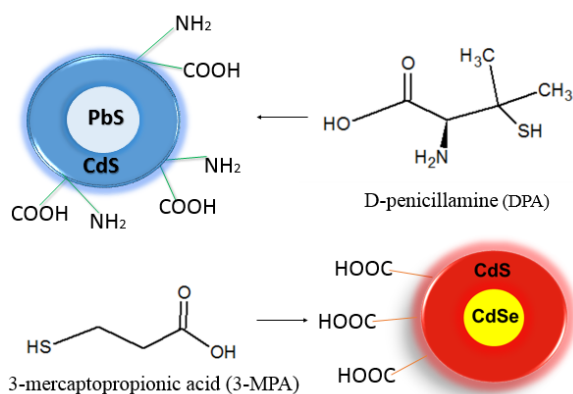


Fig. 1 Functionalization of QDs by thiol containing ligands

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V. Posters
Tuesday
15.30-17.30





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P1

DNA liquid crystals doped with AuAg nanoclusters

K. Brach, M. Waszkielewicz, J. Olesiak-Bańska, M. Samoć, K. Matczyszyn

Advanced Materials Engineering and Modelling Group, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50-370, Wrocław, Poland

Abstract

The topic of nanoparticles dispersions in liquid crystals (LCs) has been gaining considerable attention in recent years. Combining unique optical properties of nanoparticles with self-assembly and mobility of LCs may result in creation of new metamaterials.

The aim of this work was to investigate the properties of DNA lyotropic LCs doped with silver-doped gold nanoclusters (AuAgNCs). We applied UV-Vis and fluorescence spectroscopy, transmission electron microscopy and multiphoton excitation spectroscopy to characterize AuAgNCs. The LCs were investigated using polarized light, one- and multiphoton fluorescence microscopy. We show that AuAgNCs emit luminescence and second-harmonic generation under two-photon excitation. Additionally, we observed specific aggregation of nanoparticles correlated with the position of wall defects of undulated phase [1]. Detailed results of this study will be presented and discussed and compared with our previous results on bigger plasmonic nanoparticles [2, 3].

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P2

Ascorbic acid detection in aqueous solution by calix[4]arene modified QCM sensor

M. Akpınar, N. Yuksel, F. Temel, M. Inkaya, M. Tabakci

Chemical Engineering Department, Selçuk University, Konya, 42075, Turkey

Abstract

Vitamins are unheeded substances in the formation of certain chemical structures such as foodstuffs, vegetables and animal tissues. It is necessary for people and animals to grow and to lead them for a healthy life [1]. Ascorbic acid, one of the vitamins, as well as vitamin C in recent years has been newly understood its importance in the treatment of wounds, in the main care formations of the cartilage, in the bones, teeth, gums, muscles and skin [2]. For these reasons, detection of ascorbic acid has become an significant issue. Detection of substances which are biological importance are performed biosensors. In biosensor application, there are several methods which are electrochemical, calorimetric, optical and acoustic systems for sensing and interaction between bioanalyte and sensing material. Among them, Quartz Crystal Microbalance (QCM) is an acoustic microsensors which is simple, cost-effective, mass sensing device [3].

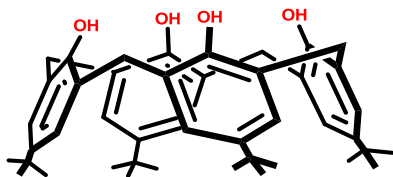


Fig. 1. Parent calix[4]arene derivative

QCM is a technique that converts the mass change on the basis of the analyte concentration to an electrical signal. There are limited studies about macromolecules even though there are many studies about polymeric materials as sensor molecules in sensor studies. One of these macromolecules, calixarenes, that can be widely used in different application fields with its unlimited derivatization, three-dimensional structure. In this study, parent calix[4]arene derivative was used as a sensing

surface of QCM system for detection of an ascorbic acid in aqueous media [4].

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P3

Newly synthesized gold nanoclusters in biological application

J. Sobska¹, M. Waszkielewicz¹, A. Podlesny², J. Olesiak-Bańska¹, M. Samoć¹,
W. Krezel², K. Matczyszyn¹

¹*Advanced Materials Engineering and Modelling Group, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland*

²*Institut de Génétique et de Biologie Moléculaire et Cellulaire, 1 Rue Laurent Fries, 67400 Illkirch-Graffenstaden, France*

Abstract

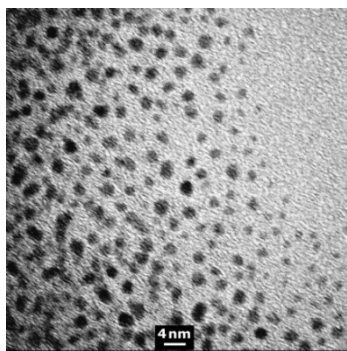


Figure 1. TEM image of the gold nanoclusters.

Nanoclusters are the nanostructures of the size around 1-2 nm, combining the properties of nanoparticles and the fluorescent molecules. Their use in nanomedicine increases due to their unique optical properties such as e.g. fluorescence and high photostability meaning that light exposure does not result in unacceptable changes of the material [1][2]. As will be presented by us those nanoparticles are suitable for applications in biology due to the low cytotoxicity and biocompatibility which allow their use without immunological rejection. Tissue imaging, the control of cancer cells, or as drug carriers are some of the examples of applications this kind of nanoparticles [1]. Interaction of neuron cell lines P19 were investigated with the use of nanoclusters of gold (Fig. 1), which have fluorescent properties. The effect of nanoparticles on cell

differentiation was measured and their effect on the innate and adaptive immune response also was characterized.

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P4

Pulsed-photoinduced optical birefringence in selected derivatives of pyrazoline

A. Popczyk, A. Szukalski, J. Myśliwiec

*Advanced Materials Engineering and Modelling Group, Wrocław University of Science and Technology,
Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland*

Abstract

Derivatives of pyrazoline are very promising organic materials for advanced technologies, especially in various photonics applications. These compounds show both unique luminescent as well as nonlinear optical properties. It has been proved that pyrazoline derivatives exhibit stimulated emission (SE), distributed feedback lasing (DFB) and random lasing (RL) phenomena. Moreover mentioned compounds characterize efficient second and third harmonic generation, but also ability of dynamic refractive index changes.[1] The chosen compounds are typical representatives of push-pull type structures with the same donor group and different acceptor group.

Here we show the experimental results of ultra-fast (in the range of microseconds) and fully reversible and efficient photoinduced birefringence changes in host/guest systems of the selected derivatives of pyrazoline embedded into PMMA matrix, measured with the optical Kerr effect experimental setup. This phenomenon allows to observe Δn dynamic modulation (changes of the refractive index) due to *trans-cis-trans* photoisomerisation and molecular reorientation process under illumination of polarized pulsed laser beam.

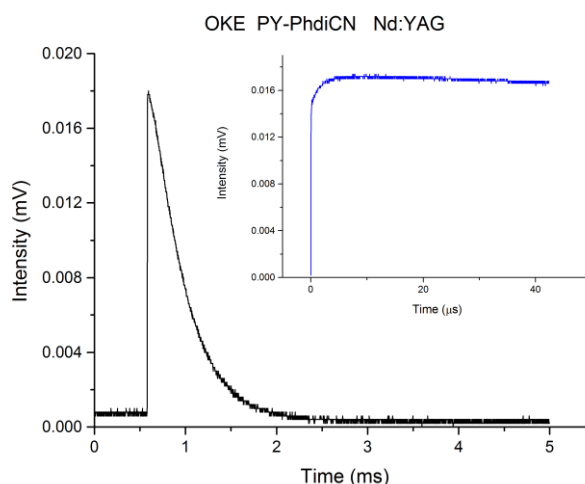


Figure 2. Dynamic photoinduced birefringence- single signal and grow (in magnification; inset).

