*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

3rd annual update of IPC research programme

[Deliverable D 3.4]

Level of dissemination: Public

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I. Introduction

Consistent with the CREATE proposal, the Deliverable 3.4 consists of an upgrade of IPC research plan consulted with the ERA Chair holder and presented to the Scientific Council of the Institute (**see annex no. 1 for details**). Due to the change in procedure, IPC no longer submits its research plans to the Ministry of Science and Higher Education. Currently, we only report the results of research and obtained funding.

II. Strategic projects

Professor Maciej Wojtkowski, his team (Physical Optics and Biophotonics Group) and the synergetic teams will continue carrying out **three**, previously reported under Deliverable 3.2, **strategic projects of huge impact on IPC**, such as:

(1) Physical Chemistry of biological evolution

(2) Research Agenda of Translational Eye Research

(3) Soft Granular Matter and Tissue Engineering

Their high level of complexity and ambition of proposed research topics requires multiannual studies. Deliverable 4.4 will detail the current status of their implementation.

III. Review and recommendations

The ERA Chair holder, Professor Maciej Wojtkowski, got acquainted with the current research programme of IPC. After thorough analysis, Professor Wojtkowski decided to extend the list of synergetic groups (i.e. groups intended for close collaboration with POB) by:

- ***Group of Cooperative catalysis*, led by Dr hab. Adam Kubas**

Dr Adam Kubas has been developing computational methods for chemistry. Inspired by the ERA Chair holder's work, he has undertaken a new research topic aimed at an analysis of a structure of a retinal protein. Dr Kubas's group seeks theoretical tools and concepts for the use in the growing field of cooperative catalysis. The use of high-level quantum chemical methods enables to provide quantitative data of controllable accuracy allowing for *in silco* design of efficient catalysts. Professor Wojtkowski initiated collaboration between dr Kubas and Professor Palczewski (the University of California, Irvine (USA)) to start work on (photo)catalytical E/Z-isomerization of retinoid derivatives. The geometric configurations of retinoids have an enormous impact on their chemical and biological properties.

The lab visit of Dr Kubas to the Palczewski's lab took place in 2019 as one of the lab visits carried out under the CREATE project. The collaboration will be further strengthened as Dr Michał Kochman (from the Palczewski's lab) will start his postdoctoral fellowship at Dr Kubas' group. Michał's work will focus on the development of ultra-fast methods for the theoretical description of the excited state dynamics using machine learning techniques.

Except for the inclusion of the other research group into synergetic groups of Professor Wojtkowski, further analysis led Professor Wojtkowski to the establishment under the Department of Physical Chemistry of Biological Systems of a new research group, i.e.:

- ***Group of Living Materials,*** **led by Dr Jan Paczesny**

Inspired by the interdisciplinary activities of the ERA Chair holder, Dr Paczesny introduced to the research agenda of IPC the studies on virus stability. The newly set group, recently, has received from the National Science Center (NCN) a grant funding - Sonata Bis to research modulation of stability of virions. Bacteriophages, i.e., viruses which hosts are bacterias, were chosen as model viruses. Within hours a single bacteriophage can multiply in millions of copies inside bacteria using biochemical machinery of the host. It usually ends with the death of bacteria. In each bacterial cell, up to a few hundred copies are formed and released, causing a bacteria-killing cascade, which is difficult to stop. The bacteriophages are used as active ingredients in biocontrol agents, in phage therapies (against drug-resistant bacteria), as sensing elements of biosensors, carriers of genetic information in gene therapies, or in phage display method. Importantly, some species are regarded as great models routinely utilised for studies on viruses attacking eukaryotic (also human) cells.

The research activities of the Department of Physical Chemistry of Biological Systems, headed by Prof. Wojtkowski, enabled the intensification of the activities of synergetic and prospective groups, causing changes in the research activities of the entire IPC. This is confirmed by the synergies of the research plans of the abovementioned groups and joint research projects. Specific joint research projects will be reported under D.4.4.

