*The **CREA**tion of the Department of Physical Chemistry of Biological Sys**TE**ms [CREATE]*

666295 — CREATE — H2020-WIDESPREAD-2014-2015/H2020-WIDESPREAD-2014-2

Upgraded research programme of IPC

[Deliverable D.3.1]

Level of dissemination: Public

Warsaw, June 2017

This project has received funding from the *European Union's Horizon 2020 research and innovation programme* under grant agreement No 666295

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1. <u>Current IPC research programme</u>

The Institute of Physical Chemistry of the Polish Academy of Sciences (IPC) carries out interdisciplinary research in the field of chemistry inspired by biology, nanotechnology, medicine, pharmacy and environmental protection. Although the primary purpose of establishing IPC was to conduct fundamental research in physical chemistry, IPC refocused to carry out research at the boarder of chemistry, physics and biology with possible application to medical industry, nanotechnology, and environmental protection. Change of IPC profile – from phenomenology to applications – can be seen in increasing number of patents and papers published in journals with varied expertise.

27 research groups (206 scientists) carry out ca. 100 projects, including joint projects with companies. Once per year, each team presents their scientific plans for the future, taking in consideration possible alignments with other disciplines. **[More information on the research programme can be found in the attachment no.1.]**

However, a *sine qua non* of well-functioning multidisciplinary institution is a policy fostering open collaboration between research groups, which allows for knowledge and skill transfer. Taking a look at IPC from this perspective – IPC still needs to take some steps to support internal collaboration.

Therefore, the ERA Chair holder – Professor Maciej Wojtkowski, has been engaged in the review of the current IPC research programme to propose some measures, enhancing the interdisciplinary approach, and selecting promising research teams for further collaboration.

2. **Review and recommendations**

The ERA Chair holder, Professor Maciej Wojtkowski, got acquainted with the current research programme of IPC by meeting representatives of the research groups, and studying their present research programme and plans.

Based on conducted analysis, Professor Wojtkowski decided to divide IPC research groups into three categories:

- **synergetic groups:**

By the synergetic groups are meant research groups, which are interdisciplinary, and strive towards biological or medical applications. Research conducted by synergetic groups are close to the research of the Department of Physical Chemistry of Biological Systems.

The scope of reaseach activity of synergetic groups gives an open field for complementary collaboration. These groups have already been carrying out research in the field of chemistry inspired by biology, nanotechnologies and medicine, coresponding with the interdiciplinary approach of IPC.

- **prospective groups:**

Second category (prospective groups) relates to larger, well-established research groups, which present high potential for: **1)** a growth in the new research direction, e.g. biology, having potential for direct collaboration with Professor Wojtkowski's Group in the future; **2)** a deployment of research results to industrial applications.

- **others:**

The other groups, not specified under the first or the second category, consider physical chemistry as a main scope of their studies, hence their interdisciplinary potential is currently limited from the point of view of the ERA Chair holder.

The general idea behind division of IPC research groups into 3 categories it is as follows:

Due to the IPC policy guaranteeing researchers' freedom of choosing research field (among others - part of obligation related with implementation of principles of the European Charter for Researchers and the Code of Conduct for the Recruitment of Researchers underlying the logo "*HR Excellence in Research*"), direct influence of the IPC Director or the ERA Chair holder on the groups which are not interested in collaboration, is limited. For this reason Professor Wojtkowski decided to build IPC potential on selected, willing to cooperate, research groups.

Nevertheless, research activity of the newly created Department of Physical Chemistry of Biological Systems led by prof. Wojtkowski enables to intensify actions of synergetic and prospective groups, inducing changes in the scope of research activity of the entire IPC.

Synergetic groups

The following groups were indicated as synergetic:

- ***Laser Centre*, prof. Czesław Radzewicz / dr. hab. Angulo Gonzalo**
  Close cooperation on the development of new light sources, dedicated to two-photon eye imaging has already been started. Together with this group the ERA Chair holder applied for, and gained, a significant funding from the Foundation for Polish Science. To consolidate this cooperation, the ERA Chair holder plans to hire an exprienced researcher, who will be conducting his research in the Laser Centre lab.
- ***Microfluidics and Complex Fluids*, prof. Piotr Garstecki**
  The ERA Chair holder is interested in supporting research aimed at development of new techniques dedicated to guide the evolution of bacteria, conducted by the *Microfluidics and Complex Fluids* research team.
- ***Soft Condensed Matter*, prof. Robert Hołyst**
  This group carries out research aimed at application of nano-materials in chemistry and biology research. In the collaboration with the ERA Chair holder's team, synergy between both groups will be maintained by joint research on intracellular dynamics.
- ***Surface Nanoengineering for chemo- and bio- sensors*, dr hab. MEng. Joanna Niedziółka-Jönsson**
  The group of Professor Wojtkowski and the *'Surface Nanoengineering for chemo- and bio-sensors'* Group will carry out research on large nanorods. The aim of the research is to develop technique of imaging of cerebral circulation (here: in mouse and rat brains).

Prospective groups

Research groups which present high potential for:

a) a growth in the new research direction, e.g. biology:

- ***Molecular films research*, prof. Włodzimierz Kutner**
  Amid the research of this group are the bioinspired intelligent molecularly imprinted polymers (MIPs) for selective chemosensing. This research field has potential for collaboration of the two groups.

- ***Charge Transfer Processes in Hydrodynamic System*, dr hab. Martin Jönsson-Niedziółka**

  Under a following research topic: bioelectrocatalytic processes by enzymes both under static and hydro-dynamic conditions, this group studies the enzyme reactions aimed at applications in sensing and biofuel cells, as well as fundamental studies of enzyme kinetics.

- ***Spectroscopic and microscopic (STM/AFM) studies of intermolecular interactions*, dr hab. Robert Nowakowski**

- ***Photophysics and spectroscopy of photoactive systems*, prof. Jacek Waluk.**

b) a deployment of research results to industrial applications:

- ***Organometallic and Materials Chemistry*, prof. Janusz Lewiński**
- ***Catalysis for Sustainable Energy Production and Environmental Protection*, dr hab. MEng. Juan Carlos Colmenares.**

Professor Maciej Wojtkowski has proposed to the abovementioned research groups joint research projects, and currently works are continued to transform joint research plans into proposals.

Consistent with the CREATE proposal, the Deliverable 3.1 consists of an upgrade of IPC research plan (consulted with major stakeholders and the ERA Chair holder) reported to the Polish Ministry of Science and Higher Education. However, due to the change of a procedure of reporting research plans to the Ministry of Science and Higher Education (now are reported only research tasks to be financed directly from the funds of the Ministry, which are very limited) – jointly planned research projects of Professor Wojtkowski and research groups selected for collaboration were only partly included in this document [see Annex I. for details]. Specific joint research projects will be fully reported to the CREATE Project Officer under Deliverable 4.1 *"Joint research plan with a schedule and identified source of funding"* (due date: Oct., 2017), and its updates (Deliverables: 4.2, 4.3, 4.4).

The IPC research programme – with a special focus on research portfolio of synergetic and prospective research groups – was also presented to the managers of collaborating companies with a request for a review. The exemplary opinion is presented below:

Dear Sirs,

The portfolio of projects planned in the Institute of Physical Chemistry consist of very wide spectrum of topics. Remarkable feature of some of these topics is multi-disciplinary approach. These topics are focused not on the specific discipline of science but rather on widening human knowledge. Exploring the borders of bio-chemistry and physics together seems to be the most efficient way of solving real-life problems.

Especially interesting subjects from the business perspective might be those who seeks for the new sensors or sensing methods. Worth noticing is that very different approaches are present here: starting from imprinting bio-molecules into polymers, through high-end nanotechnology and coming back to laser-based techniques.

I hope some of the presented topics will continue and succeed not just on scientific field but also as mature business-applied technologies.

With best regards, Marcin Izydorzak – ***CEO at Scope Fluidics Sp. z o.o.***

Dear Madams,

With a great interested I read the research program of the Institute of Physical Chemistry Polish Academy of Sciences. It is focused on many important aspects of our everyday life from new sensors for medicine and industry to new photovoltaic and photocatalytic devices, as well as deep and thorough fundamental science.

As a business representative of photonic industry I found very interested topics related to optical techniques, such new microscopy methods or development of lasers sources. For me, this means that the Institute of Physical Chemistry is opened for many disciplines and promotes multidisciplinary approach. Having all strong teams from different disciplines (organic and inorganic chemistry, physical optics, spectroscopy, biology) under one roof creates great opportunity for new discoveries and practical use of scientific knowledge.

With kind regards,

Michał Nejbauer – ***CEO at FLUENCE Sp. z o.o.***

ANNEX 1.
IPC research programme reported to the Ministry of Science and Higher Education

This project has received funding from the *European Union's Horizon 2020 research and innovation programme* under grant agreement No 666295

Thematic team 2 – Professor Kutner

PROSPECTIVE GROUP

1. New DNA analogues generated by the programmed transfer of oligonucleotide sequence information into molecularly imprinted polymers.

We will develop and produce genetically important new DNA analogues[1] with sequences longer than hexanucleotide sequences. To this end, we will transfer the oligonucleotide sequence information in a programmed manner to molecularly imprinted polymers (MIP) produced by electropolymerization. We will confirm this transfer using new chemical sensors that selectively recognize these oligonuceotides. In these sensors layers of the produced MIPs will serve as recognition elements.[2]

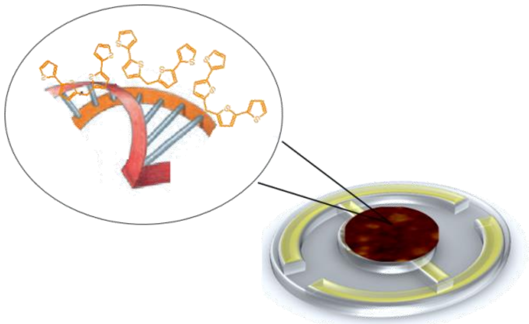


Diagram 1. The programmed transfer of oligonucleotide sequence information to molecularly imprinted polymers (MIP) in order to produce DNA analogues, on the example of a piezomicro-gravimetric chemical sensor with a layer of MIP selectively recognizing oligonucleotide sequences.

Literature:

- Bartold, K., Pietrzyk-Le, A., Huynh T.-P., Iskierko, Z., Sosnowska, M., Noworyta, K., Lisowski, W., Sannicolò, F., Mussini, P. R., Cauteruccio, S., Licandro, E., D'Souza, F., and Kutner, W., *ACS Appl. Mater. Interfaces* **2017**, *9*, 3948-3958.
- Huynh, T-P., Pietrzyk-Le, A., Bikram K. C. C, Noworyta, K. R., Sobczak, J. W., Sharma, P. S., D'Souza, F., Kutner, W., *Biosens. Bioelectron.* **2013**, *41*, 634–641.

