UNIVERSITY
OF WARSAW

RESEARCH GROUPS
FACULTY OF CHEMISTRY
UNIVERSITY OF WARSAW

WCh
Faculty of Chemistry
University of Warsaw

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Editor:
Karolina Dudzińska, MSc

Language Editor:
Karolina Piecyk, PhD

Cover design:
Justyna Makowska, MSc

Photos of Research Groups:
Rafał Chojnacki, BSc

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Authorities

Dean

Prof. Andrzej Kudelski, PhD DSc
e-mail: akudel@chem.uw.edu.pl

Vice-Dean for Student Affairs

Prof. Beata Krasnodębska-Ostręga, PhD DSc
e-mail: bekras@chem.uw.edu.pl

Vice-Dean for Financial Policy and Development

Zbigniew Rogulski, PhD DSc
e-mail: rogul@chem.uw.edu.pl

Vice-Dean for Research and International Relations

Prof. Rafał Siciński, PhD DSc
e-mail: rasici@chem.uw.edu.pl

Head of Doctoral Studies

Prof. Michał Cyrański, PhD DSc
e-mail: mkc@chem.uw.edu.pl

HISTORY OF THE FACULTY OF CHEMISTRY, UNIVERSITY OF WARSAW

Zbigniew Wielogórski, PhD (translation: Katarzyna Jakubowska, MSc)

The history of Warsaw academic chemistry begins with the foundation of Medical School (known also as Faculty of Academical Medicine) in 1809. It became Faculty of Medicine when Royal University was founded in 1816. The statute of Royal University from 1818 placed chemistry at Faculty of Philosophy at Third Department – Natural Sciences. At that time students attended a course of chemistry with applications that was taught by professor Adam Maksymilian Kitajewski. It is worth mentioning that chemistry lectures and practical classes were also obligatory for medicine, pharmacy and law students.

Changing attitude of the occupant towards the University affected the development of natural sciences including chemistry. After closure of Royal University chemistry was offered first at Pharmacy School, then, at Polish Medical and Surgical Academy, at Main School and finally at Russian-language Imperial University of Warsaw that was founded in 1869. The events of World War I brought reopening of the University in 1915, however, it was under German influence. In 1918 the University of Warsaw was reorganized in the independent state of Poland. Chemistry was then offered at Faculty of Philosophy, which was divided in 1927 into two faculties: Faculty of Liberal Arts and Faculty of Mathematics and Natural Sciences. Chemists conducted research and taught classes at Faculty of Mathematics and Natural Sciences, but in 1951 they transferred as a new faculty emerged, Faculty of Mathematics, Physics and Chemistry. In 1955 the next division brought the foundation of University of Warsaw Faculty of Chemistry.

In late 1910's growing number of University of Warsaw students, including chemists, resulted in overcrowding of the premises that were then mainly located on Krakowskie Przedmieście Street. There was an urgent need for expansion and, as a consequence, Chemistry Building located on Pasteura Street in Ochota district was built. However, some time passed before it could have been used by the academic community because of the World War II. The history of the building started in 1934 when the University was given a plot with a surface area of 13.526 m^2 that was located on the corner of Pasteura and Wawelska Streets. Hypothecary address for the plot was 17 Wawelska Street and it was next to the Radium Institute. In this place the Chemistry Building was built, however, it was not the first location that had been considered. Back in 1919 there was an intention to grant University of Warsaw a part of area called 'Pole Mokotowskie' that was then used as landing ground. In December 1922 an architect Tadeusz Zieliński developed a design for an academic town. That design was mainly fulfilled by the middle of the last century as today's Ochota Campus. In 1924 the area was already set, however, financial crisis in Poland in 1928-1929 prevented the construction. At that time only a dormitory in Narutowicza Square was built. Thanks to many people's efforts, among others University of Warsaw Rector professor Stefan Pieńkowki and University of Warsaw professors: Kazimierz Jabłczyński, Wiktor Lampe and Mieczysław Centnerszwer and Warsaw University of Technology professor – architect Aleksander Bojemski, and also thanks to the support of chemistry professors: Republic of Poland President Ignacy Mościcki and Minister Wojciech Świętosławski and also Deputy Prime Minister chemical engineer Eugeniusz Kwiatkowski the construction of the Chemistry building began on 19 September 1935. It is worth stressing out that the excavation were done according to the original design that was changed in 1936 as the construction of the building was split into two stages. As a result, the building was smaller and did not reach Wawelska Street and Miecznikowa Street. Except the expansion from 1960's the second stage of the construction never happened and the whole original design was never completed. The construction works were going fast. The foundation stone was laid by Republic of Poland President Ignacy Mościcki on 29 May 1936 and the dedication ceremony took place already on 23 June 1939. Unfortunately, the new and modern Chemistry Building could not be used for a long time as in September 1939 the World War II started and the building was situated on the brink of Warsaw defence. Since the first days of occupation the Germans started robbing equipment, furniture and

research apparatus. The building became a backup field hospital and in May 1941 a Wehrmacht field hospital that had one thousand beds was organised there in order to prepare for the German-Soviet War. Wounded soldiers were transported from railway station to the hospital by trams as tram line was specially built for this use. Little is known about what happened in the building during the war, however, devastation of the rooms done by the occupant could be clearly seen after the war. During Warsaw Uprising the Chemistry Building did not suffer much damage, the field hospital had been evacuated at the end of July 1944 and a few Wehrmacht soldiers that occupied the Radium Institute were of no interest to Polish forces in Ochota district. At the end of 1944/beginning of 1945 just before leaving the building, the Germans blew up a part of it. From the first days after the war efforts have been made to rebuild the Chemistry Building and start teaching classes for the first postwar year of students. These were first classes since the opening ceremony that had taken place 6 years before! Unfortunately, the postwar reality was unfavourable. Because there was no appropriate facility and there was a field hospital in the Chemistry Building during German occupation Ministry of Public Security intended to organise a hospital there. It took much effort to convince the officials that this would be unreasonable, since the building was originally designed with chemical research in mind. It was argued that before the war professors and architects made journeys to Western European countries to find the best designs and solutions for such a research facility and then implement them for the Chemistry Building. Moreover, special construction materials were used and specific equipment was provided in order to create a modern research facility that would preserve its excellence for many years to come. Strong walls and efficient installation still make it possible to modernise the building and adapt it to today's needs. Finally, the building was granted to University of Warsaw at the end of July 1945. The reconstruction of destructed rooms and complement of windows and doors that were looted by locals begun. Thefts happened even despite the presence of armed guards. Professor Wiktor Kemula made extraordinary contribution to the reconstruction and renovation of the building. He was a landlord for many years and made great effort to obtain funds for necessary works. Finally, the reconstruction of the part of the building that had been blown up finished in 1951. However, some laboratories and lecture halls were functioning before that time making it possible for many students of Faculty of Mathematics and Natural Sciences to learn. Furthermore, some research departments of Faculty of Geology took refuge in the Chemistry Building for several years.