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P5

Highly selective detection of zinc ions by fluorescein-benzothiazole based fluorescent sensor

B. Tabakci, S. Erdemir

Chemistry Department, Selçuk University, Konya, 42075, Turkey

Abstract

As the second most abundant metal ion, zinc is actively involved in diverse biological activities, such as structural and catalytic cofactors, neural signal transmitters or modulators, regulators of gene expression and apoptosis [1]. Any disruption in the bio-availability of zinc in the mammalian system may cause serious diseases such as Alzheimer's, Parkinson's, immune deficiency, growth retardation etc., while excess accumulation of zinc in human body owing to environment pollution may lead to health hazards and therefore its accurate and sensitive detection is an intense area of research [2]. Considerable attention has been devoted to the development of fluorescent chemosensors for Zn^{2+} detection, because fluorescence techniques can offer distinct advantages such as low cost, simplicity, good sensitivity, and capability of real-time detection [3]. Also, although a large number of Zn^{2+} selective fluorescent sensors have been well established, many reported Zn^{2+} sensors still encountered a difficulty in distinguishing Zn^{2+} from Cd^{2+} [4], because Cd^{2+} is in the same group in the periodic table with Zn^{2+} and usually induces a



Fig. 1. The proposed mechanism for Zn^{2+} detection by FB

comparable fluorescent response to that of Zn^{2+} . Therefore, development of novel molecular fluorescent sensors that can clearly distinguish Zn^{2+} from Cd^{2+} is still challenging and imperative. Thus, in this study, an efficient fluorescent sensor based on fluorescein-benzothiazole (FB) for Zn^{2+} ion was synthesized and characterized systematically. FB exhibited selective and sensitive recognition toward Zn^{2+} in MeCN- H_2O ($v/v = 2/1$) over other cations via FRET, which was mainly due to the spirolactam ring-opening power of Zn^{2+} .

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P6

Structure and morphology of the blends of hexyl-substituted perylene diimide with poly(3-hexylthiophene)

D. Chlebosz¹, W. Goldman¹, M. Mezger², G. Glaßer², A. Kiersnowski¹

¹Faculty of Chemistry, Wrocław University of Science and Technology, Wrocław, Poland

²Max Planck Institute for Polymer Research, Mainz, Germany

One of the key factors governing self-assembly and crystallization of molecules and macromolecules bearing alkyl and aromatic moieties is the architecture of alkyl substituents and π -interactions between aromatic parts^{1,2}. It was already demonstrated that interactions between alkyl chains of N-substituted aromatic diimide derivatives (ADI) and poly(3-hexylthiophene) P3HT may drive formation of different crystalline structures in P3HT:ADI blends^{3,4}. In this work we discuss how the precipitation order and sequential crystallization controls the crystalline morphology of the blends.

The study was focused on the blends of *N,N'*-dihexyl-3,4,9,10-perylenedicarboximide (PDInC6) with P3HT. Crystal structure and morphology of the blends were studied by, respectively, X-ray diffraction and electron microscopy. In order to gain insight into phase transitions we used differential scanning calorimetry. Results of our experiments indicate that phase transition temperatures as well as packing of molecules in different crystalline phases and mesophases, were found related to compositions of the blends. As revealed by means of scanning electron microscopy, the blend composition also exerted an influence on the crystal morphology (Fig. 1). For instance: the P3HT:PDInC6 (5:1) blend formed relatively uniform films with granular morphology while in the (1:1) blend we observed elongated needle-like crystals. We attribute this behavior to inhibition of crystal growth due to limited diffusion rate of small molecules in polymer solutions as well as strong π - π interactions between P3HT and PDInC6.

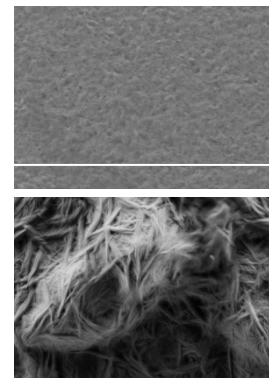


Figure 1. Crystal morphology of P3HT:PDInC6 (5:1) (a) and (1:1) (b) blends

Acknowledgement

This work was supported by National Science Centre, Poland through the grant DEC-2013/08/M/ST5/00914

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P7

Sensing abilities of chiral calixarene coated QCM sensors towards chiral amine derivatives in aqueous solution

E. Ozcelik¹, F. Temel¹, S. Erdemir², B. Tabakci², M. Tabakci¹

¹Chemical Engineering Department, Selçuk University, Konya, 42075, Turkey

²Chemistry Department, Selçuk University, Konya, 42075, Turkey

Abstract

Amines are important compounds and they are used in synthesis pesticides, drugs, polymers, surfactants, cosmetics. These amines, which are used, can cause environmental or soil contamination. For this reason, detection of amines has become an significant issue for the environment [1]. Biosensors are analytical device which can be used for biological sensing of target analytes. There are several methods for biosensor applications which are electrochemical, calorimetric, optical and acoustic systems for sensing and interaction between analyte and sensing element [2]. In these methods, Quartz Crystal Microbalance (QCM) is an sensor device which is simple, easily, low cost. This method has been used for gas and liquid sensing applications [3]. There are limited numbers studies about macromolecules as biochemical sensors even though there are many studies about polymeric materials.

Among macromolecules, calixarenes (n=especially 4, 6, and 8) are such cyclic oligomer consist of phenol units and are very well known as attractive excellent ionophores because they provide a unique three-dimensional structure with almost unlimited derivatization possibilities [4]. In these study, it was prepared some chiral calix[4]arene derivatives (Fig. 1) to use as coating materials in QCM system. Thus, it was obtained new chiral calix[4]arene modified QCM sensors, and then it was investigated their sensing abilities toward some chiral amine derivatives such as R/S-phenylethylamine and R/S-phenylpropylamine in aqueous solution.

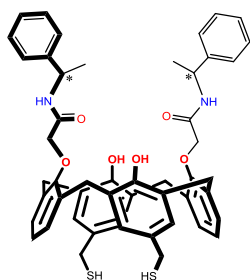


Fig. 1. Chiral calix[4]arene derivatives were used in this study.

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P8

Adsorption of azo dyes from aqueous solutions by calixarene magnetic nanoparticles

E. Akceylan, O. Sahin, B. Tabakci

Department of Chemistry, Selçuk University, Konya, 42075, Turkey

Abstract

Environmental problems have become increasingly critical and frequent, due to population growth and increased industrial activity associated with contamination of natural waters which is one of the major problems of modern society [1]. Chemicals such as dyes and pigments are widely used for coloring in various sectors of industry including textile manufacture, leather tanning, paper production, food technology and cosmetics manufacture.[1,2]

However, some synthetic dyes may be pathogenic if they are consumed in excess. It has also been shown that synthetic precursors, intermediates and degradation products of these dyes could be potential health hazards. Owing to both their toxicity and their carcinogenicity. Because of that reason, in this study, calixarene magnetic nanoparticles [3] have been synthesized (Fig. 1) and investigated their adsorption properties towards azo dyes at different pH values.