The IPC research programme – with a particular focus on the research portfolio of new synergetic research groups – was presented to the CEO of collaborating companies with a request to express their opinions:

pt. 26.06.2020 17:42

P

phageconsultants@phageconsultants.com

Dr. Jan Paczesny research

Do mkuczynska@ichf.edu.pl

To whom it might concern

This email is to confirm that the research conducted by a team led by Jan Paczesny ("Living material") at the Institute of Physical Chemistry of the Polish Academy of Sciences is of interest to Phage Consultants and Acteryon companies. Jan Paczesny is working on means of stabilization and deactivation of bacteriophages. This issue is vital as phages might be our enemies (e.g., in biotechnological plants, where they interfere with bacteria-based processes of production of active substances) or allies (in phage therapies or biocontrol applications, where phages act as antibacterial agents). Phage Consultants is a company dealing with bacteriophage infections in biotechnological plants, and the company is interested in the introduction of new means of bacteriophage deactivation. Acteryon is working on the utilization of bacteriophages in biocontrol application, and the company is interested in increasing the stability of phage formulations.

I am a CEO of Phage Consultants and CEO of Acteryon.

Yours sincerely
Macin Łoś

Phage Consultants

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To whom it might concern!

This email is to support Jan Paczesny and his team named "Living materials" as a research group that focuses on solutions of high application potential. We collaborate to introduce new antibacterial coatings that might be applied to decrease the formation of bacteria biofilms at the surface of dental materials.

I express this opinion as CEO of "Jan Łyczek Indywidualna Praktyka Stomatologiczna".

Yours sincerely
Jan Łyczek, PhD, MSc

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June 30, 2020

Dear Prof. Wojtkowski

I write today to express my strongest support of the scientific work you are performing in collaboration with Dr. Adam Kubas.

We believe that this research carried out by Dr. Adam Kubas is extremely important in understanding the mechanisms of vision and thus furthering the development of new pharmaceutical technologies toward the treatment of eye diseases and delaying the process of visual aging. The calculations of geometric configurations of molecules are key components for triggering the phototransduction and have enormous impact on visual activity. Considering the synergies between the expertise of Dr. Kubas' group at the Institute of Physical Chemistry of the Polish Academy of Sciences and Prof. Palczewski's science team at the School of Medicine, University of California Irvine, we offer our strongest encouragement to continue the collaboration between these groups.

Sincerely,

Vida M. Tripodo
Director

ANNEX

IPC research programme

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

Research group 1 – Plasmonic nanostructures for bio-spectroscopic analysis

Dr hab. Agnieszka Kamińska

Research task

1. SERS (surface-enhanced Raman spectroscopy) studies of the benign and malignant pleural fluids in relation to the stage of lung cancer

Research task description

The purpose of the research is a quantitative and qualitative analysis of obtained SERS data in terms of the stage of cancer and the possibility of differentiation based on the observed spectral changes. The tests will include the analysis of pleural fluid samples of various origins, including those caused by infections (e.g., pneumonia, tuberculosis, liver or kidney disease as controls) and benign and malignant tumours. SERS spectra will be collected by the sample mapping method. In the analysis of the obtained spectra, we intend to use the principal component method (PCA), which will allow distinguishing spectra of different samples.

Research group 2 – Living Materials

Dr Jan Paczesny

Research tasks

1. Modification of virus stability
2. Biology inspired inanimate systems

Research task description

1. Grant Sonata Bis (leader Jan Paczesny) regarding modification of virus stability. Depending on needs, one has to fight or support viruses. Viruses will be stabilised by external linkers. We search for both chemical and physical factors affecting the stability of model viruses - bacteriophages.

2. Under the OPUS grant (leader Jan Paczesny) research will be conducted on responsive chemical systems, primarily on thin films of specially designed nano-objects. In the Sonata grant (leader Konrad Giżyński) the main task is the controlled formation of colloidal chains using dielectrophoresis as well as magnetic and capillary forces.