University of Warsaw Faculty of Chemistry that was inaugurated in October 1955 was the first self-contained faculty of chemistry in Poland. Chemistry Building that is located at 1 Pasteura Street became its premises. There were numerous attempts to expand the building according to an architectural plan that was created before World War II, however, the results were not as spectacular as expected. In 1964 a new part of a building was commissioned, but south and north wings that were on the original blueprints will probably never be built.

In the mid-1950's the Faculty Council started to discuss expansion into a new building where radioactive elements and compounds would be studied. According to optimistic assumptions the new building was supposed to be commissioned in 1959, however, it happened in 1965. The Radiochemistry Building is located on Żwirki I Wigury Street.

In 2010 the first stage of construction works on The University of Warsaw Biological and Chemical Research Centre (CNBCh UW) began. The second stage of construction works ended in 2014. The premises of the Centre is connected with University of Warsaw Faculty of Biology by an above-ground walkway and the Radiochemistry Building is somehow build into the CNBCh UW building. The Centre is a joint venture of University of Warsaw Faculty of Biology and University of Warsaw Faculty of Chemistry.

It is worth reminding that the first plans for campus in Ochota district were drawn in late 1922. The first building to be built on Ochota Campus was the Chemistry Building. The construction works started in 1935.

Over the years a few thousands of students have graduated from Faculty of Chemistry, a significant number of doctoral students have been promoted and numerous researchers and scientists have got their degrees and scientific titles.

DESCRIPTION OF THE FACULTY OF CHEMISTRY, UNIVERSITY OF WARSAW

Karolina Dudzińska, MSc (translation: Karolina Piecyk, PhD)

The Faculty of Chemistry of the University of Warsaw is one of 21 faculties of the University of Warsaw providing full-time and post-graduate (extramural) education.

The Faculty runs the following fields of study:
- Chemistry – undergraduate and graduate studies
- Chemistry (in English) – graduate studies with the characteristics of individual study
- Medical Chemistry – engineering studies (some classes in English)
- Energetics and nuclear chemistry – undergraduate and graduate studies (conducted with the Faculty of Physics)
- Chemical instrumental analysis – engineering studies
- Applied chemistry – three-semester MA studies.

The Faculty of Chemistry also co-creates fields of study with other Faculties of the University of Warsaw:
- Nanostructure Engineering (Faculty of Physics) - undergraduate and graduate studies
- Environmental Management (in English) (Faculty of Biology and Faculty of Management) – graduate studies
- Inter-faculty Studies in Environmental Protection - undergraduate and graduate studies (conducted by UCBŚ UW together with 9 UW Faculties)
- Sustainable Development (in English) - graduate studies
- Forensics and Forensic Science (Faculty of Biology and Faculty of Physics, Faculty of Law and Administration, Faculty of Psychology, Center for Forensic Sciences, University of Warsaw) – graduate studies.

Postgraduate studies at the Faculty:
- Postgraduate studies in Chemical Metrology (co-created with the Polish Center for Accreditation and the Central Office of Measures)
- Postgraduate Studies – Applications of Chemistry in Environmental Protection (advanced chromatographic course)
- Postgraduate studies in Evidence Law, Forensics and Related Sciences as part of the Center for Forensic Science

and III degree studies:
- Individual PhD studies at the Faculty of Chemistry,
- TRI-BIO-CHEM PhD studies,
- RadFarm PhD studies,
- PhD studies "Implementation doctorates".

The history of teaching chemistry at the academic level dates back to the early nineteenth century. In 2009, 200 years have passed since the commencement of this activity in Warsaw. Initially, chemical studies were conducted as part of the then Faculty of Philosophy of the University, and in the 1950s, an independent Faculty of Chemistry was created at the University of Warsaw, with its own, specially built building at Pasteura Street 1. A few years later, the Faculty was expanded with the Radiochemistry building at ul. Żwirki i Wigury 101. Today the Faculty of Chemistry is a part of Ochota campus, which also contains following faculties: Mathematics, Computer Science and Mechanics (MIM), Biology, Physics and Geology, Center for Biological and Chemical Sciences, and Center for New Technologies. There are also two dormitories and a Sports and Recreation Center.

The Faculty of Chemistry of the University of Warsaw is one of the best chemical faculties in Poland, as evidenced by numerous rankings, including those conducted by the Ministry of Science and Higher Education. The Faculty of Chemistry has the A+ scientific category, which is intended for reference centers conducting research at the highest world level. The faculty also had the status of KNOW (National Leading Scientific Center), which was granted for 5 years (2012-2017). This status was granted to the Warsaw Academic Chemical Consortium, which included the Faculty of Chemistry of the University of Warsaw and the Faculty of Chemistry of the Warsaw University of Technology. The establishment of the consortium was determined by the deep conviction of its founders about the special role of chemistry in the development of modern science. In addition, the Faculty received support for the years 2017-2019 in the form of the POWER project - A program to develop the competences of Students of the natural faculties of the University of Warsaw and the Faculty of Chemistry of the Warsaw University of Technology. The main goals of this program was to acquire and expand professional competence and teamwork skills. As part of Measure 3.1 Competences in higher education, the National Center for Research and Development announced a competition for projects in the "University of the Young Explorer" program. An application submitted by the Faculty of Chemistry of the University of Warsaw entitled The "University of the Young Chemist" received funding from the National Center for Research and Development. The project is implemented together with the Future in Science Foundation. As part of this project, support was provided to Students from all over Poland, planning to tie their future with the natural and exact sciences, in particular with chemistry. The offer is offered to schools from areas with a diverse population, and at least half are children from rural areas or small towns. The main goal of the "University of the Young Chemist" project is to increase the competence and skills of youth in mathematics and natural sciences, in particular chemistry. The main goal of the project is to inspire youth to be creative, approach various research problems in a unconventional manner, to familiarize themselves with the university and inspire to work in a field of chemistry. This project is a response to the growing needs of the growing economy and the dynamically changing labor market.