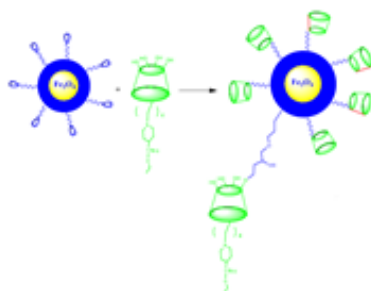


Fig 1. A schematic representation of calixarene magnetic nanoparticles

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P9

Synthesis and spectral properties of fluorine based calix[4]arene

O. Sahin, M. Sahin, E. Akceylan

Department of Chemistry, Selçuk University, Konya, 42075, Turkey

Abstract

Selective signalling of transition metal ions and anions has potential analytical applications in many fields like chemistry, medicine, biology and environment [1]. Among the numerous analytical methods that are available for the detection of cations, flame photometry, atomic absorption spectrometry, ion sensitive electrodes, electron microprobe analysis, neutron activation analysis, etc., are expensive, often require samples of large size and do not allow continuous monitoring [1,2]. Fluorescence spectroscopy is an attractive tool owing to its sensitivity, selectivity, versatility and relatively simple handling [1,2].

Calix[4]arenes are important macrocyclic compounds and also ideal platforms for the development of complexing agents for metal ions [3]. Calixarenes substituted on the upper or lower rim may show selective cation recognition dependent on the cation ligating group. This group, known as the ionophore, may be a crown ether, amide, Schiff base, or other functional group [3]. In this study, fluorogenic fluorene functionalized calix[4]arene were synthesized (Fig. 1). This compound was examined for its fluorescent properties toward different metal ions (Na^+ , Li^+ , Mg^{2+} , Ni^{2+} , Ba^{2+} , Ca^{2+} , Cu^{2+} , Pb^{2+} , Zn^{2+}) by UV, NMR and fluorescence spectroscopy.

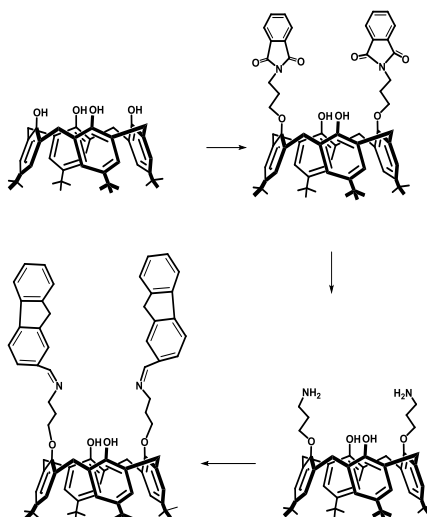


Fig 1. Synthesis of fluorene based calix[4]arene.

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P10

Influence of graphene on the human immune cells in vitro

I. Dudek, Z. Wichrzycka, P. Rzodkiewicz, A. Stangret, M. Skoda, D. Szukiewicz

Department of General & Experimental Pathology with Centre for Preclinical Research and Technology (CEPT), Medical University of Warsaw, ul. Pawińskiego 3C, 02-106 Warsaw, Poland

Abstract

Graphene can be used as an innovative biomedical material in drug delivery and as a scaffold for cells in tissue engineering [1,2,3]. The discovery of the influence of graphene on human immune system cells seems to be the most important thing. These cells are the first line of contact with the nanomaterial and they are responsible for the occurrence of possible adverse reactions to graphene. An understanding of the interaction of nanomaterials with immunological systems is vital for preclinical evaluation as well enabling future rational designs of nanomaterials [2]. We examined if three commercially available graphene nanosheets respectively: flakes 1 (average flake thickness (AFT):5-30nm, specific surface area (SSA):60 m/g²), flakes 2 (AFT:60 nm, SSA:<15 m²/g) and 3 (AFT:8 nm, SSA:100 m²/g),- can caused DNA damage *in vitro* in cultures of isolated human lymphocytes. The cells were treated with 6.25–30 mg/ml of the nanomaterials for 24, 48 and 72 h. The genotoxicity of graphene was conducted by the micronucleus test [4]. The dose-dependent increase in DNA damage and micronuclei was not observed. None of the treatments significantly affected cell count or the mitotic index. Moreover, we examined of impact graphene on activation and morphology of lymphocytes via Lymphocyte Transformation Test. We noticed that only high doses of graphene could enhanced activation and proliferation of lymphocytes as concanvalina A. Moreover, only the flakes 1 could enhanced the lymphocytes proliferation and that 72-h treatment was the most effective. We concluded that graphene is not genotoxicity and the manner of interaction between nanomaterial and lymphocytes is strictly dependent on the concentration of a solution, sheet dimensions and time of incubation.

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P11

Development of low bandgap small molecules and conjugated polymers for efficient organic solar cells

P. Krajczy

*Department of Medicinal Chemistry and Microbiology, Wrocław University of Science and Technology,
Wyb. Wyspiańskiego 27, 50-370 Wrocław, Poland*

Abstract

Recent years, a lot of research considering organic solar cells (OSCs) have been done and this significant increase of attention around OSC is related to their potential for low cost fabrication, tuneable flexibility, lightweight and friendly for environment energy conversion [1]. For this purpose, scientist from around the world try to getting better the interaction between donor – acceptor in bulk – heterojunction (BHJ) architecture, where the main emphasis is on the development of new donor materials. Donor materials usually occur as π – conjugated polymers, consist of heterocyclic building blocks like benzodithiophene, benzotriazole, benzoxadiazole or diketopyrrolopyrrole [2,3]. However, not only polymeric structure could act as the donor material in HBJ blend. The area of small molecule materials, recently has greater impact in construction of highly effective organic photovoltaic devices.

Since the molecular design of organic photovoltaic materials is the main strategic pushes the development of low band gap molecules, there are several others methods improving the power conversion efficiency (PCE) of resulting photovoltaic device [4]. Regarding to the important parameters that good material for OSC purpose has to exhibit, the ideal donor material should have broad range of adsorption matched to the solar spectrum, deep HOMO level, low bandgap and fast hole mobility. The literature studies and subsequent experiment assumes to firstly calculate the energy levels using DFT method and next to obtain new, two-dimension-conjugated molecules that can exceed the PCE of currently synthesised materials.

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P12

Characteristics of spherulites and fibrils obtained from β -lactoglobulin and hen egg white lysozyme

M. Grelich, M. Rzaša, K. Brach, J. Olesiak – Bańska, K. Matczyszyn,
M. Samoć

Advanced Materials Engineering and Modelling Group, Faculty of Chemistry, Wrocław University of Science and Technology, Wyb. Wyspiańskiego 27, 50-370 Wrocław, Poland

Abstract

There is a wide range of proteins which under mildly denaturing conditions, such as low pH and elevated temperatures, undergo misfolding and aggregating into amyloid fibrils. Such structures have been related to some neurodegenerative diseases such as Alzheimer's, Parkinson's or Huntington's disease. *In vitro* they can be formed from several proteins, including β -lactoglobulin (BLG), hen egg white lysozyme (HEWL) and bovine insulin [1].