Research group 3 – Physical Optics and Biophotonics Group

Professor Maciej Wojtkowski

Research task

Introduction of biomarkers for monitoring therapy against brain tumour using OCMA imaging technique.

Research task description

Aim of the research: to develop new, non-invasive methods of monitoring brain glioma therapy using OCM microangiography technique.

Methods: between 2018 and 2020, we have developed a new OCM instrument dedicated to imaging of the brain circulation system of rodents in three dimensions. In this project, we will analyse the signals obtained from the OCMA device and look for biomarkers to monitor therapy aimed at

stopping brain tumour development. The experimental system is currently installed in the M. Nencki Institute of Experimental Biology where we can perform animal studies.

Research group 4 – Surface Nanoengineering group

Dr hab. inż. Joanna Niedziółka-Jönsson

SYNERGETIC GROUP

Research task

Surface modification of signal transducers to study molecular interaction

Research task description

The aim of the research is to modify the surface of optical fibre probes to be used as transducers to study molecular interaction and detection of (bio)molecules. In our research, we will use an interferometry method to determine the rate constants of association and dissociation reactions.

Moreover, we will use the surface plasmon resonance of metallic nanostructure to study molecular interaction between peptides and proteins, and bacteriophage adhesin and lipopolysaccharides with the help of UV-vis spectrometry in suspensions.

Research group 5 – Phase behaviour and dynamics in polymer solutions

Professor Jacek Gregorowicz

Research task

Ionic liquids as solvents in polymer technology – continuation

Research task description

Within the project in 2021, we plan to continue investigations of surfactants aggregation, mainly ionic surfactants, in dilute solutions (micellisation) and investigations of lyotropic liquid crystalline phases form by these surfactants in hydrophilic ionic liquids. We aim at understanding how the structure of a surfactant, the structure of an ionic liquid and water present in a system influence the aggregation process. The investigations of the aggregation processes will obey measurements of surface tension, ^{1}H NMR chemical shifts and diffusion coefficients. Investigations of liquid crystalline phase will be performed with use of optical microscopy, DSC and X-ray diffractometry. In addition investigations of micellisation processes with confocal microscopy is planned.

Research group 6 – Nanoelectrochemistry group

Dr hab. Wojciech Nogala

Research task

Development of Faradaic current measurement method with fluorescence microscopy

Research task description

The number of Faradaic electrons monitored during single entity charge transfer processes is often below the currently available detection limits. We plan to use bipolar microelectrode setup, coupled with optical detection of the electrogenerated fluorophore, to overcome the limitations of electrochemical detection of single entities. We will utilise the fact that a single fluorescent molecule can be easily detected, and that the quantum yield of some fluorescent molecules can be

enormously enhanced or quenched (switched on or off) by electron transfer. This will enable the charge transfer to/from individual electroactive molecules to be studied.

Research group 7 – Chemistry in Confined Spaces

Dr Volodymyr Sashuk

Research task

Photoisomerisation of azobenzenes under dual confinement

Research task description

The aim of the task is to study the photoisomerisation of azobenzenes on the surface of gold nanoparticles in the presence of organic macrocyclic compounds. The kinetics of the process and the degree of isomerisation depending on the curvature of the surface and the size of the macrocyclic cavity as well as the presence of functional groups will be investigated.

Research group 8 – Dynamics of light-induced bimolecular reactions

Dr hab. Angulo Gonzalo

SYNERGETIC GROUP

Research tasks

1. Chemical Manoeuvres in the Dark
2. Chemical Reactions under Weird Photoselection

Research tasks description

1. Chemical reactions have been extensively studied in sub-nanoseconds after photoexcitation. However, studies of fast chemical transformations in the ground electronic states, in which most of the chemistry takes place are scarce. It is possible now to improve this thanks to infrared sub-picosecond light sources and transient Raman probing, a technology developed in the Laser Centre. This allows to selectively excite vibrationally the ground state of molecules in solution to trigger a chemical reaction and monitor the changes in their nature over time as the reaction proceeds. This task is performed in collaboration with a group 27. Our task will be planning and analysing the experiments.