2. Efficient polymer chromophores for photovoltaic cells

We will develop a new strategy for the synthesis of efficient chromophores for organic and hybrid photovoltaic cells. These chromophores have common molecular features.[1] They are difficult to synthesize (Diagram 1).[2] Therefore, we will generate them from various functional monomers by electrochemical copolymerization. These monomers facilitate beneficial processes and minimize those that are unwanted in photovoltaic cells. We will develop a quick and easy way to prepare photoactive polymer materials.

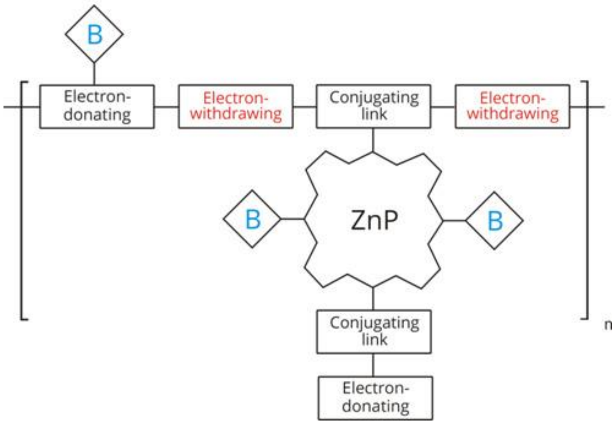


Diagram 1. Simplified structural formula of an efficient polymer chromophore of a photovoltaic cell. ZnP – zinc porphyrin, B – volumetric non-conducting substituent.[1]

Literature:

- Obraztsov, I., Kutner W., and D'Souza F. *Solar RRL* **2017**, DOI: 10.1002/solr.201600002.
- Chao, Y. I. H., Jheng, J.-F., Wu, J.-S., Wu, K.-Y., Peng, H.-H., Tsai, M.-C., Wang, C.-L., Hsiao, Y.-N., Wang, C.-L., Lin, C.-Y., Hsu, C.-S., *Adv. Mater.* **2014**, *26*, 5205.

3. Recognition layers of molecularly imprinted polymers (MIP) with an incorporated redox probe for the construction of new generation electrochemical sensors

In electrochemical assays of non-electroactive analytes an external redox probe is often employed.[1] Bonding of the analyte in the MIP causes swelling of the polymer thus closing its pores.[2] Therefore, diffusion of the probe through the MIP layer to the electrode is made more difficult. For conductive MIP layers this analyte bonding does not block diffusion, however, it does change the charge transfer resistance.[3] Therefore, we propose to covalently immobilize the probe (e.g. ferrocene) on the MIP. This will make it possible to carry out assays without the need to add a probe to the test solution, which will significantly enhance these assays.

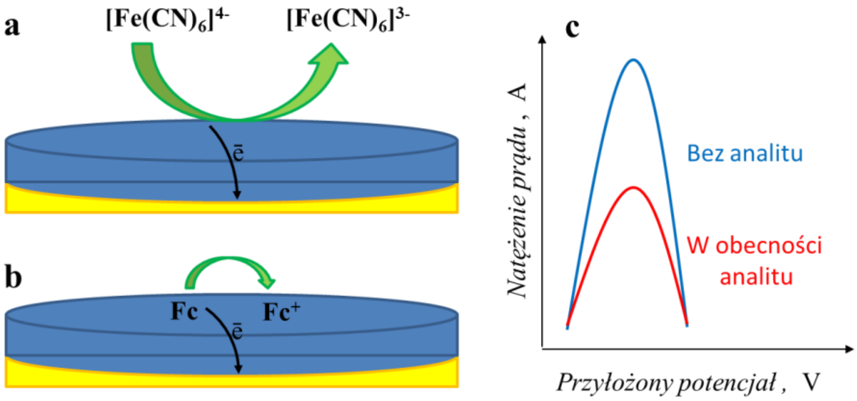


Figure 1. Principle of operation of chemical sensors with a MIP recognition layer and the use of an (a) external and (b) internal redox probe and (c) analitycal DPV signal in the presence and absence of the analyte.

Literature:

- Cieplak, M.; Kutner, W., *Trends Biotechnol.* **2016**, *34*, 922-941.
- Yoshimi, Y.; Narimatsu, A.; Nakayama, K.; Sekine, S.; Hattori, K.; Sakai, K., *J. Artif. Organs* **2009**, *12*, 264-270.
- (a) Cieplak, M.; Szwabinska, K.; Sosnowska, M.; Bikram, K. C. C.; Borowicz, P.; Noworyta, K.; D'Souza, F.; Kutner, W., *Biosens Bioelectron* **2015**, *74*, 960-966; (b) Huynh, T. P.; Bikram, K. C. C.; Lisowski, W.; D'Souza, F.; Kutner, W., *Bioelectrochemistry* **2013**, *93*, 37-45.

4. Chemical sensors for the selective determination of p-synephrine

We will develop and produce chemosensors with MIP recognition layers for the selective determination of *p*-synephrine **1** – a harmful dietary supplement[1,2] with an adverse effect on the circulatory system.[3] One study indicates that consumption of **1** is safe, and that it is *m*-synephrine that is responsible for the adverse effects.[4] However, the risk of using **1** and the fact that octopamine – its analogue – is an illegal doping agent, suggest that **1** will also be prohibited.[5] Therefore, a method of selective detection and determination of *p*- and *m*-synephrine in both synthetic and biological samples is required. Figure 1 shows the proposed structural formula of an example pre-polymerization complex. **1**.

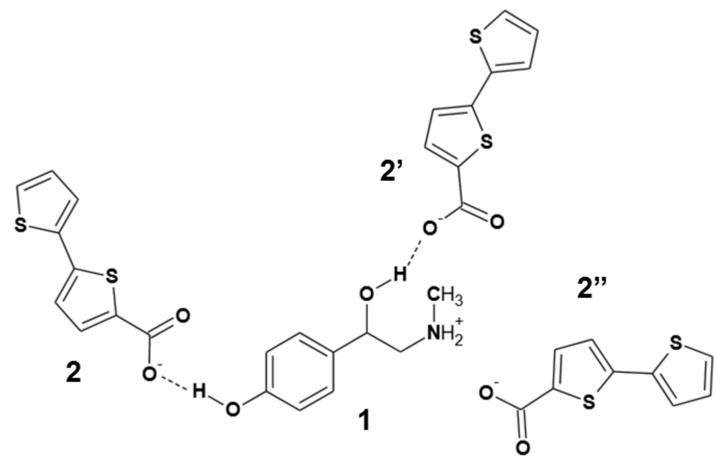


Figure 1. Proposed structural formula of the pre-polymerization complex of p-synephrine 1 with three molecules of functional monomer, 2,2'-bithiophene-5-carboxylic acid 2, 2', 2''.

Literature:

- Arbo, M. D.; Schmitt, G. C.; Limberger, M. F.; Charao, M. F.; Moro, A. M.; Ribeiro, G. L.; Dallegrave, E.; Garcia, S. C.; Leal, M. B.; Limberger, R. P., *Regul. Toxicol. Pharmacol. RTP* **2009,** *54*, 114-117.
- Arch, J. R., *Eur. J. Pharmacol.* **2002,** *440*, 99-107.
- Rossato, L. G.; Costa, V. M.; Limberger, R. P.; Bastos Mde, L.; Remiao, F., *Food Chem. Toxicol. Intern. J. BIBRA* **2011,** *49* (1), 8-16.
- Stohs, S. J.; Preuss, H. G.; Shara, M., *Oxid. Med. Cell. Longev.* **2011,** *2011*, 482973.
- WADA, Monitoring Program Available: http://www.wada-ama.org. **2009**.

5. Electrophoretic production of layers of ZnO nanoparticles and their application to Raman surface-enhanced spectroscopy (SERS).

We will electrophoretically deposit variously sized ZnO nanoparticles, synthesized in ZT09 and surface-modified with selected organic ligands, on solid substrates. We will examine the structure and morphology of the resultant layers using SEM and XRD. We will also examine their absorption and fluorescence. Next, we will plasma remove the ligands from the surfaces of these nanoparticles. We will use layers prepared in this manner with their improved surfaces as substrates for SERS study of selected model compounds. We will also endeavour to dope these layers with metals (Ag, Au) and we will investigate the effect of this doping on the SERS signal strength.

6. Chemical sensors for the selective detection and determination of peroxide explosives

We will design and synthesize molecularly imprinted polymers (MIP) with triacetone triperoxide. This compound has explosive properties. It can be easily synthesized under domestic conditions. This is why terrorists often use it as an explosive. There is therefore a need to develop and produce a chemosensor for the selective detection and determination of this triperoxide. We will use MIPs imprinted with it as the detection elements of our chemosensors. Preliminary DFT calculations indicate that functional monomers of bis (bithiophene) containing an amine group (Fig. 1) are best suited for the preparation of these MIPs.

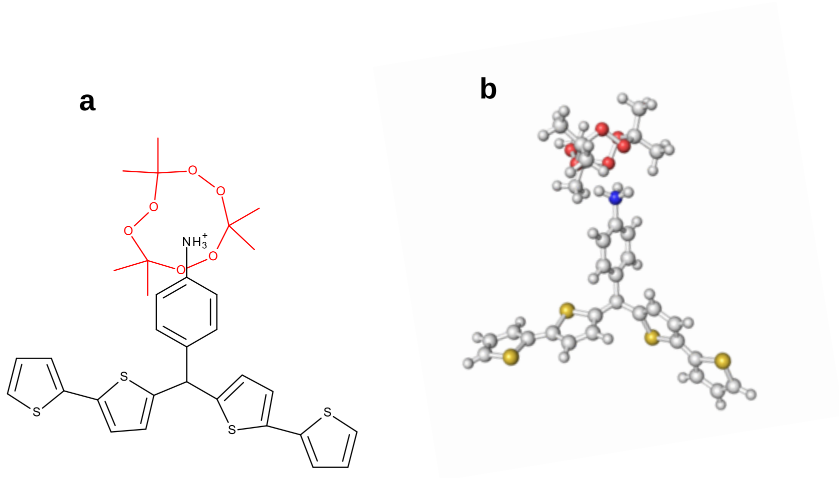


Figure 1. (a) Structural formula of the triacetone triperoxide complex with the functional monomer 4-bis(2,2'-bithienyl)methylalanine and (b) DFT-optimized structure of this complex.