In years 2014-2017, the Faculty was placed on the first place in the Ranking of the “Perspektywy” in the group of chemistry. In addition, in 2017 and 2018 the field of study “chemistry” - first-cycle studies, submitted to the Program "Studies with the Future" by the Faculty of Chemistry of the University of Warsaw, obtained the Certificate and Quality Label "Studies with the Future" awarded by the jury under the patronage of the Foundation for the Development of Education and Higher Education. In addition, in 2018 the Advanced Instrumental Methods and Measurement Techniques - engineering studies (currently Chemical Instrumental Analysis) obtained the Accreditation Certificate “Studies with the Future”. In 2017, the Faculty of Chemistry of the University of Warsaw also signed a cooperation agreement with BASF Polska Sp. z o. o.. This cooperation creates content for the website: CHEMIATOMY.PL and the facebook profile of BASF Polska under the name "chemiatomy", and promotes the Website and facebook profile of BASF Polska under the name "chemiatomy", run and administrate by BASF Polska. The goal is to promote chemistry with rich multimedia content, interactive illustrations, games and state-of-the-art web applications, as well as to facilitate its understanding, especially by young generations.

An important element of the Faculty of Chemistry at the University of Warsaw is interdisciplinary research conducted at the Center for Biological and Chemical Sciences of the University of Warsaw, which is a platform for cooperation between the faculties of Biology and Chemistry. This platform allows to build solid link between science and the economy. The faculty guarantees a high level of education, access to modern equipment and cooperation with scientists with extensive scientific achievements. This is evidenced, for example, by the number of scientific papers on various subjects, published in the best international scientific journals. By studying at the Faculty of Chemistry, you can have the chance to meet outstanding, passionate scientists and join numerous scientific activities and become a co-author of publications. The Faculty of Chemistry conducts scientific research and studies in the field of physical, nuclear and radiation chemistry, theoretical and crystallography, inorganic and analytical, organic and chemical technology.

The Faculty of Chemistry of the University of Warsaw develops scientific cooperation with many foreign research centers. The Student has the opportunity to undergo a several-month scientific internship in European academic centers under the Erasmus program. The ECTS credit system applicable throughout the European Union make it easier for the Student to study abroad and guarantee the recognition of his exams and credits.

Studies at the Faculty of Chemistry of the University of Warsaw are two-cycle studies. They consist of 6 and 7 semesters Bachelor's studies (1st degree) and 3 and 4 semesters Master's studies (2nd degree). During undergraduate studies, some subjects are necessary to obtain comprehensive chemical education, and therefore some subjects are mandatory such as mathematics, physics, the basics of general, inorganic, organic, physical, quantum or analytical chemistry. During undergraduate studies, the Faculty offers a large selection of lectures and laboratory classes so that the Student can develop their individual passions and create their own "path" of study. There is an extensive laboratory program, which allows to learn about various research methods. To start a master's degree, the Student must pass an entrance examination. During the second degree studies, some subjects are mandatory (recommended in accordance with the subject of specialization), the Student decides about the selection of other subjects according to his interests. During the second semester, a specialization is chosen within 8 thematic blocks, in which the Student will perform a diploma thesis. In addition, during the master's degree the Student may participate free of charge in the classes of the pedagogical block, which includes psychology, pedagogy, chemistry didactics and internships in schools. Completion of this course give authorization to teach chemistry in primary and secondary schools (in accordance with current law). Internships are also offered to Students in scientific and research or industrial institutions. For Students who want to continue their education, there is the possibility to continue their scientific path at the Doctoral School.

Studies at the Faculty of Chemistry of the University of Warsaw guarantee a broad and thorough education, which is crucial in getting an interesting job. Graduates from the Faculty of Chemistry find jobs in various industries, state laboratories and schools and various types of colleges. Chemistry is not an easy science and therefore there is a great demand for specialists in various fields related to it. Chemists are sought after by companies related to modern industry (supervision and quality control), or administrative units operating in environmental protection, by medical, pharmaceutical, forensic laboratories, or food control, and other entities where 'open mind' and knowledge of exact sciences is essential. Organic chemists are essential in the innovative economy related to new materials, in biochemistry research laboratories and in pharmaceutical and cosmetics companies (synthesis and quality control). Chemists associated with theoretical chemistry and crystallography find employment at universities, research institutes, computer centers in administration and banking, i.e. in all areas of the labor market where computer is the basis of creative work.

The following Student organizations operate in Faculty of Chemistry:
Student Government - the main goal of the Student Government Board of the Faculty of Chemistry of the University of Warsaw(ZSS WCh UW) is to represent Students of the Faculty of Chemistry before the authorities and take care of their interests. It consists in issuing opinions on matters related directly to studies, in addition, ZSS WCh UW delegates Students to the Scholarship Committee, Faculty Council and Chemistry Didactic Council. Animation of Student life is another equally important task. ZSS WCh organizes various events aimed at the integration of Students, such as: thematic competitions with prizes, Student eve, integration events, as well as a Science Camp. The Science Camp in Chęciny, which is both integrative and scientific, is supported by the Faculty. The local government also organizes campaigns enabling Students to buy sweatshirts and aprons with the Faculty's logo. In addition, the Management Board conducts training on the rights and obligations of Students and training on USOSweb service for newly admitted Students. It provides advice and support to Students in difficult life situations.
Students' Scientific Club "Fulleren" - has been active at the Faculty of Chemistry with breaks since 1986. It brings together Students of the Faculty of Chemistry and the College of MISMaP. "Fulleren" is associated in the Academic Association of Chemistry Students as a representation of the University of Warsaw.

"Fulleren" organizes, among others meetings with well-known scientists, science camps in attractive tourist destinations and trips to domestic and foreign conferences.

A Student at the Faculty of Chemistry may apply for the following scholarships: social, social in an increased amount due to residence in the Student's home or other facility than the Student home, special scholarship for disabled persons, rector's scholarship for Students with good results in science and sport. In addition, any Student in a random situation may apply for a grant. Students of the Faculty of Chemistry of the University of Warsaw from outside Warsaw can also apply for accommodation in University dorms located close to the Faculty.

Studies at the Faculty of Chemistry of the University of Warsaw offer an opportunity not only for scientific but also for comprehensive development. If a Student wants to improve its knowledge of foreign languages, the University offers four semesters of free language course in any language. Inside the Ochota Campus a modern University of Warsaw Sport and Recreation Center is located where the Student can find a gym, fitness center, sports hall with fields for team games (volleyball, basketball, badminton, handball), swimming pool and climbing wall. Music enthusiasts, however, during the day can sign up to the Academic Choir operating on the Ochota Campus, and in the evenings they can go to the nearby University Club Proxima, where concerts and Student events regularly take place.