2. A polarised pulse of light excites electronically only a set of molecules in a sample with the proper spatial orientation. This depends strongly on the intensity of the pulse. Despite known for a long time, there are few examples of this phenomenon and, to our knowledge, no studies of how this affects the dynamics of chemical reactions and the observables in experiments monitoring fluorescence and transient absorption in the sub-nanosecond and sub-picosecond time scales. The effects are expected to strongly correlate with molecular size and the relaxation characteristics of the medium. We plan to study them, both from a theoretical and an experimental point of view.

RESEARCH GROUP 9 – Coordination metal complexes and functional materials

Professor Janusz Lewiński

PROSPECTIVE GROUP

Research tasks

1. Synthesis and characterisation of hybrid organic-inorganic lead and lead-free halide perovskites.
2. Development of new catalytic systems for CO2 photoreduction based on ZnO nanocrystals derived from organometallic approaches

Research tasks description

1. We aim to raise the challenge of further development of novel multicomponent inorganic-organic lead halide perovskites and investigations on their physicochemical properties of the bulk crystals and perovskite thin films. As lead toxicity is one of the key challenges facing lead halide perovskites, our research effort will also be devoted to developing low toxic metal halide perovskites and their derivatives for photovoltaic applications. Particular attention will be paid to the development of mechanochemical synthetic procedures for the preparation of perovskites as it avoids solvent usage and allows shortening of reaction times, and simultaneously increasing the purity of the product.

2. Very recently, we have developed novel organometallic synthetic procedures for high quality and processable quantum-sized ZnO crystals. The resulting ZnO NCs possess many advantages over materials synthesised using standard sol-gel technique. For instance, they exhibit ultra long-live electron-hole separation, which makes them highly prospective for photocatalytic applications. Now we will focus on the development of novel catalytic systems for CO2 photoreduction based on ZnO nanocrystals.

Research group 10 – Soft Condensed Matter

Professor Robert Hołyst

SYNERGETIC GROUP

Research task

Development of new catalytic systems for CO2 photoreduction based on ZnO nanocrystals derived from organometallic approaches

Research task description

Non-equilibrium systems are characterised by energy fluxes across these systems. We want to establish a relation between energy stored in such a system and the value of the fluxes.

Research group 11 - Microfluidics and Complex Fluids Research Group

Professor Piotr Garstecki

SYNERGETIC GROUP

Research tasks

1. Modification of polycarbonate (PC) microchannels in microfluidic systems to obtain conductive surfaces, including for electrochemical analysis
2. Synthesis of surfactants for microbiological research in two-phase microfluidic systems

Research tasks description

1. Polycarbonate – due to its properties (including high mechanical strength, ease of processing,

commercial availability or low price) – is one of the most commonly used materials for the production of microfluidic systems. The aim of the research work in 2021 will be to develop and optimise the PC modification method for obtaining conductive surfaces. The modification will involve the use of a series of sequential chemical reactions. This approach will open new research opportunities combining the advantages of microfluidics and, e.g., electric current techniques.

2. In microfluidic systems in which two-phase systems (droplets) are used, stabilisation of the interface is necessary. The addition of a surfactant stabilises the surface of the drops and prevents their coalescence. The aim of the research is the synthesis of surfactants that can be used for microbiological studies in two-phase microfluidic systems. Our goal is the synthesis of surfactants, which – in addition to droplet stability and biocompatibility – will prevent (reduce) the transfer of molecules between droplets. Transfer of molecules between the drops is a very unfavourable phenomenon, so obtaining surfactants that minimise such transfer is of utmost importance.