7. Electrochemical deposition of semiconductor layers with plasmonic elements for the photocatalytic decomposition of water (continuation)

We will continue our research on TiO_2 layers doped with non-metals and $BiVO_4$ semiconductor layers deposited on plasmonic structures. We will examine the structures resulting from the electrophoretic deposition of gold nanorods and the deposition of layers of gold in inverted opal structures. We will use these layers for the photoelectrocatalytic decomposition of water. Our research thus far confirms the possibility of producing these layers on solid gold substrates. However, no attempt has yet been made to deposit such layers on plasmonic structures.

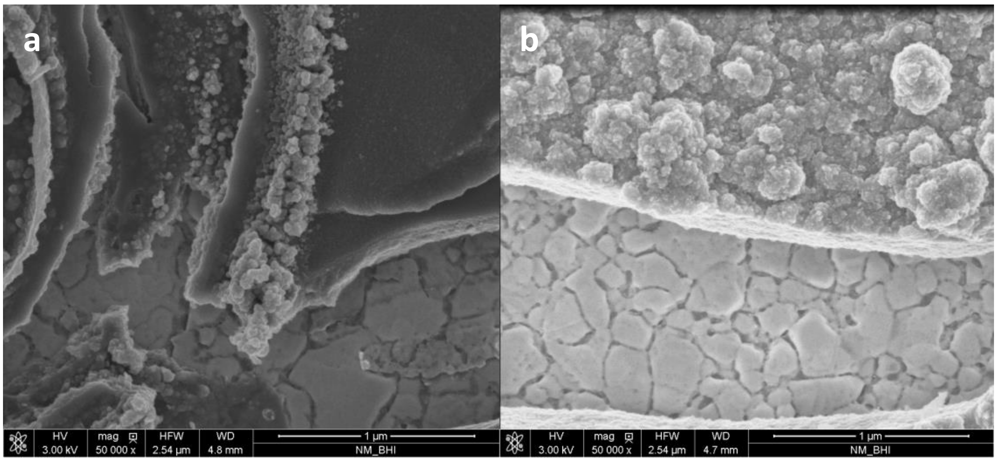


Figure 1. SEM images of a layer of TiO_2 deposited from a solution of 25 mM $TiCl_3$ and 0.1 M KNO_3 in (a) potentiodynamic and (b) potentiostatic conditions.

8. Improvement of the method of producing molecularly imprinted polymers with enhanced surfaces

We will perfect a procedure for preparing layers of molecularly imprinted polymers (MIP) with improved surfaces. After optimization, we will apply this procedure to increase the active surface area of designed and constructed MIP layers for the identification of selected hormones in the plasma. After coupling with selected transducers, we will use these layers as components recognizing chemical sensors. These sensors should exhibit an analytical efficiency (sensitivity, detection, response time, etc.)[1] greater than the efficiency of chemosensors with non-extended surface areas of recognition layers.

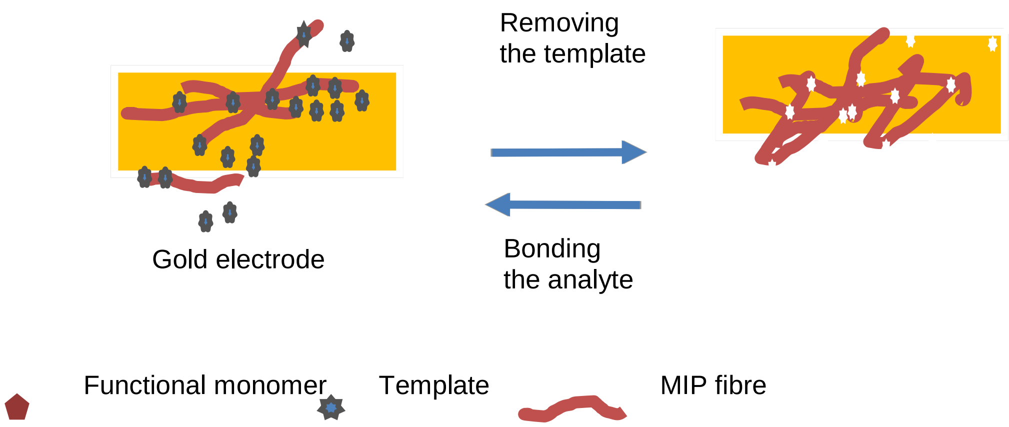


Figure 1. Production of nanostructured molecularly imprinted polymer.

Literature:

- M. Dabrowski, M. Cieplak, P. S. Sharma, P. Borowicz, K. Noworyta, W. Lisowski, F. D'Souzab, A. Kuhn, W Kutner, *Biosens. Bioelectron*. **2017**, 94, 155-161.

Thematic team 4 – Dr. hab. inż. Joanna Niedziółka-Jönsson

SYNERGETIC GROUP

Modification of surfaces to construct (bio)sensors

The purpose of the research is to synthesize new materials and to modify solid surfaces so as to be able to use them as receptor layers for the detection of (bio)molecules.

The effect of the presence of native and additionally introduced oxide layers, the modification to resonance properties, light propagation and the sensitivity of optical systems [1,2,3] will be investigated.

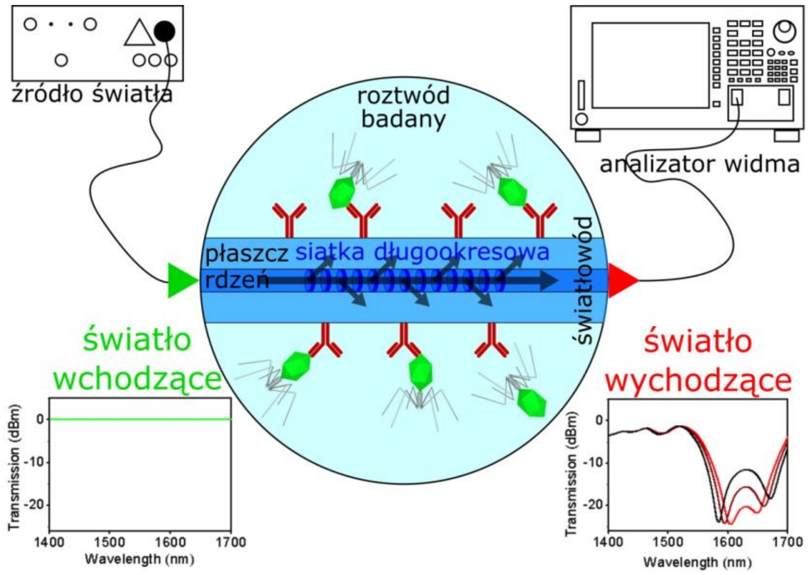


Figure. Diagram of measurement system for the detection of bacteriophages on long-period fibre grating.

We plan to synthesize metallic nanostructures, to use their localized plasmon resonance for the detection of significant analytes, i.e. viruses, environmental pollutants using UV-vis spectrophotometry, both in solutions [4,5], and following their surface immobilization [6].

Literature:

- M. Dominik, A. Lesniewski, M. Janczuk, J. Niedziolka-Jonsson, M. Holdynski, L. Wachnicki, M. Godlewski, W.J. Bock, M. Smietana, "Titanium oxide thin films obtained with physical and chemical vapour deposition methods for optical biosensing purposes", Biosensors & Bioelectronics, 93 (2017) 102-109.
- R. Różycki-Bakon, M. Koba, P. Firek, E. Roźniecka, J. Niedziółka-Jönsson, M. Śmietana, "Stack of nano-films on optical fiber end-face for label-free biosensing applications", Journal of Lightwave Technology, 34 (2016) 5357-5363.
- M. Janczuk-Richter, M. Dominik, E. Roźniecka, M. Koba, P. Mikulic, W. J. Bock, M. Śmietana, J. Niedziółka Jönssona, „Long-period fiber grating sensor for detection of virus concentration" Sensors and Actuators B, 250 (2017) 32-38.
- A. Lesniewski; M. Los, M. Jonsson-Niedziółka, A. Krajewska, K. Szot, J.M. Los, J. Niedziolka-Jonsson; Biocon. Chem., 25 (2014) 644-648.
- P. Kannan, M. Los, J. M. Los, J.oanna Niedziolka-Jonsson; Analyst, 2014, 139 (14), 3563 -3571.

- J. Matyjewicz, A. Lesniewski, J. Niedziolka-Jonsson; Electrochemistry Communications, 48 (2014) 73-76.

Thematic team 5 – Professor Gregorowicz

Research subject: Phase behaviour and dynamics in polymer solutions.

Research plans for 2018

Ionic liquids as solvents in polymer technology – continuation.

Surfactants forming aggregates in ionic liquids can facilitate the dissolution of chemical substances and polymer materials that are practically insoluble in these solvents. As part of this task we plan to continue our study of the aggregation of surfactants in diluted solutions (micellization) and of lyotropic liquid-crystalline phases produced in concentrated solutions of ionic surfactants in hydrophilic ionic liquids. The aim of the research is to establish how the structure of the surfactant, the structure of the ionic liquid and the water content in the system affect the processes of aggregation.

The aggregation studies will involve measurements of surface tension, ^{1}H NMR chemical shifts, diffusion measurements (PFG NMR technique). The research on liquid-crystalline phases will involve optical microscopy, DSC and X-ray diffraction.

Thematic team 7 – Dr. Sashuk

1. Research task

The light controlled anisotropic organization of colloids

2. Aim of research

Controlling the process of self-assembly in a solution poses quite a challenge [1]. This is due to the isotropy of the medium in which the given process takes place. Our aim is to direct self-organization in colloidal solutions.

3. Description and methodology, literature

In our studies we plan to use gold nanoparticles with longitudinal morphology, so-called nanorods. They have at least two crystallographic planes with varying strengths of bonding of molecular adsorbates. We intend to use this property for the selective adsorption of suitably functionalized organic ligands. One of the ligands will be terminated with a macrocyclic ring, and the other, containing an azobenzene group, will act as a photorelay. Under normal conditions, the photorelay in the *trans* conformation will be threaded through the macrocyclic ring causing the arrangement of the nanorods to be side-by-end, *Fig.1.* After irradiation of the system we expect isomerization of the photorelay to the *cis* form and its exit from the macrocyclic gap due to geometric effects. We also expect that the light-induced change in the dipole moment of the photorelay depending on its spatial position will cause the nanorods to be arranged side-by side or end-to-end, *Fig. 1*. On stopping irradiation, this system should return to the initial perpendicular configuration. The nanorods and the ligands will be prepared according to the procedures set out in the literature and our own procedures based on typical retrosynthetic algorithms. The modification of the nanorod surfaces with an organic layer will take place by the formation of gold-sulphur bonds. The self-assembly process will be monitored by UV-Vis spectroscopy and SEM.

[1] Yi, C.; Zhang, S.; Webb, K.T.; Nie, Z. Anisotropic Self-Assembly of Hairy Inorganic Nanoparticles, *Acc. Chem. Res.*, **2017**, *50*, 12-21.