Amyloid fibrils are ordered aggregates based on a common structural motif - intermolecular β -sheets running along the fibril axis. The fibrils are above a few micrometres in length, with diameters between 5 – 15 nm, relatively stiff and nonbranched [1, 2]. These structures are often found arranged into large spherical aggregates called spherulites. They tend to be from a few to tens of μm in diameter and consist of a central core which is surrounded by radially oriented amyloid fibrils [3].

In this study results concerning fibers and spherulites obtained from BLG and HEWL are presented. The aggregates were investigated using SEM, AFM, optical microscopy, UV-Vis absorption spectroscopy and autofluorescence. These techniques are useful to study structural properties as well as formation of fibers or spherulites [4, 5]. The influence of preparation conditions on the final structure of amyloids was determined and protein autofluorescence was investigated as a marker of protein aggregation.

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P13

Synthesis and optical properties of water soluble CdS tetrapods

M. Chachuła, D. Wawrzyńczyk

Advanced Materials Engineering and Modelling Group, Faculty of Chemistry, Wrocław University of Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland

Abstract

Fluorescent, colloidal semiconducting nanoparticles are interesting candidates for optical bioprobes in imaging and sensing applications. Unfortunately, most commonly used hot injection based synthesis techniques yields hydrophobic nanoparticles, and for any biorelated application further surface functionalization steps are necessary [1].

This is why, we have synthesized CdS semiconducting quantum dots (QDs) directly in water solution by heating under reflux technique [2]. We have used three types of organic stabilizing ligands: L-penicillamine, D-penicillamine and Rac-penicillamine, molecules which additionally showed optical activity. We used transmission electron microscopy imaging to investigate the morphology of the synthesized particles (Fig.1). The obtained CdS QDs had tetrapod-like shapes with sizes 15.40 ± 0.99 nm, 12.70 ± 0.59 nm and 12.96 ± 0.62 nm. We have also investigated spectroscopic properties of obtained CdS tetrapods, what included the measurements of UV-Vis absorbance, fluorescence spectra and luminescence decays. Chiral, water soluble CdS nanotetrapods are expected to have a range of potential applications in bioimaging and sensing chiral drugs due to their unique optical properties [3].

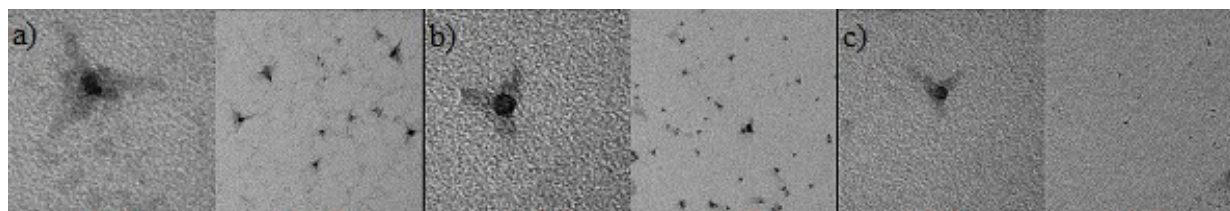


Fig.1. TEM images of a) L-penicillamine, b) D-penicillamine, c) Rac-penicillamine stabilized CdS nanotetrapods.

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P14

Nanomaterials modified by carbon quantum dots for photocatalytic degradation of air pollutant

M. Kobyłański¹, A. Malankowska¹, J. P. Narváez Mejía^{1,2}, A. Zaleska-Medynska¹

¹ Department of Environmental Technology, Faculty of Chemistry, University of Gdansk, 80-308 Gdansk, Poland

² Ingeniería Ambiental, Facultad Ingeniería Civil Ambiental, Escuela Politécnica Nacional, Ecuador

Abstract

Carbon quantum dots (C QDs) are very interesting materials, which have an ability to convert visible or near-infrared light to UV region [1]. Consequently nanomaterials modified by C QDs could be active under visible light. Titanium dioxide nanostructures are promising materials, utilized in application related with photocatalytic degradation pollutant present in the gaseous phase. However the bad gap of titanium dioxide is about 3,2 eV and this material could be utilize only under UV light. The photocatalytic properties of nanostructures could enhance when the semiconductor's surface will be modified by C QDs and make it possible for materials based on titanium dioxide to be active under visible light[2].

The aim of this work was synthesis of titanium dioxide spheres modified by C QDs and investigation of the photocatalytic activity during photodegradation of toluene as model pollutant.

The light sources were LED diods emitting irradiation $\lambda > 375$ nm, 415 nm and 465 nm. The characterization of materials includes photoluminescence properties, FTIR, UV-Vis spectra and SEM images of obtained nanostructures.

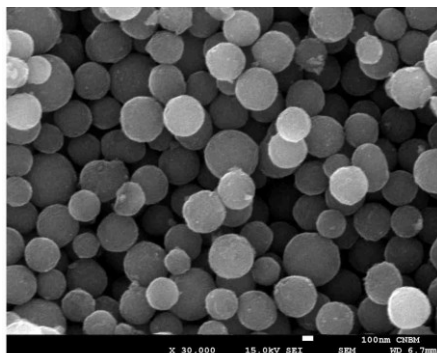


Fig. 1. SEM image of TiO₂ spheres

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Acknowledgments

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P15

The influence of homogenization process on lasing performance in polymer-nematic liquid crystal emulsions

M. Lipka, A. Adamów, L. Sznitko, J. Myśliwiec

Advanced Materials Engineering and Modelling Group, Faculty of Chemistry, Wrocław University of Science and Technology, Wyb. Wyspiańskiego 27, 50-370 Wrocław, Poland

Abstract

Here we report on the results of studies of amplified spontaneous emission in polymer-liquid crystal emulsions based on mixtures of poly(vinyl alcohol) and 5CB nematic liquid crystal doped with three luminescent dyes: DCM, Coumarin 504 and Coumarin 540. The mixture of dyes was used in order to extend the range of stimulated emission spectra. We have investigated the emission properties of four samples with different size and distribution of liquid crystal micro droplets, controlled by the length of time exposure on ultrasounds during the homogenization process. We have designated the threshold conditions for stimulated emission occurrence and compared the emission spectra obtained below as well as above threshold conditions. Additionally the emission spectra were transformed to the chromaticity diagram CIE XYZ 1931 in order to visualize the broadening of stimulated emission spectra of studied emulsions.

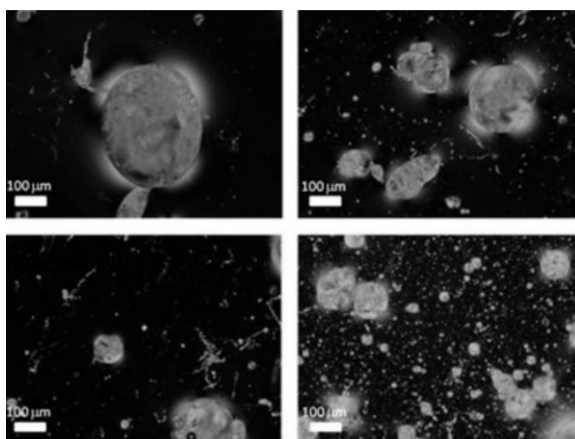


Fig. 1. LC domains micrographs of investigated emulsions

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P16

Liquid crystal in biological systems

M. Piksa, K. Brach, J. Olesiak-Bañska, K. Matczyszyn

Advanced Materials Engineering and Modelling Group, Faculty of Chemistry, Wrocław University of Technology, Wyb. Wyspiańskiego 27, 50-370 Wrocław, Poland

Abstract

In the late 1940s the discovery of the hydration of duplex DNA resulting in formation of DNA liquid crystal (LC) phases has been announced. This research caused interest of researchers who characterized solutions of duplex B-form DNA by optical, x-ray and magnetic resonance methods. Numerous studies of long DNA have revealed formation of an isotropic phase, chiral nematic, uniaxial columnar and higher-ordered columnar liquid crystal phases and crystal phases [1].