Research group 12 – Organisation and synthesis of nanoparticles

Dr hab. Marcin Fiałkowski

Research task

Self-assembled membranes obtained at the liquid-liquid interface

Research task description

Our task is to develop a synthetic path to obtain a thin membrane at the interface between two liquid phases. To achieve this goal, we plan to utilise the phenomenon of self-assembly of gold nanoparticles. We will employ properly functionalised nanoparticles displaying amphiphilic properties. Within the task, we will select the appropriate ligands and the crosslinking agent. We plan to develop a synthetic protocol to obtain a membrane separating either two immiscible or two miscible liquid phases.

Research group 13 – Physical chemistry of complex systems

Dr hab. Wojciech Góźdź

Research task

Investigation of the influence of restricted geometry on behavior os systems composed of molecules with competing interactions

Research task description

We will investigate the formation of ordered structures composed of a cluster of colloidal particles in confined geometry. We will examine the deformation of vesicles composed of amphiphilic molecules, caused by attachment to flat surfaces. We are going to use molecular simulations and minimisation of free energy functionals to study these systems.

Research group 14 – Charge transfer processes in hydrodynamic systems

Dr. hab. Martin Jonsson Niedziółka

PROSPECTIVE GROUP

Research tasks

1. Using flow injection microfluidics to investigate the inhibition and regeneration of enzymes
2. Properties of Pillar[n]arenes in liquid-liquid electrochemistry

Research tasks description

1. The goal of the task to investigate the timescale of inhibtion and recovery of enzyme function using a microfluidic system where the concentration of inhibitor can be changed rapidly. This can give us clues to the mechanism of the inhibition and eventually be of help to better understand and protect enzymes from deactivation.

2. We are looking into the properties of Pillar[n]arenes, prepared by the Sashuk group, as carriers for transfer of small molecules across the liquid-liquid interface. There are reports of Pillar[n]arene complexes formed in a single phase with specific analytes. We investigate if this influences the transfer potential of these analytes if the pillararene is present in the second phase.

Research group 16 – Dynamics of nanocrystal structure induced by surface chemistry

Dr hab. Zbigniew Kaszkur

Research tasks

1. Ex-situ and in-situ powder diffraction studies of the structure of nanocrystalline catalytic materials
2. Atomistic simulations of metal, alloy clusters and multilayers– fragments of fcc, bcc lattice and systems containing 5-fold symmetry axis

Research tasks description

1. The studies target measurement and interpretation of a subtle peak evolution of metal nanocrystals during the catalytic reaction at their surface. This evolution reflects the structural atomistic mechanism of chemical reaction in heterogeneous catalysis and is interpreted using atomistic simulations.

2. Besides explaining a subtle evolution of diffraction pattern during the chemical reaction, atomistic simulations are to explain defect structure in fcc/bcc multilayers. The methodology of this research is based on the diffraction method developed in our group. It enables measurement and interpretation of a metal nanocrystal surface process in-situ [1-5].

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

Research group 17 – Environmental Chemistry Group

Dr hab. Rafał Szmigielski

Research task

Chemical characterisation of particulate matter (PM) at the suburban site near the capital city of Warsaw

Research task description

Low emissions of the particulate matter are among critical sources of the air pollution in suburban areas during autumn and/or winter episodes. The work aims to conduct 2-week field measurements aimed at the collection of the respirable fraction (PM2.5) of atmospheric aerosol in Podkowa Leśna and the determination of its main components. This project will extend the scientific knowledge on the smog formation in Poland and support its monitoring in the ambient air.

Research group 18 – Functional Polymers

Dr Piyush Sindhu Sharma

Research tasks

1. Evaluation of the new class of functional monomers for fabrication of electrochemical devices (new).
2. Electrochemical polymerisation at the air-liquid interface as a method for fabrication of selective membranes for protein biomarkers determination.