4. Diagram illustrating the research task

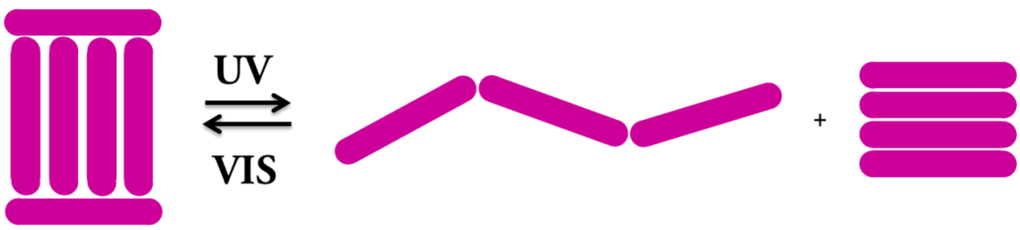


Figure 1. Schematic diagram of light-dependent organization of nanorods in liquids.

Thematic team 8 – Dr. hab. Angulo Gonzalo

SYNERGETIC GROUP

1. The Team's research task

The experimental study of the dynamics and kinetics of photo-induced reactions of electron and proton transfer and energy transfer, initiated by one or two light pulses in liquid solutions and other non-ordered media.

Experimental and theoretical studies of intramolecular reactions using the generalized Langevin equation

2. Aim of research

To improve the physical description, and thus also the possibilities of predicting the course of the reaction.

3. Description and research methods, literature.

Upconversion fluorescence and transient absorption on a short timescale. Stationary electron spectroscopy.

Influence of the excitation light intensity on the rate of fluorescence quenching reactions: pulsed experiments. Gonzalo Angulo, Jadwiga Milkiewicz, Daniel Kattnig, Michał Nejbauer, Yuriy Stepanenko, Jan Szczepanek, Czesław Radzewicz, Paweł Wnuk and Günter Grampp, *Phys. Chem. Chem. Phys.*, **2017**, 19, 6274—6285.

How good is the generalized Langevin equation to describe the dynamics of photo-induced electron transfer in fluid solution? Gonzalo Angulo, Jakub Jędrak, Anna Ochab-Marcinek, Pakorn Pasitsuparoad, Czesław Radzewicz, Paweł Wnuk, Arnulf Rosspeintner, arXiv:1704.06066.

4. Figure illustrating the research task

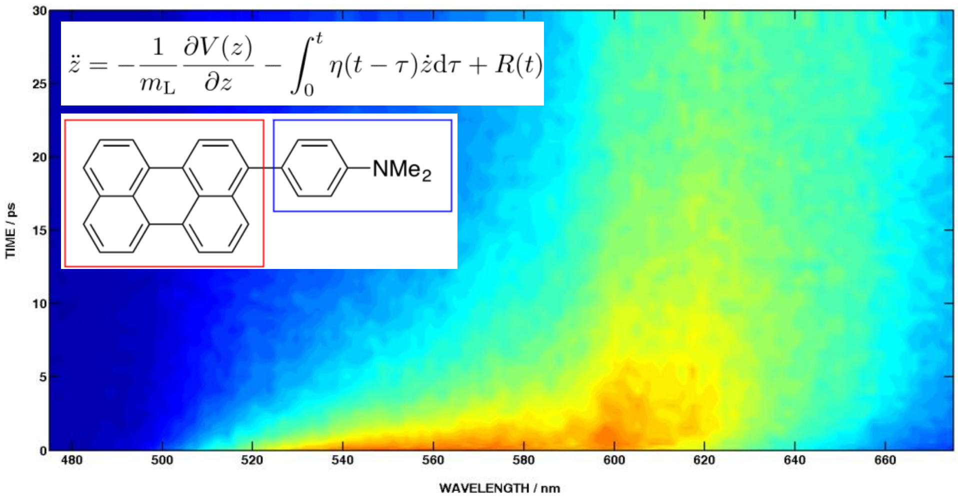


Fig. Evolution of fluorescence of a molecule of perylene-DMA excited by light of wavelength 485 nm in a mixture of glycerol and DMSO of viscosity 5 cP. Fluorescence moves towards the longer wavelengths, which is a consequence of solvent relaxation caused by transfer of the charge from DMA to perylene. The generalized Langevin equation describes this process well.

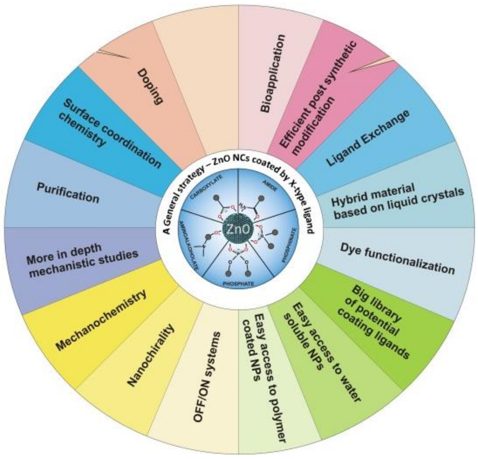
THEMATIC TEAM 9 - Professor dr. hab. inż. Janusz Lewiński

PROSPECTIVE GROUP

The projects implemented in our team concentrate on the synthesis and characterization of defined inorganic-organic organometallic precursors and their transformation into functional materials. In 2016 these studies will be carried out under the following thematic tasks:

1. Obtaining and functionalizing ZnO nanoparticles

We plan to continue research into the design and synthesis of novel molecular precursors of ZnO nanoparticles and their controlled transformations towards well-defined ZnO quantum dots with the desired morphology and physicochemical properties. The topic includes broadening the research to include new ligands and bimetallic systems to improve the luminescence properties and stability of the quantum dots obtained. In addition, functionalized ligands or biodegradable polymers terminated with reactive functional groups, making it possible to obtain bioconjugates, will be used in the studies. Selected systems will be investigated in biological tests to determine their cytotoxicity or widely understood biocompatibility.

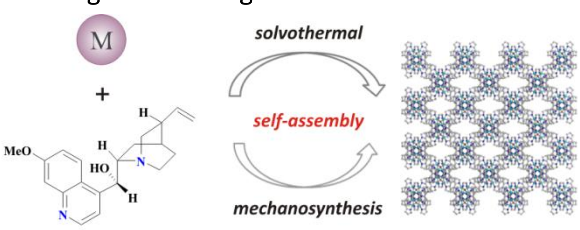


A separate issue to be developed within the topic will be the production of materials based on ZnO nanoparticles for use in organic catalysis and photocatalysis.

2. Construction of microporous functional materials

In the past decade one of the most dynamically developing areas of inorganic and materials chemistry has been the construction in a predictable manner of extensive metal-organic frameworks (MOFs).

In this area of research we plan to develop the synthesis of microporous functional materials using alternative methods to the commonly used solvothermal chemical transformations. To this end, alongside the original *chimie douce* methods developed in our team, we will use mechanosynthesis to efficiently produce complex materials by direct chemical reaction with solid reactants using mechanical force. It is planned to develop this strategy to obtain homochiral coordination polymers and microporous materials based on main group and transition metal complexes as well as alkaloid ligands of cinchona bark. In addition, some of the research will be directed towards the use of well-defined $Zn_4O(RCOO)_6$ complexes as the basic building blocks in the mechanochemical synthesis of model and new MOF materials.



***Publications*:**

- P. Krupiński, A. Kornowicz, K. Sokołowski, A. M. Cieślak, J. Lewiński, „Applying mechanochemistry for bottom-up synthesis and host-guest surface modification of semiconducting nanocrystals: A case of water-soluble β-cyclodextrin-coated zinc oxide", *Chemistry – a European Journal*, 2016, 22, 7817–7823.

- A. Grala, M. Wolska-Pietkiewicz, W. Danowski, Z. Wróbel, J. Grzonka, J. Lewiński,” ‘Clickable’ ZnO nanocrystals: the superiority of a novel organometallic approach over the inorganic sol–gel procedure”, *Chemical Communications*, 2016, 52, 7340–7343.

Thematic team 10 – Professor Hołyst

SYNERGETIC GROUP

1. The application of biological material in chemistry.
2. The aim of the research is to show how living matter and biological material in general can be used in chemical research. Examples are bacterial sensors based on bioconjugates consisting of fluorescent and magnetic nanoparticles with attached bacteriophages – viruses that recognize bacteria, described in our paper BIOCONJUGATE CHEMISTRY 28, 419-425 (2017),
3. Our study methods involve the use of nano-materials in research at the point of contact between biology and chemistry. Typical equipment used in our research includes fluorescence correlation spectroscopy, SEM, TEM, Taylor dispersion analysis, the Langmuir-Blodgett trough, the flow cytometer, a bacterial culture laboratory. We will analyze the effect of the presence of needle-shaped nanoparticles on bacterial culture (fig.1).

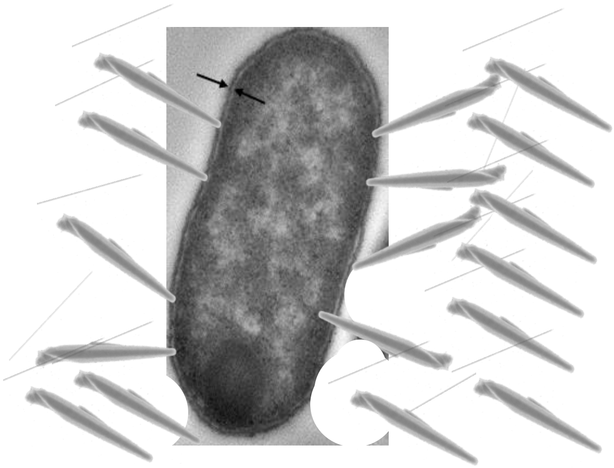


Fig.1 E.coli bacteria subjected to the action of nano-needles of zinc oxide (illustrative image).
Nano-needles SEM image, bacteria TEM image.

Thematic team 11 - Professor dr. hab. Piotr Garstecki

SYNERGETIC GROUP

The research tasks of Team 11 for 2018 include:

1. Work on the fundamental problem of fluid mechanics in the microscale, in particular we are working on the characterization of the velocity of droplet flow in microcapillaries, taking into account the influence of a whole range of factors including fluid viscosity, surface tension, the presence and amount of surfactant, channel cross sectional shape and continuous flow velocity.
2. The development of new methods of micro-fabrication and modification of surface chemistry. As part of this task, we are carrying out a continuum of work ranging from methods of microfabrication through photolithography and soft lithography, mechanical machining, pattern transfer by casting or imprint, and methods for modifying the polymer surface of the microchannels.
3. The development concepts of new research programmes. In this task, in particular, we will continue work on discovering and developing new surfactants to better stabilize the emulsions used in biological experiments and surfactants actively responding to environmental stimuli - temperature, light or, for example, pH of the solution. We are also interested in using techniques developed in our team towards the possibility of guiding the evolution of bacteria.