Isotropic liquid occurs at low concentration of DNA and it is characterized by randomly oriented DNA molecules. With an increase of DNA concentration the increase of molecules organization is observed. The formation of DNA LC phases is a consequence of that phenomenon. The most commonly observed LC phase is the cholesteric one which turns itself into a columnar hexagonal phase for higher DNA concentrations [2].

Cholesteric and columnar hexagonal liquid crystalline DNA phase formation may be easily observed in appropriately prepared LC cells containing DNA solution (CDNA = 60mg/ml) under the polarizing microscope. It gives possibility of observing phase transitions and determining pitch of cholesteric phase.

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P17

Synthesis and biological applications of chiral azobenzenes derivatives

M. Ziemianek^{1,2}, M. Deiana¹, Z. Pokładek², M. Samoć¹, P. Młynarz², K. Matczyszyn¹

¹Advanced Materials Engineering and Modelling Group, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland

²Department of Bioorganic Chemistry, Faculty of Chemistry, Wrocław University of Science and Technology, Wyb. Wyspiańskiego 27, 50-370 Wrocław, Poland

Abstract

Azobenzene (AB) derivatives can occur in either *trans* (E) or *cis* (Z) conformation, however at equilibrium in the dark, this moiety exists in the more stable *trans* isomer. Irradiation with UV light induces a molecular geometry change leading to the *cis* isomer formation, which can revert back to the *trans* state thermally or upon irradiation. Azobenzene derivatives are ideal for use as molecular photoswitches, due to the different spectral properties of the *trans* and *cis* conformers. ABs are commonly used as biological tools to direct and manipulate a wide range of bio-events^{1,2}.

We present the synthesis and biological studies of photoresponsive chiral azobenzene units embedded into human serum albumin (HSA). We showed that the resulting switchable supramolecular complex provides potential for fuelling new devices that combine well-defined 3D structure afforded by the chiral host with the ability to trigger the physicochemical response of the resulting material.

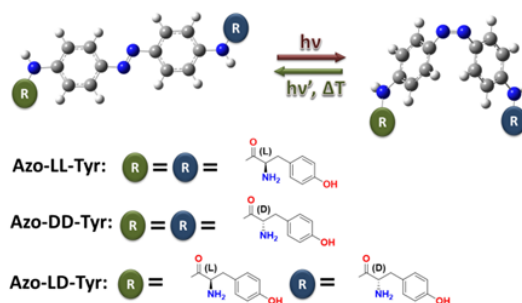


Figure 1. Structure of the synthesized azobenzene derivatives.

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P18

Photothermal stability of triangular gold nanoparticles

M. Klekotko, J. Olesiak-Bañska, K. Matczyszyn, M. Samoć

*Advanced Materials Engineering and Modelling Group,
Faculty of Chemistry, Wrocław University of Science and Technology,
Wyb. Wyspiańskiego 27, 50-370 Wrocław, Poland*

Abstract

Noble metal nanoparticles have unique physical and chemical properties dependent on their size and shape, which make them attractive for use in a wide range of applications. The usage of these structures is often related with the laser irradiation of the sample. Therefore, the influence of the laser beam on the morphology of the nanostructures should be examined.

This work presents the results of the femtosecond laser irradiation of triangular gold nanoparticles (GNPs). In our research, we compared the photothermal stability of the gold nanoprisms synthesized using biological and chemical methods. Bio-mediated synthesis involved a mint extract as a source of reducing, structure-directing and stabilizing agents [1]. For the chemical method, we applied a three-step protocol, involving chemicals commonly used in the synthesis of nanostructures [2]. The morphological changes of the GNPs exposed to the laser beam were followed by absorption spectroscopy and transmission electron microscopy. As seen in Fig.1, irradiation of triangular GNPs with femtosecond laser pulses can lead to various structural changes of the NPs.

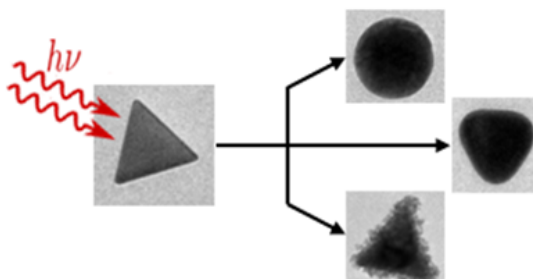


Fig. 1. Morphological changes of the triangular nanoparticles irradiated with a femtosecond laser beam.

Acknowledgements

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P19

Synthesis, spectroscopic and polymerization kinetics studies of benzannulated difluoroboranyls

B. Jędrzejewska, B. Ośmiałowski

University of Technology and Life Sciences, Faculty of Chemical Technology and Engineering
Seminaryjna 3, 85-326 Bydgoszcz, Poland, borys.osmialowski@utp.edu.pl

Abstract

In general difluoroboranyl derivatives (compounds carrying BF_2 group) exhibit high fluorescence quantum yields. Substituent or π -conjugated spacer responsible for transmission of the charge from donor to acceptor may modify some of their properties. The **D-A** molecules (**D**onor-**A**ceptor) exhibit solvatochromic behavior due to the said charge transfer, which is larger in excited state than in ground state of subjected molecule. Some other properties as, for example, maximum of absorption or fluorescence, fluorescence lifetimes and quantum yield of fluorescence may be modified by a variety of methods.

Aromaticity, in general, is a molecular property that greatly influences properties of many organic molecules. The same is realized for dyes especially when *benzo* ring is added to the *chromophore*. Thus, recently we have shown that the position of benzannulation and the number of *benzo* rings attached to the pyridine core may be used to tune the properties of compounds. The figure below shows the absorption maxima for pyridine (**1**), quinoline (**2**), isoquinoline (**3**) and phenanthridine (**4**) BF_2 -carrying derivatives. It is easy to see that spectra shift to the red when benzannulation takes place.

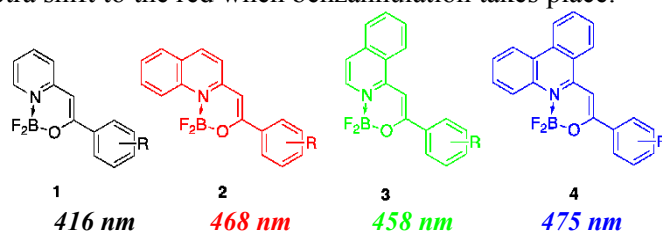


Fig. 1 The BF_2 -carrying heterocycles benzannulated at the pyridine and their absorption maxima in ethyl acetate (R=4-NMe₂)

The aim of this study was to test if difluoroboranyls can be efficient sensitizers of photopolymerization. Thus, the trimethylolpropane triacrylate (TMPTA) was used as a monomer and phenyltriethylborate salt as an electron donor. The results show **D-A** molecules carrying BF_2 group can be successfully used to photoinitiate radical polymerization.