At the Faculty of Chemistry, University of Warsaw, people with varying degrees of disability can study and study. Didactic buildings and social facilities have been adapted to the needs of the disabled - ramps, elevators, automatic doors and toilets have been installed. In addition, the laboratory rooms have been equipped with a small infrastructure supporting teaching, such as a laboratory table with a movable table top or a mirror system. Near the Faculty there is a modern dormitory, which has rooms fully adapted to the needs of the disabled. It is also possible to rent specialized equipment and software from the University of Warsaw to facilitate learning at home, as well as free transport by adapted bus. The Faculty's authorities are open to the needs of the disabled - they try to provide the disabled with the opportunity to participate in all areas of the Faculty's life, so that they are treated on an equal footing with other Students. Methods and forms of education are selected flexibly, depending on the individual needs and predispositions of the Student. Most of the lecturers provide Students with teaching materials in electronic form. The e-learning platform is also intensively developing at the Faculty. There are learning materials and instructions. Creating friendly atmosphere for the disabled to study and function in the academic community is one of the priorities of the Faculty's authorities.

For many years, the Faculty of Chemistry of the University of Warsaw has been involved in the promotion of chemistry. The numerous activities include: Open Day at the Ochota University Campus, Open Day at the University of Warsaw, Lectures on interesting chemistry, Meetings with interesting chemistry, Science Festival, participation in the Science Picnic of the Polish Radio and the Copernicus Science Center, participation in the International Fair of Analytical and Measurement Techniques (EuroLab). There are also poster sessions at the Faculty every year, i.e. a research group session and a Student session (master's thesis). In addition, according to the schedule of the organization of the academic year, a ceremonial Inauguration of the academic year and a solemn graduation of graduates takes place every year at the Faculty of Chemistry. In addition, during the holiday season, the Dean's Team organizes a Summer Picnic at the Faculty of Chemistry for employees, PhD Students and Students. This is a great opportunity to integrate the entire faculty community. An important event is also the Department Christmas Eve, where in the pre-Christmas season everyone gathers in the main hall of the building at Pasteura Street by a beautifully decorated Christmas tree, traditionally they share a wafer, make Christmas wishes and eat Christmas Eve dishes together. University of Warsaw Ochota Open Day (DOKO) is a special event integrating the community of UW units located on the so-called Ochota campus. Since 2019, it has been operating under a new name - Ochota UW Campus Discovery Day. It is a joint venture of five faculties: Biology; Chemistry; Physics; Geology and Mathematics, Computer Science and Mechanics and cooperating units: Center of New Technologies; Heavy Ion Laboratory; Biological and Chemical Sciences Center; College of Inter-Fa-

culty Individual Studies in Mathematics and Natural Sciences and the University Center for Research on the Environment and Sustainable Development. Everyone interested in mathematics and natural sciences can: visit research laboratories unavailable on a daily basis, learn how to study at particular campus departments, listen to inspiring lectures of scientists, take part in interesting scientific workshops and unforgettable experience demonstrations. In addition, all information about studying at the Ochota Campus can be obtain from deans, Students and employees of the University of Warsaw. For many years, the Faculty of Chemistry has been conducting a series of lectures in various fields of chemistry for secondary school Students throughout the entire academic year (named “Lectures on Interesting Chemistry”). Lectures take place in the hall of the Faculty of Chemistry and are conducted by outstanding specialists in an accessible form. Free admission, no registration required. Meetings with interesting chemistry have been conducted for several years, prepared annually by chemistry Students and employees of the Chemistry Didactics Laboratory, with the support of willing PhD Students. Toddlers and children from primary and secondary schools under the supervision of their teachers can see many attractive experiences in the Laboratory of Chemistry Didactics, actively participating in them. The purpose of these meetings is to show their participants that chemistry is an interesting and spectacular field of science and to expand their school knowledge. They present a series of experiments using completely safe substances, such as: soda, powdered sugar, oil, vinegar, milk. Children of the employees of the Faculty of Chemistry of the University of Warsaw are traditionally invited to one of them. About 200-300 people take part in the meetings every year. Every year in September, numerous lectures and demonstrations are held at the Faculty of Chemistry as part of the Warsaw Science Festival. During presentation of experiments titled "Adventure with chemistry", festival guests dressed in lab coats can watch dozens of experiments, including pyrotechnic and chemiluminescent experiments. Guests can also actively participate in experimenting in laboratory rooms. The event aims to show potential "live" science candidates and interest in it. The Science Picnic of Polish Radio and the Copernicus Science Center is the largest scientific event in Europe. Its purpose is to disseminate knowledge from various scientific disciplines by presenting interesting experiments and experiences and the latest achievements of modern scientists. The picnic allows to understand and learn science, showing it as an extremely exciting field of life, and by bringing the scientist's workshop closer, it encourages and inspires visitors to undertake independent scientific activity. Employees and PhD Students of the Faculty of Chemistry have been presenting chemical experiments addressed to a wide audience for many years. Attractions that await visitors include traffic lights – chemical traffic lights, Belousov-Żabotyński reaction, microbiological link, super-stick liquid, blue bottle, scented soaps.

The scientific and research potential of the Faculty of Chemistry of the University of Warsaw is presented at numerous scientific conferences, but also at the International Fair of Analytics and Measuring Techniques (EuroLab). EuroLab is a prestigious industry event of a business and scientific nature, organized by MT Targi Polska and co-created by representatives of the academic community, industry institutions and research centers. Traditionally, Ochota Campus of the University of Warsaw represents its offer at the fair. The Ochota Campus stand (Center for Biological and Chemical Sciences, Faculty of Biology, Faculty of Chemistry, Center for Forensic Sciences, Committee of Analytical Chemistry of the Polish Academy of Sciences) is very popular among visitors. Event organizers traditionally care for an extensive substantive program. During the three days of the fair, numerous conferences and seminars are held by prominent scientists and experts in the field of chemical analytics, biotechnology and Life Science, metrology, laboratory diagnostics and nanotechnology. The lecturers include employees of the Faculty as well as graduates working in many companies and institutions of national and international rank. An important element of showing the latest research and research group achievements is the so-called BST Poster Session, during this annual session particular scientific laboratories of the Faculty of Chemistry of the University of Warsaw and separate research groups present themselves. The Student Poster Session of Master's theses also fits into the presentation of the results of scientific research, as most diploma theses are directly related to the latest science. It is also an important element of education. The results obtained by Students are presented during a special poster session, which takes place every year at the Faculty of Chemistry. Due to the very high level of prepared posters and oral presentations (2-3 min), awards and distinctions have been granted for many years.