Thematic team 12 – Dr. hab. Fiałkowski

Self-assembly of magnetic nanoparticles (NP) on phase interfaces.

Aim: (i) To develop a method of synthesis of core-shell NPs having a superparamagnetic core and capable of adsorbing themselves on the oil-water interface; (ii) to investigate the structures created by these NPs in the presence of an external magnetic field (Fig. 1). **Method:** We will use existing methods of synthesis of NPs from iron oxide and develop the technique we have developed in our team [1] of interphase formation of NP monolayers.

Expected effects: The development of a protocol for the synthesis of stable superparamagnetic NPs and the investigation of the 2D structures they create in the presence of a magnetic field on phase interfaces.

Literature:

- T. Andryszewski, M. Iwan, M. Hołdyński, M. Fiałkowski, Chemistry of Materials 28, 5304 (2016)

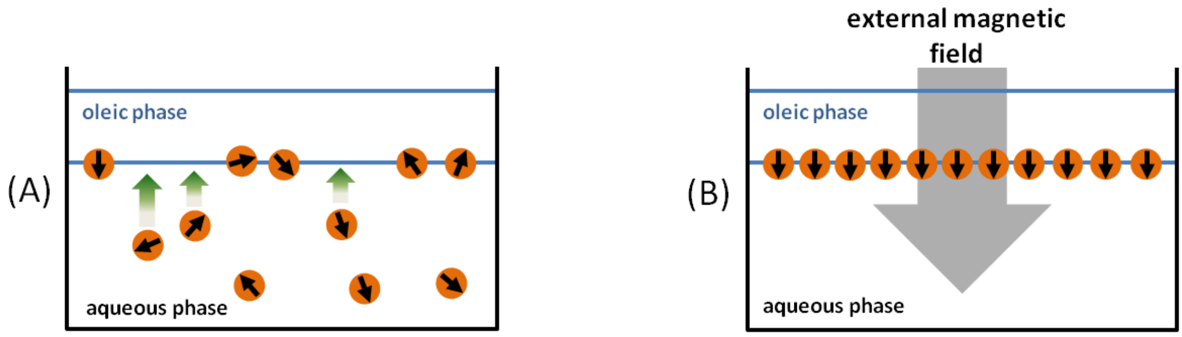


Fig. 1. Diagram of the planned experimental system for the study of superparamagnetic nanoparticles. (A) Suitably functionalized nanoparticles are introduced into the oil-water phase separation boundary where they form a stable monolayer. (B) Then, by means of an external magnetic field the nanoparticles in the monolayer assemble themselves into ordered structures

Thematic team 13 – Dr. hab. Góźdź

To create a model and investigate the short-range attractive and long-range repulsion volumetric properties of fluid. The aim of the research is to examine the creation of ordered structures built of colloid particles. An example of such an ordered structure is shown in

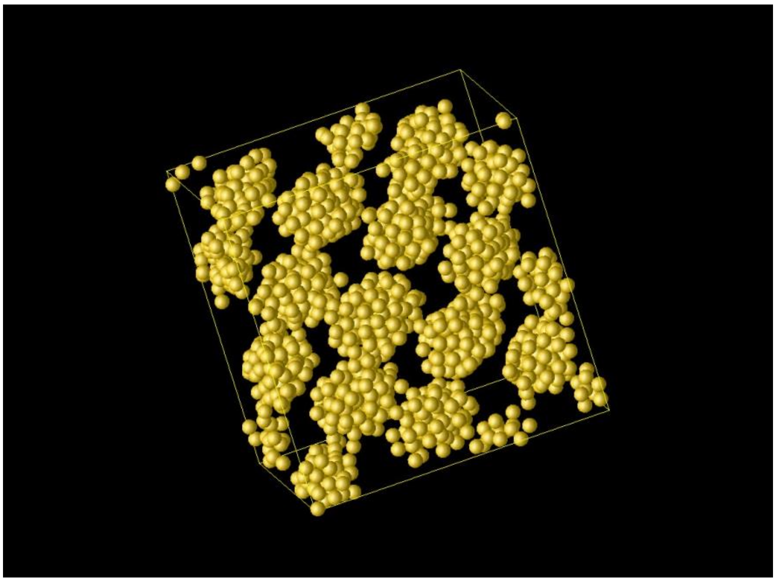


Figure 1. Monte Carlo molecular simulations will be carried out in a large canonical ensemble.

More important publications:

- Góźdź W. T., Ciach A. "Critical point calculation for binary mixtures of symmetric non-additive hard disks" , Cond. Matt. Phys. 19(1) , 13002:1-8, 2016
- A. Ciach, J. Pękalski and W. T. Góźdź, ''Origin of similarity of phase diagrams in amphiphilic and colloidal systems with competing interactions”, Soft Matter 9, 6301 (2013)

Thematic team 14 – Dr. hab. Martin Jonsson Niedziółka

PROSPECTIVE GROUP

Task 1: Detection of neurotransmitters by the spinning drop method

Aim: To design electrodes for the simultaneous detection of multiple neurotransmitters in the presence of interfering substances

Literature:

- *Anal. Methods* **6:** 7532, (2014)
- *Electrochem. commun.* **72:** 46, (2016)

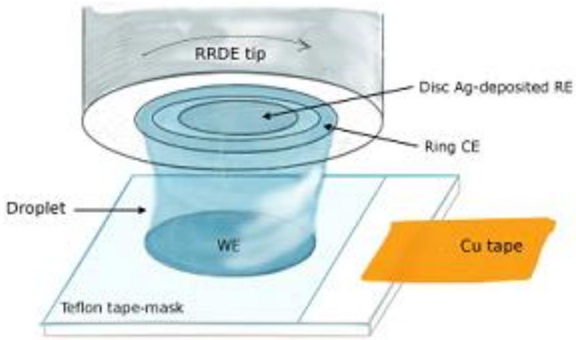


Diagram 1. Scheme of spinning droplet as a method for selective detection of low concentrated neurotransmitters in small volumes on modified electrode

Task 2: Measurement of the endogenous concentration of glutamate in *in vitro* conditions.

Aim: The development of a biosensor enabling long-term measurement of glutamate by electrochemical methods in cell culture conditions.

Literature:

- *Trends in Neurosciences*, **33:**121, 2010
- *Nature*, **420:** 812, (2002).

Thematic team 15 – Dr. hab. Jacinto Sa

Modern heterogeneous catalysis (MoHCa) for 2018

Aims:

- The synthesis and characterization by physicochemical methods of new nanocatalysts.
- The use of catalytic hydrogenation to form added value compounds. All the reactions will involve the formation and/or breaking of chemical bonds and the efficient conversion of toxic compounds into useful and non-toxic products.

Research methodology:

- Catalytic hydrogenation reactions will be carried out in a flow reactor.
- Catalytic materials will be characterized by standard physicochemical methods such as XPS, XRD, FT-IR, SEM.

Expected scientific results:

- The development of new nanocatalysts active in hydrogenation reactions
- The determination of the structure-reactivity relationship with respect to the morphology of metal nanoparticles

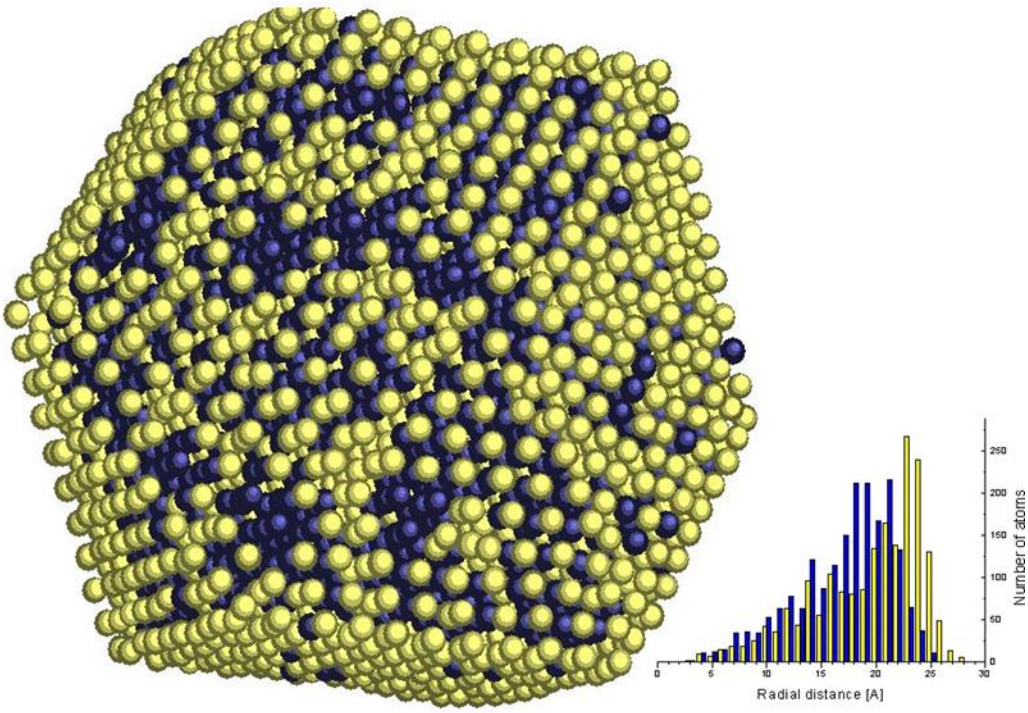
Thematic team 16 – Dr. hab. Kaszkur

Research on the dynamics of changes in the structure of nanocrystalline catalyst systems based on Pt, Ir, Au induced by chemical reaction and temperature

The aim of the research is to find the physicochemical conditions at which the structure of the surface of metal nanoparticles changes (reconstruction), changing their catalytic activity and observing its dynamics. The methodology of the study is based on the diffraction method developed in our team, enabling the observation and interpretation of surface processes in situ on metallic nanocrystals [1-5].

Literature:

- *J. Appl. Cryst.* (2017), 50, 585.
- *PhysChemChemPhys.* (2015), 17, 28250.
- *J. Appl. Cryst.*, (2014), 47, 2069.
- *RSC Adv.*, **(2014),4 (28), 14758.**
- ***Phys.Chem.Chem.Phys.* (2009), 11, 5416.**



Thematic team 17 – Dr. hab. Szmigielski

The Environmental Research Team's planned research task in 2018 will be to identify the processes of the chemical evolution of 3-methylbutane-1,2,3-tricarboxylic acid (MBTCA). This task fits into the long-term cycle of research being carried out by the Team on the mechanisms of smog formation, including its main constituents - suspended particulate matter (aerosol).