Synthesis, spectroscopic and polymerization kinetics studies of symmetrical and unsymmetrical difluoroboranyls

J. Davis¹, E. Addison¹, B. Jędrzejewska², B. Ośmiałowski²

¹Department of Chemistry, Delaware State University

²University of Technology and Life Sciences, Faculty of Chemical Technology and Engineering
Seminaryjna 3, 85-326 Bydgoszcz, Poland, beata@utp.edu.pl

Abstract

BODIPY dyes are fluorophores presenting sharp absorption and emission bands, high fluorescence quantum yields, and valuable photostabilities. In the literature there exist also reports on compounds where the BF₂-group is chelated symmetrically in NBF₂N and OBF₂O moieties. Molecules carrying the NBF₂O fragment, especially imines based on hydroxyl-containing Schiff bases, are known as well [1,2].

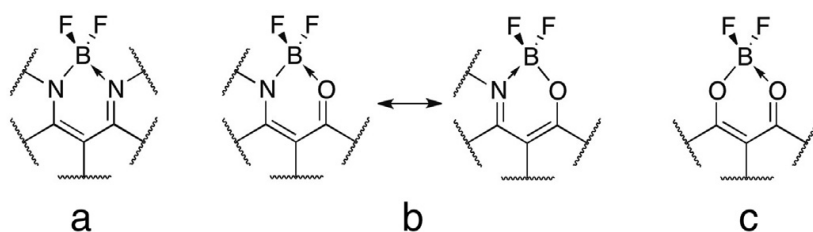


Fig. 1. The NBF₂N (a), NBF₂O (b) and OBF₂O (c) core in difluoroboranyls synthesis.

The potential of BF₂ dyes was demonstrated in several fields of science as, for example, photodynamic therapy, microscopy, molecular probing, drug delivery, laser dyes, and more [1]. Our research on difluoroboranyls concerns:

- organic synthesis and product purification,
- investigation of their spectral and photophysical properties,
- application of the selected difluoroboranyls as photoinitiators for acrylates' polymerization.

It is worth mentioning that difluoroboranyls are very rarely used in photopolymerization studies. This motivated us to test BF₂-carrying molecules as a visible light photoinitiators.

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Gold nanorods-enhanced multiphoton imaging of neurons

A. Pniakowska¹, M. Rząsa¹, T. Wójtowicz², J. Olesiak-Bańska¹, K. Matczyszyn¹

¹ *Advanced Materials Engineering and Modelling Group, Wrocław University of Science and Technology, Wyb. Wyspiańskiego 27, 50-370, Wrocław, Poland*

² *Department of Biophysics, Wrocław Medical University, Chalubińskiego 10, 50-365 Wrocław, Poland*

Abstract

Gold nanorods have received extensive attention because of their attractive applications in biomedical imaging, drug delivery, optical filters and photothermal therapy.

Our GNRs were synthesized using binary surfactants mixtures of hexadecyltrimethylammonium bromide (CTAB) and sodium oleate (NaOL). This method improves dimensional tunability and monodispersity in the seeded-growth solution. The nanorods have the dimensions: (91.2 ± 5.8) nm x (18.3 ± 1.0) nm and LSPR wavelength longer than 800 nm [1]. For biological applications, the surface functionalization of GNRs is very important because CTAB coated nanorods are toxic. We functionalized the surface of our nanorods with layer-by-layer method, with the negatively charged poly(sodium 4-styrenesulfonate) (PSS) or additional layer of positively charged poly(allylamine hydrochloride) (PAH) [2]. Gold nanorods conjugated with biocompatible ligands can enhanced optical extinction of neurons (Fig. 1). They can attach to neurons and trigger action potentials in response to pulses of light [3].

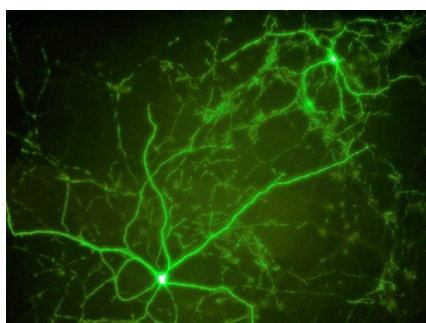


Fig. 1 Neurons fluorescence under optical microscope

In our measurements we used functionalized GNR as a photosensitizer and inject them into mouse neurons. Therefore, biological cells were treated by patch-clamp technique to inject functionalized nanoparticles and Alexa fluorescent dye. Next, we performed our measurements, which were based on multiphoton imaging of neurons under 800nm excitation. In this experiment we aimed at maximizing the separation of nanoparticles in neurons.

Although part of ligand-functionalized nanoparticles did not readily attach to all neurons, when they already bind to a cell they have highly resistant to washout and ability to high photostimulation. This kind of research have applications for therapies involving neuronal photostimulation [3].

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P22

Collagen in light amplification applications

M. Janeczko, K. Cyprych, J. Myśliwiec

Advanced Materials Engineering and Modelling Group, Wrocław University of Science and Technology, Wyb. Wyspiańskiego 27, 50-370 Wrocław, Poland

Abstract

In our work we report on the results of amplified spontaneous emission and random lasing obtained in dye-doped collagen and α -cyclodextrin systems with Rhodamine 6G used as an active material. Collagen as a complex protein forms fibril higher order structures which were used as scaffold for Rh6G dye facilitating dye aggregation inside single fibers structures leading to formation of distributed network of circular resonators connected with collagen waveguides.

With the applying the dye properties there was acquired wavelength tunable random lasing as a result of aggregation process induced by molar ratios change of α -cyclodextrin and Rhodamine 6G in range of values 100:1, 10:1 and 1:1. Produced system have been analyzed with AFM microscopy, excitation with nanosecond pulsed Nd:YAG laser. Formation of optical cavities has been confirmed and light scattering properties were analyzed with coherent backscattering experiment.

P23

Study and design of biosensors for monitoring contaminants in food and environment

S. F. Zaman, Dr. D.J. Shariff

Department of Biotechnology, BITS Pilani Dubai Campus, P.O.Box 345055, Academic City – Dubai, U.A.E

Abstract

A biosensor is defined by the International Union of Pure and Applied Chemistry (IUPAC) as a self-contained integrated device that is capable of providing specific quantitative or semi-quantitative analytical information using a biochemical receptor [1]. Environmental security is one of the fundamental requirements of our well-being. However, it still remains a major global challenge, on account of the increasing number of potentially harmful pollutants (chemical compounds, toxins and pathogens) discharges into the environment [2]. This calls for the need of a quick and cost-effective technique to be used in the detection and monitoring of pollutants. Biosensors serve as a suitable cost-effective complementary analytical tool. Biosensors can be considered as a subgroup of chemical sensors in which biological mechanism is used for analyte detection [3,4]. Nano-biosensors with dedicated miniature sensors have been developed and is a field of ongoing research. The scope of this research paper is to understand biosensors, its working in general with reference to its constituents and the use of these