Research tasks description

1. Within this task we plan to evaluate usefulness of some newly synthesised conducting functional monomers. These new monomers are based on bis-(2,2',5',2''-terthiophen-5''-yl)methane polymerizing group (Scheme 1). These monomers provide low oxidation potential. Importantly this motif stabilise cataion-radical (polaron) and dicatioan (bipolaron). Second group of monomers is based on EDOT polymerising moiety (Scheme 2). Polymerisation of these monomers should result in deposition of highly conductive, closely packed, relatively hydrophilic linear polymers. We will investigate electrochemical and spectroscopic properties of monomers as well as its polymeric films.

2. This study includes formation of surface-imprinted membranes at the air-water interface with use of the Langmuir technique. The two-dimensional electrochemical polymerisation will be devised in order to study electrochemical behavior of the formed Langmuir films. Formation of the films and their changes upon protein complexation and redox reaction will be studied by surface pressure and surface potential measurements. In the next step, the formed membranes will be transferred onto the solid substrates by using either Langmuir-Blodgett or Langmuir-Schaefer techniques. The membrane composition and morphology will be then studied by PM-IRRAS,UV-Vis and AFM techniques.

Research group 19 – Soft Granular Matter and Tissue Engineering

Dr Jan Guzowski

Research task

Investigation of mechanical properties of hydrogel microparticles and of the dynamics of their suspensions inside microchannels

Research task description

Currently, there is a lack of full knowledge about the mechanical properties of microparticles and in particular about their collective behaviour in microchannels. Such knowledge is needed to develop further techniques of cell encapsulation for applications in "3D" cell culture and drug testing. Research tasks will include (i) design and manufacturing of microfluidic devices, (ii) synthesis of hydrogel microparticles via polymerisation of droplets generated inside microchannels, (iii) tracking of changes in the elasticity of particles during their polymerisation inside a microfluidic device, (iv) observation of collective particle dynamics inflow inside a narrowing channel.

Research group 20 – Cooperative catalysis

Dr hab. Adam Kubas

Research task

Electronic structure of graphene oxide - porphyrin derivatives nanohybrids

Research task description

In this research task, we will focus on the electronic structure of the nanohybrids in the context of hydrogen photoproduction. Notably, we will investigate the nature of the charge transfer excited electronic states. The outcomes of the quantum chemical calculations will be compared with experimental data obtained by our collaborators at the Adam Mickiewicz University in Poznan (dr A. Lewandowska-Andrałojć and prof. B. Marciniak).

Research group 21 – Spectroscopic and microscopic (STM/AFM) studies of intermolecular interactions

Dr hab. Robert Nowakowski

PROSPECTIVE GROUP

Research tasks

1. Spectroelectrochemical studies on the interaction of atmospheric compounds with phospholipid bilayers
2. Integrated physicochemical methodology for tissue engineering
3. Development of novel nano-catalysts for the production of value-added products. Catalytic removal of pharmaceutical micropollutants from water
4. High-resolution microscopic studies of self-assembly and surface processes in layers of selected organic semiconductors

Research tasks description

1. The task is a continuation of already conducted research aimed at understanding the interactions of selected carcinogenic compounds, found in the air, with model biological membranes. The

studies will be performed using electrochemical techniques and high-resolution AFM microscopy in electrochemical conditions. They will be carried out in cooperation with the team 17 "Environmental chemistry", headed by dr hab. Rafał Szmigielski.

2. The research is aimed at understanding the local and macroscopic surface properties of selected biomaterials. Bioactivity and biocompatibility characteristics will be conducted using a combination of complementary measurement techniques, such as: AFM, TPR, TPO, TPD, BET. For some materials, e.g. model bone implants, DRIFT operand (Fourier transform spectroscopy with diffusion reflection) with probe molecules (e.g. CO) is planned.