STATISTICS (1/10/2019)

TEACHERS: 204

- with the title of professor – 36
- with the degree of habilitated doctor – 56
- with a doctoral degree – 112

NUMBER OF PHD STUDENTS: 134 + 25 PhD Students at the Doctoral School

NUMBER OF STUDENTS: 600

- full-time first cycle studies
  Chemistry - 287
  Medical chemistry – 69
  Chemical instrumental analysis – 59
  Power engineering and nuclear chemistry – 22
- full-time second cycle studies
  Chemistry – 149
  Chemistry (studies in English) – 5
  Power engineering and nuclear chemistry – 9

THE RATIO OF STUDENTS TO TEACHERS: 2.94

NUMBER OF CONDUCTED GRANTS: 127

85 – National Science Center (NCN)
16 – Ministry of Science and Higher Education (MNiSW)
6 – National Center for Research and Development (NCBR)
3 – National Center for Research and Development – Operational Program Knowledge, Education and Development (NCBR POWER)
5 – Foundation for Polish Science – Intelligent Development Operational Program (FNP PO IR)
4 – National Agency for Academic Exchange (NAWA)
5 – Horizon 2020 (H2020)
3 – Foreign Research Cooperation

Crystallochemistry Laboratory

UNIVERSITY OF WARSAW

WCh Faculty of Chemistry University of Warsaw

Crystallographic Group

HEAD:

Prof. Krzysztof Woźniak*, PhD DSc, Chemistry Europe Fellow

GROUP MEMBERS:

Wojciech Sławiński, PhD DSc;
Mihails Arhangelskis, PhD; Cheng Yang, PhD;
Michał Chodkiewicz, PhD; Roman Gajda, PhD;
Anna Hoser, PhD; Jan Kutner, PhD;
Maura Malińska, PhD; Damian Trzybiński, PhD;
Magdalena Woińska, PhD; Marcin Ziemniak, PhD;
Magdalena Chludzińska, MSc; Marlena Kisiała, MSc;
Małgorzata Krupska, MSc; Aleksandra Jakielaszek
PhD students: Daria Dawidziak, Paulina Marek (WUT/UW), Piotr Pacholak (WUT/UW),
Sylwia Pawlędzio, Szymon Sutuła,
Monika Wanat, Yizhi Xu
Undergraduate students: Katarzyna Bażęcka, Bożena Bednarek, Karolina Franasik, Julia Hińcz (WUT/UW), Agnieszka Huć (Wydział Geologii UW), Jakub Janiec (Wydział Fizyki), Małgorzata Kucia, Mikołaj Kuska (Wydział Fizyki), Katarzyna Polak, Agata Wróbel

RESEARCH PROFILE:

X-Ray and neutron diffraction on the solid state substances including variable temperature and high pressure studies, crystallography beyond Independent Atom Model, quantum crystallography, routine structural analysis, applications of crystallographic methods, thermodynamic profiling of molecular recognition, in particular, the solvent effects in the formation of guest-host complexes, crystallization and control of molecular crystal morphology, prediction of relative stability of interesting polymorphic structures, new methods of extracting thermodynamic properties from X-ray diffraction data and theoretical computations, treatment of thermal motion in X-ray diffraction data refinements, studies of solid substances exhibiting a significant level of crystalline disorder of different kinds (i.e. stacking faults, local structure of atom displacements or chemical short range order/disorder), structural studies on inhibition mechanisms of enzymes, macromolecular crystallography, pharmaceutical substances, mechanochemistry, prediction of crystal properties, variable temperature and high pressure studies of crystals and minerals, Pair Distribution Function investigations, phase transitions in crystals and minerals.

*e-mail: kwozniak@chem.uw.edu.pl

CURRENT RESEARCH ACTIVITIES:

Presently, we conduct structural research and studies of electron density for crystals of organic and inorganic compounds. In particular, we examine crystals of compounds of pharmaceutical importance (for example vitamin D derivatives), biochemical or biochemical significance, crystals of supramolecular compounds (rotaxanes, catenanes), macrocyclic complexes of d and f electron metal ions, crystals of model compounds used for X-ray methodological research, minerals and inorganic compounds, etc).
The aim of most of our studies is to find a correlation between the internal structure of crystals and the properties of quantitative distribution of electron density in crystals on one side, and macroscopic properties of crystals (physical, chemical, pharmaceutical, biochemical, etc) including photophysical properties of organic and organometallic materials in the solid state. We are involved in development of new approaches in X-ray and neutron diffraction methods. We study the processes of crystallization of organic, inorganic and macromolecular compounds. We also investigate dynamic properties of solids, phase transitions in the solid state, and perform crystallographic and biochemical studies of macromolecules. Finally, we also study structures and photophysical properties of materials (minerals in particular) at high pressure: determine relationships between the crystal structure at high pressure and the resulting changes of photophysical properties and the mechanism of the excimer formation in the investigated compounds. In order to understand properties of functional materials we study novel materials exhibiting a significant level of crystalline disorder of different kinds (i.e. stacking faults, local structure of atom displacements or chemical short range order/disorder). Last but not least, an important part of our studies are structural studies on inhibition mechanisms of enzymes belonging to USP family, which remove ubiquitin from eukaryotic proteins.