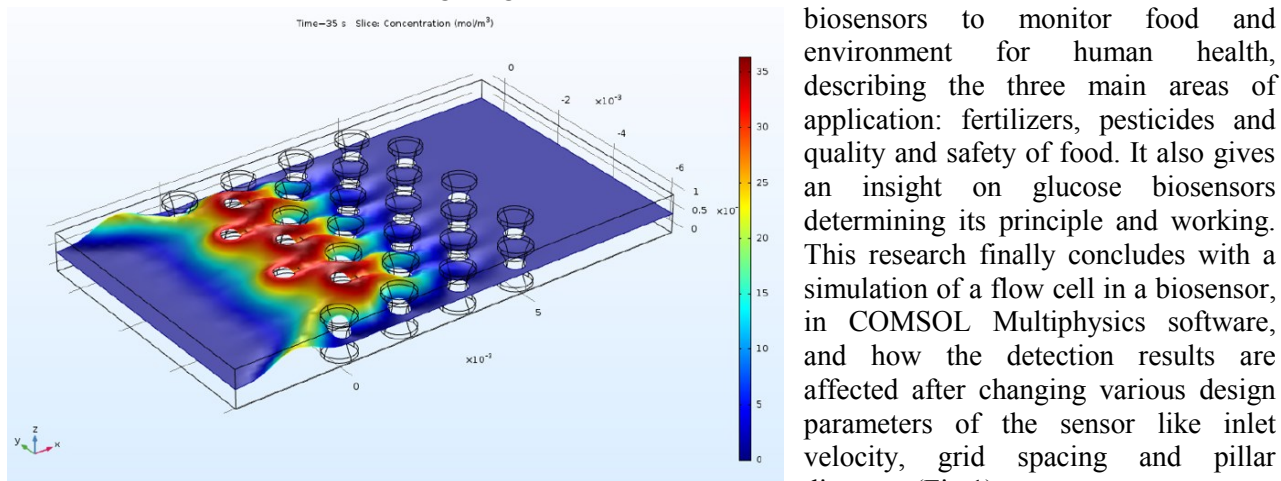


Fig.1 Structure of a flow cell in a biosensor (using COMSOL software)

biosensors to monitor food and environment for human health, describing the three main areas of application: fertilizers, pesticides and quality and safety of food. It also gives an insight on glucose biosensors determining its principle and working. This research finally concludes with a simulation of a flow cell in a biosensor, in COMSOL Multiphysics software, and how the detection results are affected after changing various design parameters of the sensor like inlet velocity, grid spacing and pillar diameter (Fig.1).

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P24

Co₃O₄ on Ag₃PO₄ surface – a step towards photocatalytic cofactor regeneration?

K. Kinastowska¹, M. Grzelczak², W. Bartkowiak¹

¹Department of Quantum and Physical Chemistry, Wrocław University of Technology, Wyb. Wyspiańskiego 27, 50-370 Wrocław, Poland

²CIC biomaGUNE, Paseo Miramón 182, 20009 San Sebastián, Spain

Artificial photosynthesis is a tempting approach for non-enzymatic regeneration of cofactors – molecules serving as electron/proton carriers in numerous enzymatic reactions. In such an attempt introduction of a powerful and economical photocatalyst is of key importance.

Semiconductor particles, in which light-generated electrons and holes may participate in water oxidation and cofactor reduction respectively are particularly desired, especially if they absorb in visible range. However, finding a single, visible-active catalyst with band-gap position suitable for the overall process is very challenging. Thus, combining two different materials, each selective for one of half-reactions, to create a complete, specialized system is an interesting concept.

Microcrystalline silver phosphate (Ag₃PO₄) was reported as an effective photocatalyst for water oxidation and organic dyes degradation under visible-light¹. What is more, presence of appropriate co-catalysts on Ag₃PO₄ surface can additionally boost its photocatalytic activity, also towards organic dyes². Nevertheless, from the perspective of cofactor regeneration, organic compounds decomposition is unfavorable as cofactor stability in the reaction environment is essential.

We propose decoration of Ag₃PO₄ surface with cobalt oxide nanoparticles (Co₃O₄ NPs) as a double-role co-catalyst that increases the system selectivity for water and limits its affinity for MB resulting in enhanced water oxidation and reduced MB decomposition (Fig. 1). We present microscopic, spectroscopic and photoelectrochemical characteristics of prepared material. We also show evaluation of Ag₃PO₄@Co₃O₄ water oxidation performance in presence of MB and compare it with the results obtained for bare Ag₃PO₄. Moreover, we prove the photocatalyst-mediated nature of MB degradation in a set of experiments with the use of optical band-pass filters.

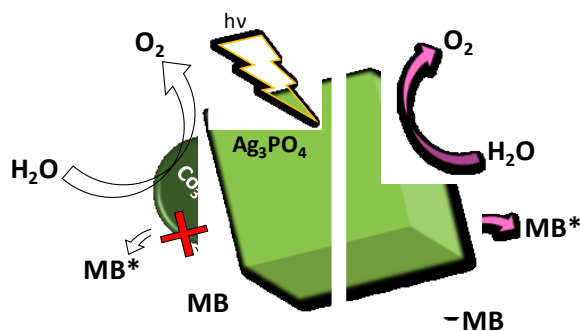


Fig. 1 Schematic illustration of proposed photocatalytic system improvement.

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Tiophene and tetrathiafulvalene derivatives – 3rd order nonlinear optical characterization

M. Michalski¹, A. Szukalski², A. Ayadi³, A. El-Ghayoury³, J. Myśliwiec²

¹ *Optical and Photonic Engineering, Department of Fundamental Problems of Technology, Wybrzeże Wyspiańskiego 27, 50-370, Wrocław, Poland*

² *Advanced Materials Engineering and Modelling Group, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50-370, Wrocław, Poland*

³ *Laboratoire MOLTECH-Anjou, University of Angers, UFR Sciences, UMR 6200, CNRS, Bat. K, 2 Bd. Lavoisier, 49045, Angers Cedex, France*

Abstract

Optical Kerr Effect (OKE) is one of the third order nonlinear optical effects based on photoinduced anisotropy of refractive index which could be used e.g. for all optical switch [1].

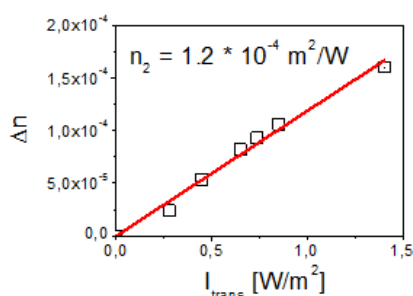


Fig. 1. Dependence of photoinduced optical birefringence versus pumping beam intensity for tiophene derivative

Here we show the OKE phenomenon studies for selected tiophene and tetrathiafulvalene derivatives. An active material was doped in to the PMMA matrix as a typical guest-host system. Due to the fact, that these compounds have active centres in a form of π -type multiple bonds, there is possible to observe the multiple and reversible photoinduced conformational *trans-cis-trans* changes (in the range of single milliseconds). Knowing values of Δn photoinduced birefringence changes in a function of I pump beam intensity, it is possible to calculate the nonlinear n_2 optical refractive index (c.f. Fig. 1).

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P26

Statistical analysis and optimization with response surface methodology of photocatalytic activity of ZnO/polypyrrole nanocomposite

E. Özbay, İ. Erdoğan, H. Kamış

Selcuk University, Department of Chemical Engineering, Konya, Turkey

Abstract

Domestic and industrial wastes are threatening the environment health day by day. According to the World Bank, 17 to 20 percent of industrial water pollution comes from textile dyeing and treatment. Photocatalysis is seen as a great potential for this wastes [1]. Photocatalysis is generally based on the light absorption of semiconductor metal oxide photocatalyst, such as ZnO and TiO₂, to excite the electrons from valence band to conduction band and create electron-hole pairs [2]. Researchers have focused on increasing the degradation rates of pollutants by combining nanoparticles with conductive polymers to achieve synergetic and complementary behaviours in recent years [3].