3. The main part of the proposed research will focus on hydrogenation reactions conducted in a continuous flow mode of importance in industry and environmental protection, on novel catalysts containing noble metals (e.g. Pd, Pt, Ag). The aim will be, e.g.: i) to determine the structure-reactivity relationship concerning the morphology of metal nanoparticles; ii) the effect of doping on the catalytic performance of metal/support systems.

4. This is a continuation of microscopic (STM) studies of self-assembly of low and high molecular weight organic semiconductors with potential application in electronics. The subject of research is a new organic semiconductor with a complex topological and/or electronic structures. We also plan to extend investigations to single or multi-component adsorption systems showing, e.g. the possibility of a surface chemical reaction.

Research group 22 – Charge transfer in biological systems and at the interfaces

Dr Piotr Zarzycki

Research task

Design and structural studies of the host-guest pharmaceutical cocrystals

Research task description

The goal will be to tailor the structure and properties of the host-guest cocrystals based on the confinement of the targeted drug molecules within different supramolecular cavities. The project will include synthesis, optimisation of crystal growth, X-ray crystallography and solid-state characterisation of the host-guest cocrystals.

Research group 23 – Modified electrodes for potential application in sensors and cells

Professor Marcin Opałło

Research task

Electrochemical properties of nanomaterials suspensions

Research task description

Research on electrochemical detection of selected suspended nanomaterials will be continued. Experiments will be performed in forced convection conditions: inflow systems and at rotating disc electrode. If it is possible, results will be compared with those obtained in quiescent conditions. For experiments in flow systems, specially designed devices made by 3D printing technology will be employed.

Research group 24 – Complex Systems and Chemical Processing of Information

Professor Jerzy Górecki

Research tasks

1. Stationary structures, phase transitions and complex time evolution in confined systems.
2. Information processing using networks of chemical reactions.

Research tasks description

1. Identification of stationary structures, phase transitions and characterisation of a complex time evolution of systems with specific interactions (SALR - Short range Attraction and Long range Repulsion type, interactions mediated by concentrations of surface-active molecules), in systems that are confined within a small space: The research will combine theoretical methods of statistical physics, microscopic computer simulations using molecular dynamics and experiments with self-propelled objects on the water surface. Such problems as aggregation in systems with competing interactions or pattern formation by core-shell particles will be concerned.

2. We plan to continue theoretical studies, simulations and experiments on information processing using reaction networks coupled by the exchange of reactants and products. Results previously obtained for oscillatory chemical media will be generalised by considering more complex types of nonlinear dynamics like multistability or the existence of many attractors. Genetic algorithms will be used to optimise a network for a specific task. We expect to identify the class of algorithms that can be efficiently executed using reaction networks. The developed concepts of chemical information processing will be verified in the experiment with Belousov-Zhabotinsky reaction.

Research group 25 – Laboratory astrochemistry

Professor Robert Kołos

Research task

Photochemistry of simple pnictogen-bearing compounds of astrochemical importance

Research task description

Vinyl isocyanide (H2C=CHNC), phosphabutyne (C2H5CP), as well as vinyl- and ethylidynearsine (H2CCHAsH2 i HCCAsH2) will serve as the precursors for low-temperature photochemical investigations in solidified inert gases (e.g. Ne, Ar, Kr, Xe, N2, H2). Product detections shall rely on IR absorption, Raman scattering, and on electronic absorption/luminescence measurements. Identification of the newly formed species will be assisted, aside of the isotopic labelling, with quantum chemical calculations (mainly at the DFT level) pertinent to molecular structures, energetics, spectroscopy, and photoreaction channels.

Research group 27 – Laser Centre

Dr hab. Yuriy Stepanenko

SYNERGETIC GROUP

Research task

Chemical Manoeuvres in the Dark

Research task description

Chemical reactions have been extensively studied in sub-nanoseconds after photoexcitation. However, studies of fast chemical reactions in the ground electronic states, in which most of the chemistry takes place are scarce. It is possible now to improve this, thanks to infrared sub-picosecond pump - transient Raman probing, a method developed in the Laser Centre. This allows to selectively excite vibrationally the ground state of molecules in solution to trigger a chemical reaction and to monitor the changes in their nature over time as the reaction proceeds. This task is performed in collaboration with group 8. Our task will be performing time-resolved experiments and analysis of the results.