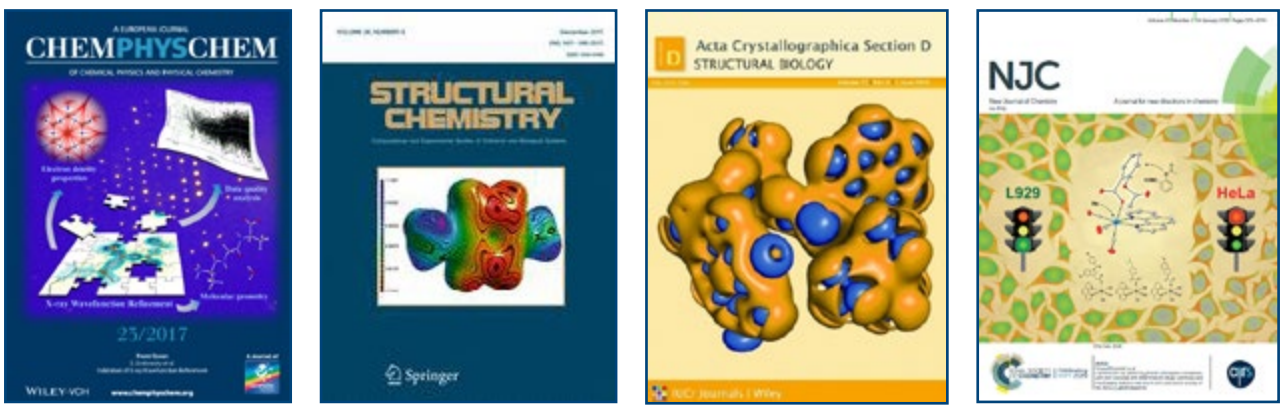

Fig. 1. (left) Front Cover: ChemPhysChem, vol 18 (2017), M. Woińska, D. Jayatilaka, B. Dittrich, R. Flaig, P. Luger, K. Woźniak, P. M. Dominiak, S. Grabowsky, Validation of X-ray Wavefunction Refinement, pp 3334 –3351, (left) Front Cover: Structural Chemistry, vol. 28, issue 6 (2017), R. Gajda, K. Woźniak, Charge density studies p-phenylenediammonium, pp. 1607–1622, (center left) Front Cover: Acta Crystallographica D, vol. 72, issue 6 (2016), M. Malinska, Z. Dauter, Transferable aspherical atom model refinement of protein and DNA structures against ultrahigh-resolution X-ray data, pp 770-779 (center right); Front Cover: J. Skiba, A. Kowalczyk, P. Stączek, T. Bernaś, D. Trzybiński, K. Woźniak, U. Schatzschneider, R. Czerwieniec, K. Kowalski, Luminescent fac-[Re(CO)3(phen)] carboxylato complexes with nonsteroidal anti-inflammatory drugs: Synthesis and mechanistic insights into the in vitro anticancer activity of fac-[Re(CO)3(phen)(aspirin)], New Journal of Chemistry, 43 (2019) 573-583 (right).

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4. S.A. Morris, G.P.M. Bignami, T. Tian, M. Navarro, D.S. Firth, J. Cejka, P.S. Wheatley, D.M. Dawson, W.A. Sławiński, D.S. Wragg, R.E. Morris, S.E. Ashbrook, In situ solid-state NMR and XRD studies of the ADOR process and the unusual structure of zeolite IPC-6, Nature Chemistry. 9(10) (2017) 1012.
5. A.A. Hoser, A.Ø. Madsen, Dynamic quantum crystallography: lattice-dynamical models refined against diffraction data. I. Theory, Acta Cryst. A72 (2016) 206–214.

6. M. Woińska, S. Grabowsky, P.M. Dominiak, K. Woźniak, D. Jayatilaka, Hydrogen atoms can be located accurately and precisely by routine X-ray crystallography, Science Advances. 2(5) (2016) 1600192.
7. W. Fabiola Sanjuan-Szklarz, A.A. Hoser, M. Gutmann, A.Ø. Madsen, K. Woźniak, Yes, one can get better quality structures from routine data collections, IUCr Journal. 3 (2016) 61-70.
8. M. Malińska, K.N. Jarzembska, A.M. Goral, A. Kutner, P.M. Dominiak, K. Woźniak, Interplay between sunitinb malate crystal packing, charge density distribution, and protein-ligand interactions in sunitinib-containing biological systems, Acta Crystallographica. D70 (2014) 1257-1270.
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Czochralski Advanced Crystal Engineering Laboratory (aceLAB)

HEAD:

Prof. Michał K. Cyrański*, PhD DSc

GROUP MEMBERS:

prof. Tadeusz M. Krygowski, PhD DSc (emeritus);
Łukasz Dobrzycki, PhD DSc;
Arkadiusz Ciesielski, PhD;
Michał A. Dobrowolski, PhD
PhD students: Grzegorz Cichowicz,
Sylwia Kutyła, Kamila Pruszkowska,
Patryk Rzepiński, Paweł Socha

RESEARCH PROFILE:

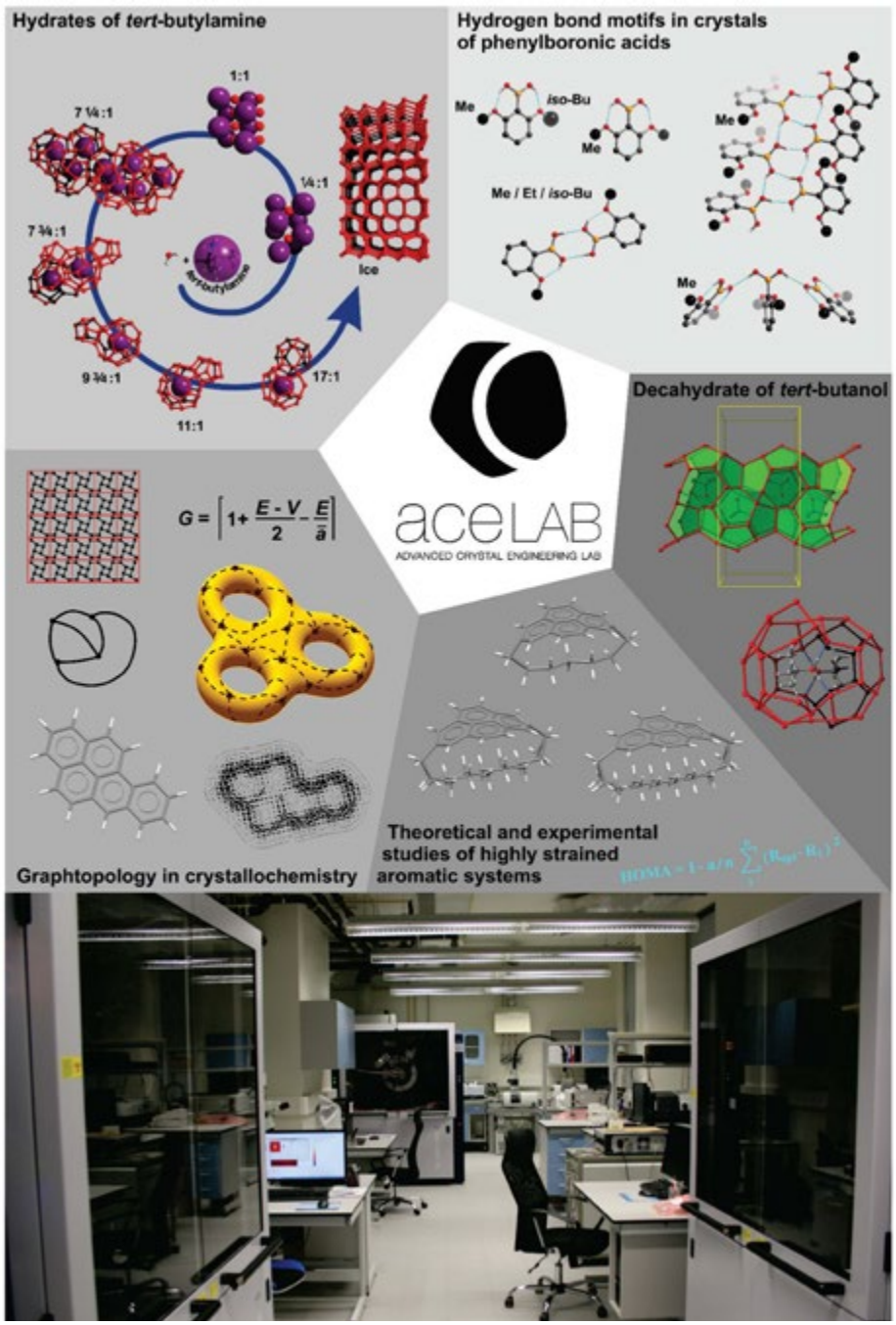
Our scientific interest covers a broad spectrum of problems in structural chemistry of small organic compounds, physical organic chemistry, chemical crystallography, crystal engineering and forensic science as well.