In this study, statistical analysis of the effect of Polypyrrole/ZnO nanocomposites on photocatalytic activity was performed. Photocatalytic degradation of Methylene Blue (MB) dye using synthesized Polypyrrole/ZnO nanocomposites is investigated and percentage degradation of MB dye is modelled by using Response Surface Method. A central composite design (CCD) with response surface methodology (RSM) was applied to evaluate the relationships between operating variables, such as catalyst concentration, pH and dye concentration, to identify the optimum operating conditions.

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Ligand-induced plasmonic chirality

M. Rakoczy, J. Olesiak-Bańska, M. Waszkielewicz, M. Samoć

Advanced Materials Engineering and Modelling Group, Faculty of Chemistry, Wrocław University of Science and Technology, Wyb. Wyspiańskiego 27, 50-370 Wrocław, Poland

Abstract

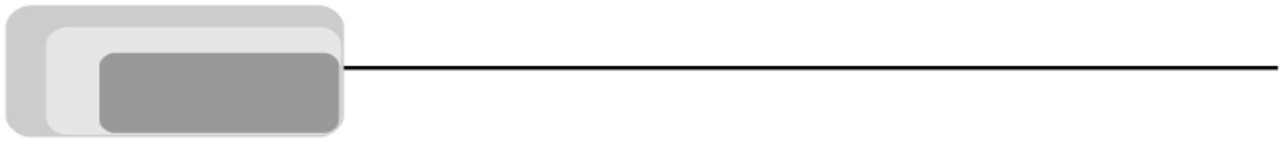
Circular dichroism (CD) involves the interaction of chiral species with circularly polarized light and is crucial in investigation and discrimination of biological molecules. The plasmonic effect can be used to define circular dichroism (CD) enhancements for chiral induced molecules. When a chiral ligand interacts with a nonchiral metallic particle, this leads to field enhancements that can both influence the CD of the ligand and transfer the chirality and thus the CD activity from electronic transitions of the molecule to surface plasmon resonance absorption of the metallic particles. Normally weak molecular CD response is strongly amplified [1,2] The interactions between a metal nanoparticle and a chiral absorber hold multiple applications in photonics and biosensing. [3,4].

This contribution describes our investigation of plasmonic enhancements of circular dichroism by binding a chiral ligand to gold nanostructures. We synthesized gold nanorods (NRs) and nanospheres (NSs). In the case of NRs, the synthesis was based on the seed mediated method, with reduction of tetrachloroauric(III) acid with NaBH₄, in the presence of AgNO₃ and cetyltrimethylammonium bromide (CTAB) as a ligand [5] The synthesis of nanospheres also was based on tetrachloroauric(III) acid which was added to a high concentration of boiling citrate. This caused the change of colour of solution from yellow through transparent to a burgundy. The nanorods and nanospheres were characterized by UV-Vis absorption and transmission electron microscopy (TEM).

Then, partial and full ligand exchange was performed: L-cysteine, L-penicillamine and glutathione were used to coat the nanoparticles. We optimized the protocol of chiral functionalization by the analysis of CD spectra of the nanoparticles. The strongest chirality induced in the range of plasmonic absorption wavelengths was observed with L-cysteine as a ligand and a specific concentration of CTAB as a co-stabilizer of NRs.

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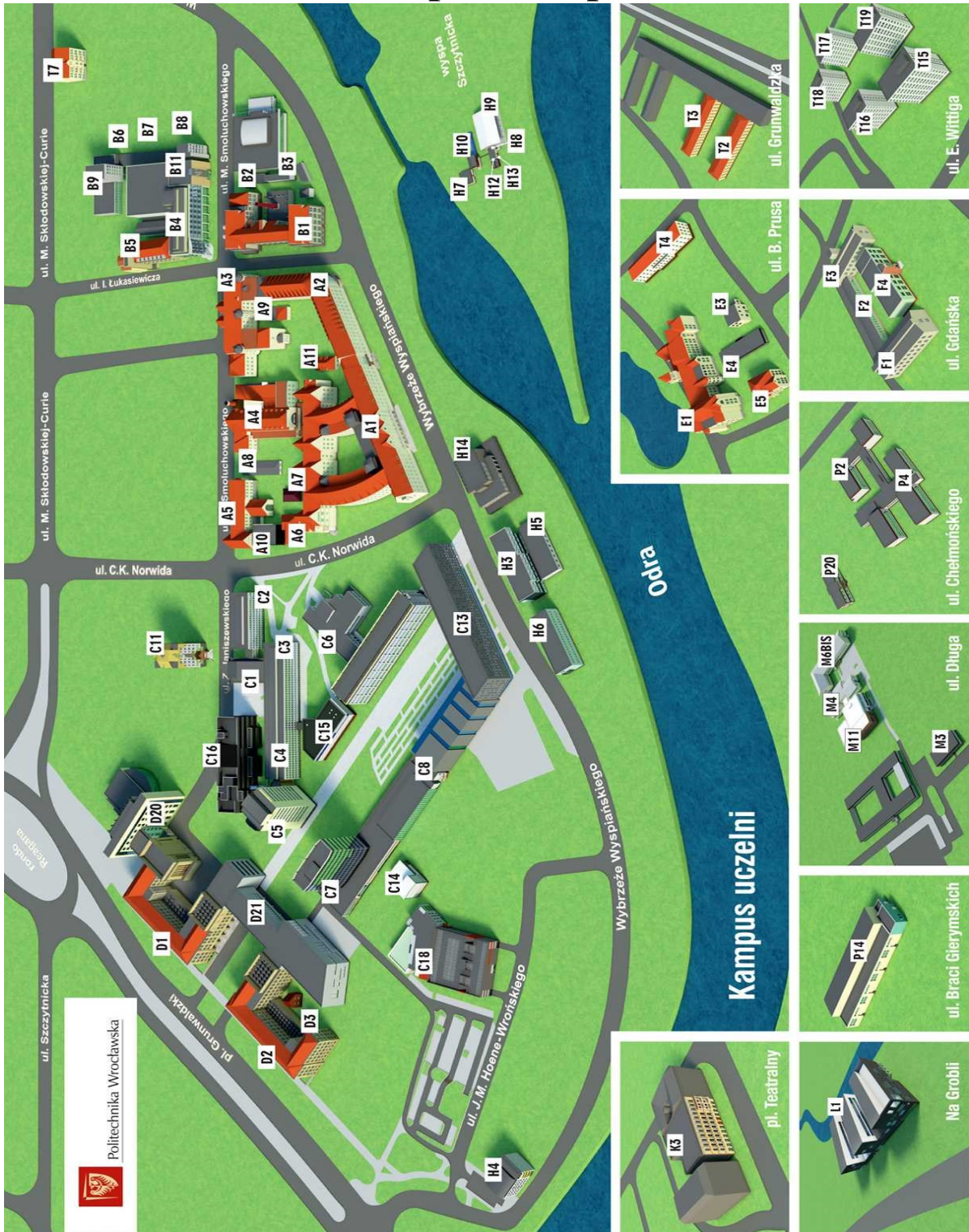




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Map of campus







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