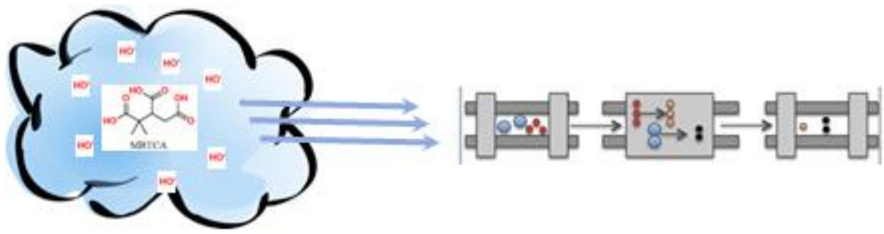


Diagram: Free radical decay of MBTCA in cloud droplets and detection of detection of emerging products

MBTCA is an important marker of aerosol aging in polluted air, resulting from complex changes in the lower atmosphere. Until recently, it was considered to be the end product of oxidation of unsaturated terpene hydrocarbons, including α-pinene, emitted by forest ecosystems in excess of 120 TgC / year. In light of the most recent research conducted in experiments under strictly controlled conditions, it was noted that MBTCA undergoes further oxidation processes in atmospheres whose pathways have not yet been investigated. In addition, MBTCA has a strong affinity for the aqueous phase, which means that this compound may undergo further conversion with highly polar hydroxyl radicals in atmospheric water droplets (rain, mist, etc.) The aim of the proposed work is to identify the unknown MBTCA disintegration paths in the gas phase and in atmospheric water droplets using hydroxyl radical chemistry and the use of tandem mass spectrometry as a diagnostic tool. In the first phase, it is planned to investigate pathways of MBTCA fragmentation in an electrospray ion source, to determine the physicochemical parameters of these processes and to identify the emerging products. In the second phase it is planned to conduct a series of MBTCA reactions in water droplets using the Fenton reaction as a source of hydroxide radicals and to identify the emerging new constituents of particulate matter.

Literature:

- Noziere, B. *at all.*, Chem. Rev., 2015.
- Wayne, R.P., Chemistry of Atmospheres (3rd Ed.), 2017.

Thematic team 21 – Dr. hab. Nowakowski

PROSPECTIVE GROUP

1. Interactions of particles of probes with hierarchical heterostructures

Rationale: The research is aimed at modifying intelligent multi-component nanostructures based on Cu, Ni and Ce, and investigating the interaction of probe particles with hybrid nanocomposites exhibiting catalytic properties. Operando DRIFT and electrochemical measurements will be carried out for the selected gas mixtures and organic solutions respectively. The synthesized new nanomaterials will be characterized in terms of activity for selected processes of oxidation of organic compounds in the gas phase and in solutions, and the results obtained correlated with structure, morphology, donor acceptor properties and the composition and distribution of active centres on the surfaces of nanostructure catalysts. We also plan to investigate them with regard to use in electrochemical sensors.

2. Molecular resolution STM imaging of the adsorption of selected ions in organic and inorganic solutions

Rationale: The aim of the project is to study the adsorption of selected ions on atomic smooth surfaces (e.g. mica, Au (111)) by imaging with an STM microscope. Measurements will be made under electrochemical conditions in selected organic and inorganic solutions and ionic fluids. Tungsten probes insulated in glass and sharpened by electrochemical etching will be prepared. These probes enable atomic imaging of the examined surfaces and are durable when working in both organic and inorganic solvents.

3. Electrochemical characteristics of selected carbon materials for use in supercapacitors

Rationale: The project concerns the preparation of carbon electrodes modified by reduced graphene oxide with nanoparticles of Cu, Ag, Ni. These electrodes will be tested for use in electrochemical capacitors.

4. Correlation of structural, supramolecular, electrochemical properties and electrical aggregation of complex electroactive compounds

Rationale: This is a continuation of STM studies started earlier of the self-assembly of small and high molecular weight electrochemical compounds with potential applications in organic electronics. The aim of the proposed project is to continue the microscopic studies of new complex organic semiconductors and to broaden the knowledge of the structural properties of the produced layers of ordered molecules by their electrochemical and electrical properties. We plan to expand our research methods to include STM in electrochemical conditions, or atomic force microscopy with related methods (with conductive probe, Kelvin microscopy). We expect that the information we obtain will bring us closer to a description of the existing electrical conduction mechanisms in the layers of the investigated semiconductors.

Literature:

- T. Jaroch, A. Maranda-Niedbała, K. Kotwica, D. Wamil, P. Bujak, A. Proń, R. Nowakowski, Self-assembly of tetraalkoxydinaphthophenazines in monolayers on HOPG by scanning tunneling microscopy, Surf. Sci. (2015) 641, 252-259
- K. Kotwica, A.S. Kostyuchenko, P. Data, T. Marszalek, L. Skorka, T. Jaroch, S. Kacka, M. Zagorska, R. Nowakowski, A.P. Monkman, A.S. Fisyuk, W. Pisula, A. Pron, Star-Shaped Conjugated Molecules with Oxa- or Thiadiazole Bithiophene Side Arms Chemistry – A European Journal (2016) 22, 11795-118062

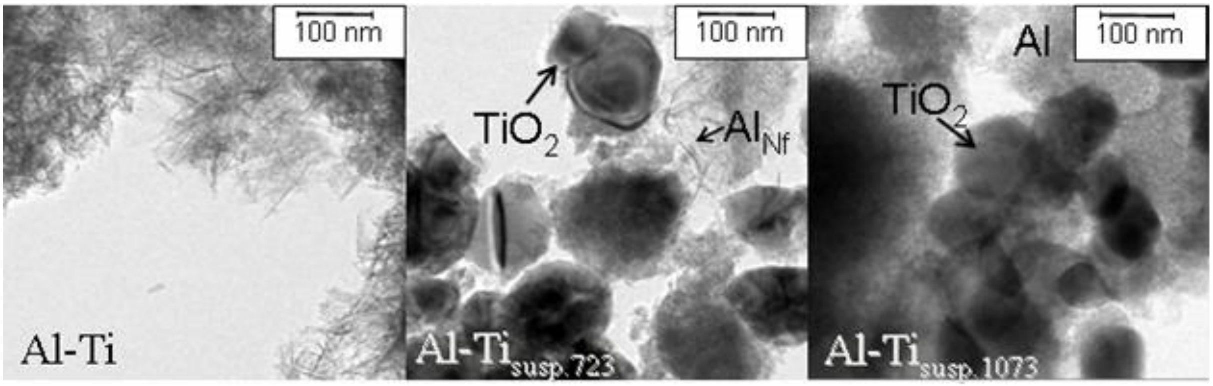


Fig. 1. TEM images of aluminium-titanium nanocatalysts (Subject 1).

Thematic team 22 - Dr. Zarzycki

1. Research task

Self-assembly, charge redistribution and interactions in supramolecular systems and at phase boundaries.

2. Aim of research

To design and obtain supramolecular systems based on macrocyclic compounds. To evaluate the effect of supramolecular modifiers on precipitation and dissolution processes of biominerals.

3. Description and methodology

We plan theoretical and experimental research on intermolecular interactions and charge transfer in the limited geometry of the macrocyclic skeleton and at the phase interface in crystallization/dissolution processes of biominerals.

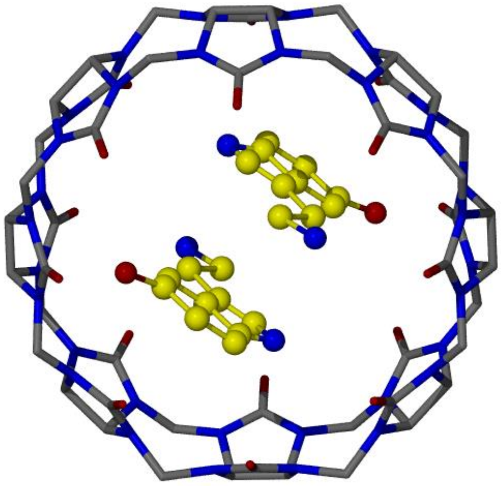


Figure 1. Two particles of serotonin in the gap in cucurbit[8]uril –crystalline structure.

Thematic team 24 – Professor Górecki

In 2018 Team 24 will pursue two directions of research:

1. The first of these will be the use of artificial intelligence techniques, and in particular genetic algorithms to design chemical systems capable of processing information. This topic will be an extension of the NCN project: **Strategies for teaching chemical classifiers based on reaction-diffusion processes** (**OPUS 8)** planned for 2015-2018. So far, the results have shown that even simple networks consisting of more than a dozen objects are able to perform non-trivial operations.

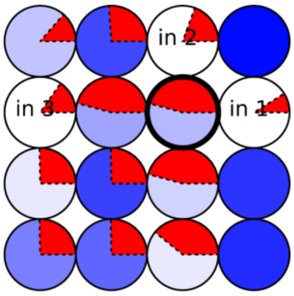


Fig.1. An example of a chemical system that recognizes the position of a point relative to a sphere, which uses drops in which the Belousov–Zhabotinsky reaction is occurring, represented in the illustration as discs, to process information. The blue colour codes the conditions of the reaction, red evaluates the quality of the result obtained by observing the time evolution of the selected drop [1].

In 2018 we plan to include a broad class of non-linear chemical processes as a medium for processing information. We also plan to investigate various strategies for reading the result based on the temporal evolution of the system. It will be important to associate the methods we develop with the concepts of Reservoir Computing [2].

2. The second subject of Team 24 will be research into the complex processes and structures enforced by influences of a specific nature. Its aim is to find out about the properties of dynamic and thermodynamic systems with heterogeneous spatially distributed particles and the processes of spatial-temporal self-organization in such systems. Within this topic we will examine:
   - The dynamics of structures composed of particles interacting by changes in surface tension caused by the gradient of surface concentration of particular molecules,
   - The process of spontaneous aggregation of charged nanoparticles with attraction at short distances, - the influence of boundary walls, charged or not, on the properties of ionic liquids and their mixtures with liquids with electrically neutral molecules,
   - Simulations of the dynamics of the structures obtained by passivation of a metal electrode under galvanostatic conditions taking into account the polarization of the metallic surface and the presence of halides,
   - Microscopic simulations of the effect of flow over the surface of a liquid on the evaporation rate.

Literature:

- K. Gizynski, J. Górecki, CMST 22(4) 167-177 (2016), DOI:10.12921/cmst.2016.0000057
- Miller, J. F., Harding, S. L., and Tufte, G. (2014). Evolution-inmaterio: evolving computation in materials. Evolutionary Intelligence, 7(1):49–67.