The research includes both theoretical investigations of such topics as aromaticity, substituent effect in chemistry, solvent effect and experimental studies on crystallization and crystal structure analysis including polymorphism, phase transitions, twinning, disorder, stability of molecular crystals. The experimental part is supported by molecular modeling including quantum-mechanical calculations (ab initio). To explain some fundamental problems in organic chemistry we also introduce and apply new theoretical approaches based on graph topology. In our research we use the following experimental techniques: single crystal X-ray diffraction, in wide range of temperatures (including room temperature high pressure investigations) combined with Raman spectroscopy; powder diffraction; calorimetric measurements (DSC, TGA/DSC). To devise and obtain novel crystal structures a world-unique IR laser supported in situ crystallization device is applied. Our particular interest is also focused on development of new methodologies and research equipment.

*e-mail: mkc@chem.uw.edu.pl

CURRENT RESEARCH ACTIVITIES:

The experimental part is primarily related to the design and physicochemical characterization of new crystalline hydrates/hydrate clathrates of small organic compounds, that are liquids at room temperature. To elaborate intermolecular interactions in the solid state, to create novel architectures, many other multi-component systems, such as supramolecular complexes of phenylboronic acids, benzenoid hydrocarbons or a clathrate-like systems formed by urea, are also investigated. The primary theoretical topics of our investigations include: relation between strain and aromaticity, energetic aspects of cyclic π-electron delocalization, definition of aromaticity, comprehensive physicochemical interpretation of substituent effect, dependence between the strength and the nature of hydrogen bond and pi-electron delocalization in model systems of biological importance. Our Laboratory is equipped with two single crystal and one powder X-ray diffractometers, Raman spectrometer, DSC and TGA/DSC instruments.



SELECTED PUBLICATIONS:

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4. Ł. Dobrzycki, K. Pruszkowska, R. Boese, M.K. Cyrański, Hydrates of Cyclobutylamine: Modifications of Gas Clathrate Types sI and sH, Crystal Growth&Design. 16 (2016) 2717−2725.
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Electron Density Modelling Group

HEAD:

Paulina Maria Dominiak*, PhD DSc

GROUP MEMBERS:

Michał Chodkiewicz, PhD;
Kunal Kumar Jha, PhD; Marta Kulik, PhD
PhD students: Urszula Budniak, Małgorzata Cabaj, Barbara Gruza

RESEARCH PROFILE:

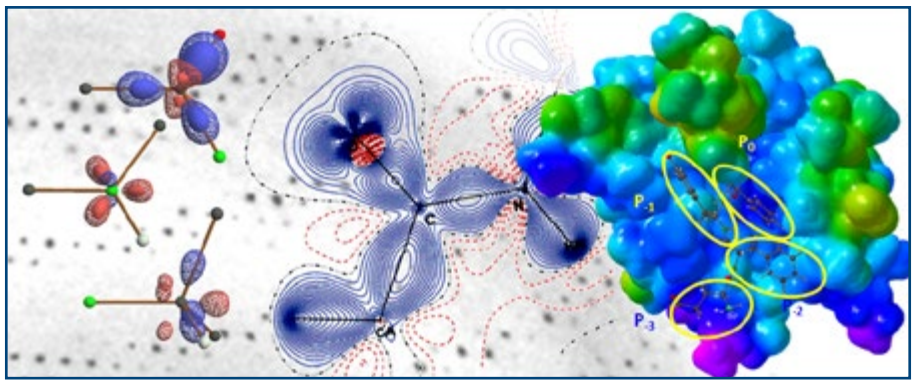
The research group works on developing new methods of electron density modelling for X-ray and electron crystallography, chemistry and structural biology.

Our primary goal is to create methods allowing to obtain more information from routinely collected X-ray diffraction data. On the one hand, these methods are intended to improve the quality of geometric data obtained from such measurements, and on the other hand, they provide access to a new type of information, i.e. to electron density and energy interactions. Our intention is that our methods of electron density modelling and intermolecular energy estimation should fill space between classical mechanics methods (force fields) and quantum mechanics methods: to be more accurate than the first, but definitely faster than the latter. We use the new methods we created (both in experiment and in theory) to understand the role of intermolecular interactions in complexes of proteins and nucleic acids and in crystals of organic compounds. Our main focus is the importance of electrostatic interactions. We are interested in the relationship between intermolecular interactions and crystals architecture, macromolecular structure or molecular recognition in the context of drug design. As part of our research, we obtain our own crystals, determine their structure by X-ray and, as far as possible, obtain experimental electron density by means of high resolution X-ray diffraction measurements on a monocrystal. In everyday practice, we combine the experiment (X-ray and monocrystalline neutrons, small molecule crystallization, DSC / TGA) with theory (classical force fields, optimization of isolated molecular geometry and periodic systems with DFT methods, topology of electron density, interaction energy with DFT- SAPT, etc.).