Research group 28 – Catalysis for sustainable energy production and environmental protection

Dr. hab. J. C. Colmenares

PROSPECTIVE GROUP

Research tasks

1. Research on the synthesis of new composite photocatalysts based on semiconductors and carbonaceous materials (e.g. biochar).
2. Study on the phenomenon of thermo-photocatalysis in environmental protection and organic synthesis.

Research tasks description

1. The aim of our research will be to use simple methods for the synthesis of composite materials based on carbon carriers (e.g. biochar from coffee/cocoa wastes, lignin-chitosan type wastes).

2. The research goal will be testing materials (from research task no. 1) in the frame of thermo-photocatalysis concept for: a. Selective oxidation of model compounds of lignocellulose components (e.g. glycerin, benzyl alcohol) to the corresponding aldehydes and ketones, and b. Oxidation of NO in air.

Research group 29 – Photophysics and spectroscopy of photoactive systems

Professor Jacek Waluk

PROSPECTIVE GROUP

Research task

Photoinduced conformational changes

Research task description

We plan to study several organic molecules that significantly change their properties after absorbing light. Among various possible photoinduced processes, those that involve conformational changes

requiring large amplitude motions seem particularly interesting. Such type of processes can be exploited for designing fluorescence sensors (e.g., viscosity or polarity probes).

The research methodology will be based on spectroscopic and photophysical measurements, using both stationary and time-resolved techniques. For the interpretation of results, quantum chemical calculations will also be performed.

Research group 30 – Nuclear Hyperpolarization of Molecular Systems and Nanomaterials

Dr. Tomasz Ratajczyk

Research tasks

1. Synthesis and properties of novel boron-based triptycene molecules for applications in materials chemistry
2. Real-time monitoring of photoreactions by the NMR-TR-NUS method integrated with a laser/UV-vis

Research tasks description

1. We will synthesise a few exemplary boron based triptycenes. For example, in the first position (i.e. 1-substituted-9-boratriptycenes), and with different bridging atoms at the second triptycene edge (i.e. 10-heteroatom-9-boratriptycenes). The influence of these substituents on the properties on the boron atom will be investigated. For instance, we would like to assess various factors that influence boron coordination properties. To do this, solid and liquid state NMR spectroscopy will be employed. Quantum chemical calculations will support the experimental results. The knowledge of interaction is necessary for the design of the novel catalytic systems and the design of functional materials.

2. Photochemical reactions are important in nature, in photocatalysis and in some functional materials. An improvement of the experimental method enabling real-time photoreactions is our goal. NMR coupled with UV-vis diode or laser will be used for that purpose. Implementation of TR-NUS (time-resolved, non-uniform sampling) will give us a possibility to follow changes in the reaction mixture and identification of photoreaction products in a better way. Anthracene derivatives, that undergo the light-induced regioselective dimerisation, as well as some molecules containing double-bound that show the E-Z tautomerism will be used as model compounds.

Research group 31 – Biophysical Chemistry: Diffusion and reactions in a crowded environment

Dr. Anna Ochab – Marcinek

Research task

Modelling of stochastic gene expression in a population of growing and dividing cells

Research task description

Modelling stochastic gene expression in a cell population taking into account cell growth and cell division, population age structure and stochastic spread of cell volume at birth and cell cycle length. Studying the influence of variable cell volume on the kinetics of chosen biochemical reactions and the coefficient of variation of protein number or concentration distribution. The research is

theoretical: a) based on a time-dependent Master equation with protein distribution between daughter cells, the probability distribution of cell cycle length and population age structure. b) Population balance equations with the possibility of the description of chemical reactions within cells.