Thematic team 25 – Professor Kołos

Task: Spectroscopy of nitriles of astrochemical significance.

Aims: A description of the electron spectroscopy of C_5N^- anions, theoretical predictions of the electron transition energy of isomers of cyanoacetylene and cyanodiacetylene, an attempt to isolate methylidophosphate (HCP) in cryogenic matrices.

Description, methodology: Analysis of IR absorption showed the presence of C_5N^- among the photolysis products of cyanodiacetylene (HC_5N) in solidified noble gases [1]; Initial experiments indicate the possibility of investigating the electron transitions of this anion by measuring the luminescence [2] induced by a tuned UV laser. This will be undertaken jointly with the Institut des Sciences Moléculaires (Orsay, France). The electronic spectra of HC_3N and HC_5N isomers will also be calculated. Synthetic work (HCP, hydrogen cyanide analogue) will be carried out in collaboration with the Ecole Normale Supérieure de Chimie (Rennes, France).

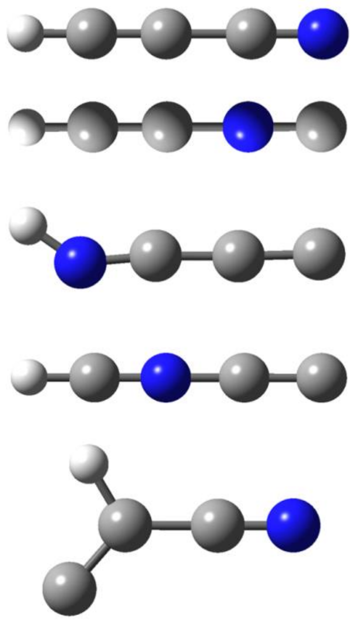


Fig. 1. Expected (DFT) structures of particles with the stoichiometry of cyanoacetylene. The electron spectrum (UV absorption) is only known for the basic isomer.

Literature

- Coupeaud, M. Turowski, M. Gronowski, N. Piétri, I. Couturier-Tamburelli, R. Kołos, J.-P. Aycard, J. Chem. Phys. 128 (2008) 154303.
- Crépin, M. Turowski, J. Ceponkus, S. Douin, S. Boyé-Péronne, M. Gronowski, and R. Kołos, Phys. Chem. Chem. Phys. 13 (2011) 16780.
- J. C. Guillemin,T. Janati, P. Guenot, P. Savignac, J. M Denis, *Angew. Chem.* **103** (1991) 191.

Thematic team 26 – Professor Pietraszkiewicz

1. Subject:

The synthesis and photophysical properties of donor-acceptor triacetylphloroglucinol derivatives.

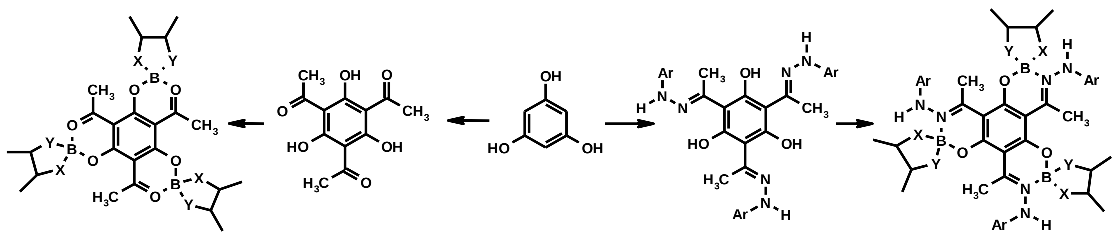
2. Aim of the research:

The aim is to investigate a new class of fluorophores with expected high photoluminescence efficiency based on the 2,4,6-triacetylphloroglucinol basic skeleton.

3. Description and methodology, literature.

Acetylation of anhydrous phloroglucinol in acetyl chloride leads to a triacetyl derivative with a high efficiency. This substrate will be used to synthesize derivatives of the Schiff base type with hydrazides and subsequent cyclization with BF_3. Triboric compounds will be converted into derivatives such as boradiazoles, boraoxazoles. The photophysical properties of the new fluorophores will be examined by fluorescence spectroscopy.

4. Figure illustrating the research task



Thematic team 27 – Professor Radzewicz

In 2018, it is planned to continue research on a parametric amplifier based on the Chirped Pulse Amplification technique in crystals with high nonlinearity. We intend to modify the preamplifier by changing the BBO crystal to a BiBO crystal. According to our preliminary calculations, this change will reduce the parametric fluorescence. The increased amplification factor in BiBO crystals will increase the stability and efficiency of the entire parametric amplifier system. Our solution will enable the construction of a compact and efficient device that produces laser pulses with a peak intensity greater than 40 TW on a central wavelength of 800nm.

Fibre optic sources of ultrasonic laser pulses.

In the course of further work on fibre optic lasers we intend to develop new structures of fully fibre optic oscillators on only positive dispersion media for a spectral range of approximately 1 µm. We plan to further investigate the effect of the spectral filtration shape on the propagation of the impulse in fully fibre optic laser cavities of completely normal dispersion. It is planned to construct an oscillator on spectral filters with Gaussian transmission curves but with different half-widths. Particular emphasis will be put on the use of photonic fibers with increased nonlinearity and reduced dispersion to construct optical fibre oscillators with completely normal dispersion. We will test new configurations of saturated absorbers based on pulse interference in polarization-supporting optical fibres. We also intend to expand the fibre optic amplifier with large core diameter fibres that will enable the pulses to be boosted to significantly greater energies while simultaneously reducing the effect of nonlinear effects on the boosted pulses.

Developing new methods of ultrafast particle spectroscopy. In particular, we are planning to expand the Ramanowski Femtosecond Spectrometer to be able to record FSRS spectra in the UV area, which will increase the sensitivity of the instrument. To this end, we have planned research to produce a low-noise coherent white light generated in calcium fluoride by a laser pulse with a wavelength of 515 nm.

Thematic team 28 – Dr. hab. Colmenares

PROSPECTIVE GROUP

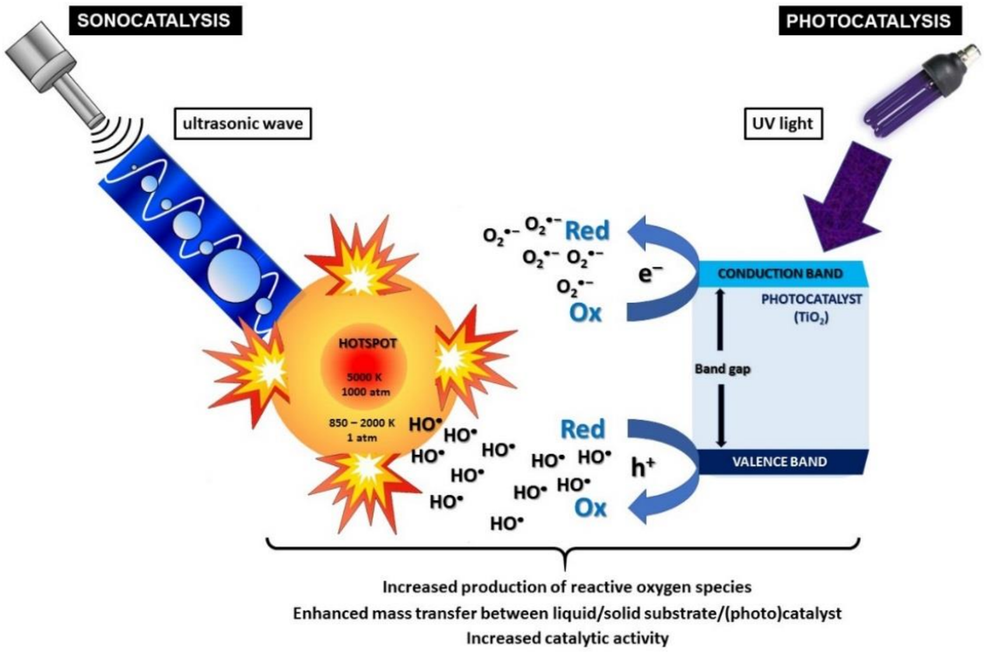


Fig.1. Schematic diagram of proof of the synergistic concept using sonochemistry and photocatalysis to convert lignocellulosic biomass.

In 2018 we plan to carry out the following research tasks:

- Optimization of our "sonophoto-embedding" method for the synthesis of multidimensional, binary and ternary hybrid photocatalysts for the degradation of organic compounds in water and air, and for the selective photo-oxidation of selected organic molecules (e.g. alcohols).
- The design and implementation of preliminary experiments to test our (in collaboration with France) proof of the concept: "The synergistic approach using sonochemistry and photocatalysis to convert lignocellulosic biomass" (Figure 1).
- Studies on the sonocrystallisation of semiconductor oxide metals (e.g. TiO2, Fe2O3): the use of acoustic cavitation for the synthesis of nanoscale crystalline metal oxides under very mild pressure and temperature conditions (e.g. 1 bar, <70°C).

Aim of the research

The aim of our research will be to investigate the use of physicochemical effects (e.g. better mass diffusion, photocatalytic regeneration, better mixing, generation of active radical chemical species) promoted by the use of ultrasound in selective and total photocatalytic oxidation reactions of selected model lignocellulose components in liquid solutions. In addition, an additional research objective will be to explore a methodology based on the synergetic action of sonochemistry and photocatalysis for the synthesis of new hybrid materials based on, among others, carbon carriers (including biopolymers) for their use in photo-catalytic oxidation processes.

Description and methodology

The proposed research methodology includes: **a.** the use of ultrasonic waves of various intensities and frequencies to assist in the photocatalytic process of selective oxidation of selected components of the structure of lignocellulose (e.g. aromatic alcohols, sugars), **b.** the preparation of innovative hybrid photocatalysts based on semiconductors (e.g. TiO_2, Fe_2O_3) and a carbon carrier (e.g. a lignocellulose biopolymer) by conventional methods (e.g. sol-gel) assisted by the unconventional, energy-efficient "sono-and/or-photo" approach (ultrasound and light sources of radiation) and their characterization by techniques such as: XRD, FTIR, HRTEM, XPS, UV-vis. A full range of basic kinetic studies (reaction of selective photocatalytic oxidation of the components of lignocellulose in the liquid phase) and studies of the stability/recycling of photocatalysts will be carried out using suitable (sono)-photo-reactors, high performance liquid chromatograph and gas chromatography.

Literature:

- A sustainable approach for lignin valorization by heterogeneous photocatalysis, Shao-Hai Li, Siqi Liu, Juan C. Colmenares and Yi-Jun Xu. Green Chemistry (Cover Page), 18(3) (2016) 594 - 607
- Heterogeneous Photocatalysis: From Fundamentals to Green Applications (Book Edition), Editors: Juan Carlos Colmenares and Yi-Jun Xu. ISBN 978-3-662-48717-4. Springer-Verlag Berlin Heidelberg, 2016 (DOI: 10.1007/978-3-662-48719-8)
- Photoactive Hybrid Catalysts Based on Natural and Synthetic Polymers: A Comparative Overview, Juan Carlos Colmenares and Ewelina Kuna. Molecules 2017, 22(5), 790; doi:10.3390/molecules2205079
- Sonocatalysis: A Potential Sustainable Pathway for the Valorization of Lignocellulosic Biomass and Derivatives, Ewelina Kuna, Ronan Behling, Sabine Valange, Gregory Chatel, Juan Carlos Colmenares. Topics in Current Chemistry (Z) (2017) 375: 41. doi:10.1007/s41061-017-0122-y
- A combined approach using sonochemistry and photocatalysis: How to apply sonophotocatalysis for biomass conversion?, Gregory Chatel, Sabine Valange, Ronan Behling, and Juan Carlos Colmenares. ChemCatChem (2017). Accepted Author Manuscript; doi:10.1002/cctc.201700297
- In Situ Coupling of Ultrasound to Electro- and Photo-Deposition Methods for Materials Synthesis, Agnieszka Magdziarz and Juan C. Colmenares. Molecules, 22(2) (2017) 216; doi:10.3390/molecules22020216
- Sonochemistry: from Basic Principles to Innovative Applications, Editors of this Topical Collection: Juan Carlos Colmenares and Gregory Chatel. Topics in Current Chemistry (2017), ISSN: 2365-0869 (Print) 2364-8961 (Online), Springer International Publishing Switzerland 2017.
- Sustainable hybrid photocatalysts: titania immobilized on carbon materials derived from renewable and biodegradable resources, Juan C. Colmenares, Rajender S. Varma and Paweł Lisowski. Green Chemistry, 18 (2016) 5736-5750.
- Synthesis of Photoactive Materials by Sonication: Application in Photocatalysis and Solar Cells, Juan C. Colmenares, Ewelina Kuna and Paweł Lisowski. Topics in Current Chemistry (2016). DOI: 10.1007/s41061-016-0062-y.

Thematic team 29 – Professor Waluk

PROSPECTIVE GROUP

Electronic and oscillation structure of molecules exhibiting light-induced transformation

The aim of the research is to understand the mechanisms of processes occurring in electronically excited states of organic molecules. In particular, it concerns conformational changes and their coupling to photoinduced charge transfer.

The study methods will include measurements of stationary and time-distributed electron and oscillating spectra. Experiments will be supported by quantum-chemical calculations.

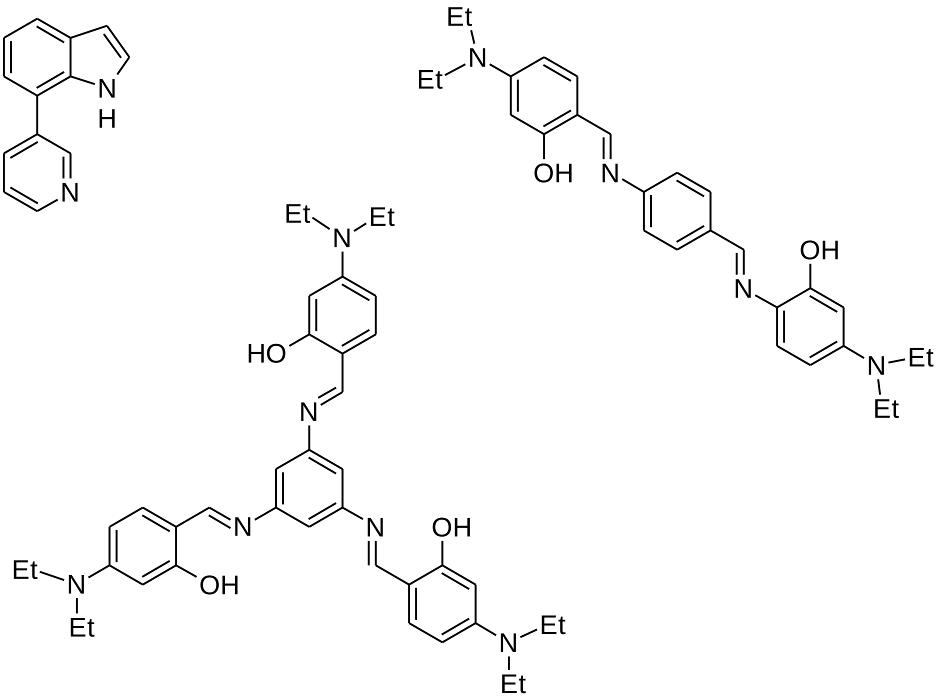
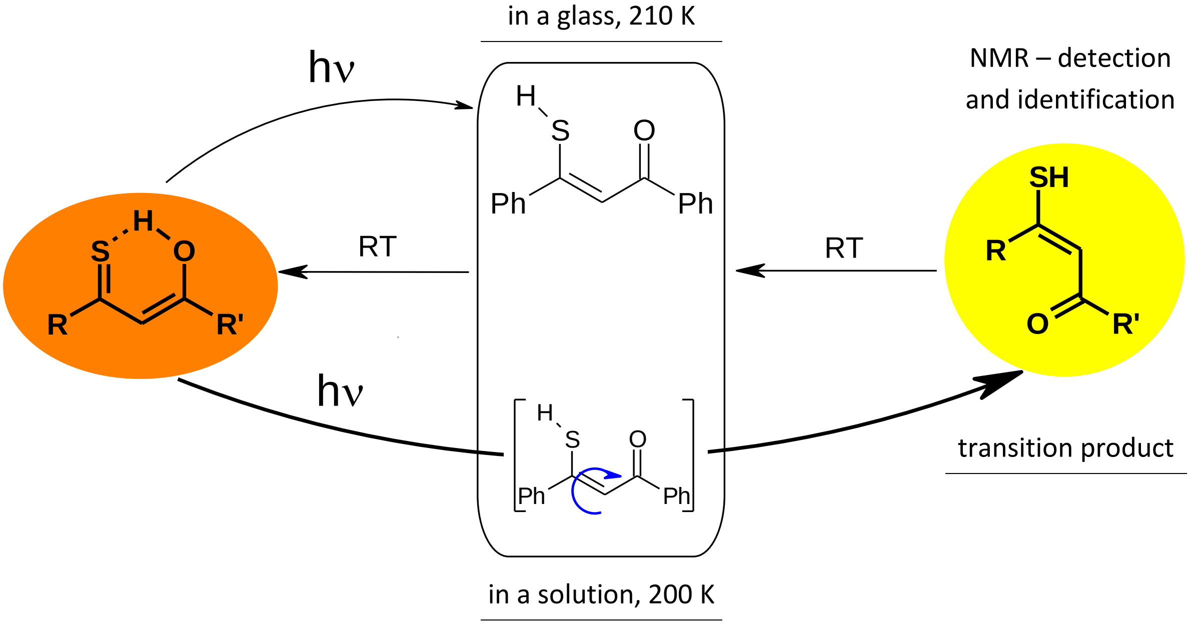


Figure 1. Examples of the molecules planned for the study of photoinduced conformational transformations.

Thematic team 30 – Dr. Ratajczak

NMR study of photochemical processes

The use of NMR spectroscopy coupled with laser photolysis is a method that in some cases enables the identification of a transition product of the photoreaction, and also allows for the suggestion of a photochemical reaction pathway of this process.



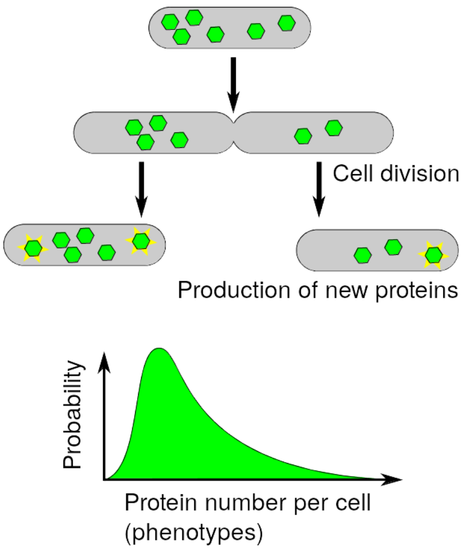
This type of analysis is possible by measuring the NMR of the sample directly exposed in the magnetic resonance cavity. In addition, lowering the temperature of the sample results in a prolongation of the lifetime of the transition product, increasing its chances of being detected and identified. Using this apparatus we would like to look at photochromic processes for selected molecules in which colour change is related to the change in molecular geometry. Examples of such molecules are β-thioxoketones and some organometallic complexes.

The aim of research using NMR spectroscopy coupled with laser photolysis is to better understand the processes that photochromic molecules undergo under the influence of light and to investigate the possibility of controlling them by changing the external conditions (e.g. solvent, wavelength of light, temperature).

Thematic team 31 – Dr. Ochab – Marcinek

Subjects to be studied:

1. Modelling stochastic gene expression in cells undergoing division.
2. Understanding how the inheritance of a random number of proteins due to cell division affects their phenotypic heterogeneity.
3. Modelling the kinetics of biochemical reactions leading to protein synthesis by means of computer simulations and mathematical description.

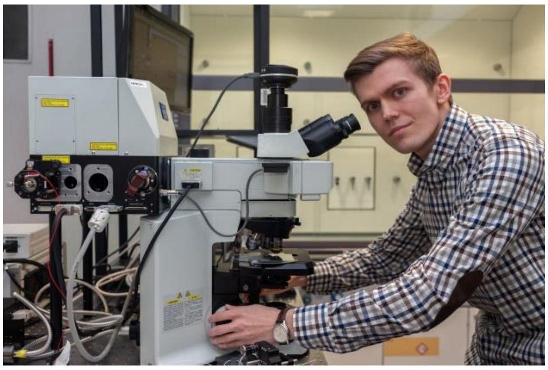


Thematic Team 32 – Professor Wojtkowski

Research task: The development of new physicochemical methods supporting biosensors.

Aim of the research: The main objective of the work will be to develop optical methods using partially coherent light and fluorescence methods to study the dynamics of intracellular structures and bacterial and viral systems.

Planned scientific and practical effects: This year we will focus our activities on the development of OCM (Optical Coherence Microscopy), a technique that makes it possible to study the dynamics of small objects. The planned effects of the research will be new imaging techniques that will enable optical imaging in living organisms.



Confocal microscope system adapted for the OCM microscope