*e-mail: pdomin@chem.uw.edu.pl

CURRENT RESEARCH ACTIVITIES:

At present, our research is mainly based on the developed in our group pseudoatom databank (University at Buffalo Pseudoatom Databank, UBDB), which enables rapid reconstruction of the electron density of organic molecules and biomacromolecules. We also work on more simplified models of electron density in the context of an even faster estimation of energy interactions and applications that go beyond crystallography. Very recently, we have moved our attention towards application of our tools to electron diffraction and single-particle cryoEM studies.



The biological systems we are currently analyzing are HIV protease complexes with small molecular ligands and IFIT protein complexes from RNA (in collaboration with the Structural Biology Group of dr Górna), starting with publicly available structures. In the case of organic crystals we work on nucleobases and their derivatives.

SELECTED PUBLICATIONS:

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2. B. Gruza, M.L. Chodkiewicz, J. Krzeszczakowska, P.M. Dominiak, Refinement of organic crystal structures with multipolar electron scattering factors, Acta Cryst A. 76 (2020) 92–109.
3. P. Kumar, B. Gruza, S.A. Bojarowski, P.M. Dominiak, Extension of the transferable aspherical pseudoatom data bank for the comparison of molecular electrostatic potentials in structure–activity studies, Acta Cryst A. 75 (2019) 398–408.
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Laboratory of Materials Technologies**

Members of our laboratory, Dean of the Faculty of Chemistry, members of the Department of Functional Materials at Ł-ITME together with representatives of the Ministry of Science and Higher Education of Poland, Łukasiewicz Research Network, Nature Photonics and partners of the Teaming for Excellence ENSEMBLE3 project.

HEAD:

Dorota Anna Pawlak*, PhD DSc

GROUP MEMBERS:

PhD Researchers: Miguel Cuerva,
Piotr Piotrowski, Monika Tomczyk
PhD students: Rafał Nowaczyński (WUT),
Piotr Paszke, Kamil Szlachetko

RESEARCH PROFILE:

Developing new methods for manufacturing photonic materials utilizing crystal growth methods. Our research focuses on metamaterials, plasmonic and materials with special optical/electromagnetic properties using top-notch characterization techniques from the macro to the nanoscale.

CURRENT RESEARCH ACTIVITIES:

We develop volumetric and micron-scale photonic materials based on: (i) self-organization mechanism in eutectic composites; (ii) directional solidification of nanocomposites made of glasses doped with optically active elements such as plasmonic nanoparticles, quantum dots and rare earth ions; (iii) solidification of microbeads to act as whispering gallery mode microresonators for microbiosensing systems or microlasers. The glass-based novel photonic materials are manufactured by the NanoParticle-Direct Doping method (NPDD) developed in our laboratory. Utilizing eutectic directional solidification, we demonstrate various optical phenomena such as photoluminescence enhancement and up-conversion, tunable narrow-band transmission switched on and off with polarization; selective plasmonic enhancement of SERS/surface enhanced Raman scattering and others.
Besides manufacturing, we characterize the optical properties of materials especially on the micron and nanoscale with techniques such as Raman, UV-VIS and infrared spectroscopy (including nano-FTIR), time-resolved luminescence and optical near-field microscopy (s-SNOM).
Our goals are to combine our knowledge and expertise to develop low-cost photonic devices with enhanced functionalities.

*e-mail: dpawlak@chem.uw.edu.pl

SELECTED PUBLICATIONS:

1. P. Osewski, A. Belardini, M. Centini, C. Valagiannopoulos, G. Leahu, R. Li Voti, M. Tomczyk, A. Alù, D.A. Pawlak, C. Sibilia, New self-organization route to tunable narrowband optical filters and polarizers demonstrated with ZnO–$ZnWO_4$ eutectic composite, Adv. Opt. Mater. 8 (2020) 1901617.
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5. K. Kołodziejak, J. Sar, K. Wysmułek, P. Osewski, M. Warczak, A. Sadkowski, M. Radecka, D.A. Pawlak, When eutectic composites meet photoelectrochemistry – Highly stable and efficient UV–visible hybrid photoanodes, J. Catalysis. 352 (2017) 93.
6. P. Osewski, A. Belardini, E. Petronijevic, M. Centini, G. Leahu, R. Diduszko, D.A. Pawlak, C. Sibilia, Self-phase-matched second-harmonic and white-light generation in a biaxial zinc tungstate single crystal, Sci. Rep. 7 (2017) 45247.
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** The Laboratory of Materials Technology was founded based on the Framework Agreement on Cooperation between the UW and the Institute of Electronic Materials Technology, now being part of the Łukasiewicz Research Network. It acts effectively as one entity (yet within two institutions) with complementary infrastructure and scientific apparatus and including key expertise in the crystal growth research area.

Structural Biology Group

HEAD:

Maria Górna*, PhD

GROUP MEMBERS:

Anna Antosiewicz, PhD; Maria Klimecka, PhD; Matthew Merski, PhD; Martyna Nowacka, PhD; Anna Trzemecka, PhD
PhD students: Daria Dawidziak, Matylda Izert, Natalia Karolak
MSc students: Mikołaj Kuska, Kamil Szostak, Patrycja Szybowska
BSc student: Piotr Twardowski

RESEARCH PROFILE:

Structural Biology, Biotechnology, Molecular Biology, Protein Crystallography, Protein purification, Protein Engineering, Protein-ligand interactions, Innate Immunity and Inflammation, Antiviral effectors, Antibiotics, Drug discovery

CURRENT RESEARCH ACTIVITIES:

We study the structure and function of proteins using structural biology methods such as protein crystallography and small angle X-ray scattering (SAXS), bioinformatics analysis and molecular dynamics simulations, as well as by functional assays both in vitro and in cell culture. We are especially interested in proteins for which little structural information is available, so that we can answer vital questions about the activity and function of these proteins. Some of our interests include proteins working on RNA, helical repeats, protein engineering and molecular diagnostics. We also use structural models of proteins to elucidate the molecular mechanisms underlying selected human diseases or to aid drug discovery. Through our findings and inventions, we would like to help combat infections or treat human inflammatory disorders.
Currently, our main research topics regard: (1) development of proteolysis-targeting compounds in bacterial systems that can lead to novel antibiotics (2) complexes of human antiviral effectors from the IFIT protein family and (3) mitochondrial post-transcriptional regulators from the FASTK protein family (3). These projects are related to studies of innate immune and inflammatory processes and developing

*e-mail: mgorna@chem.uw.edu.pl

anti-inflammatory or antimicrobial agents. We also engineer proteins for biotechnology applications and molecular diagnostics and we collaborate with the pharmaceutical industry.
More updates at https://gorna.uw.edu.pl

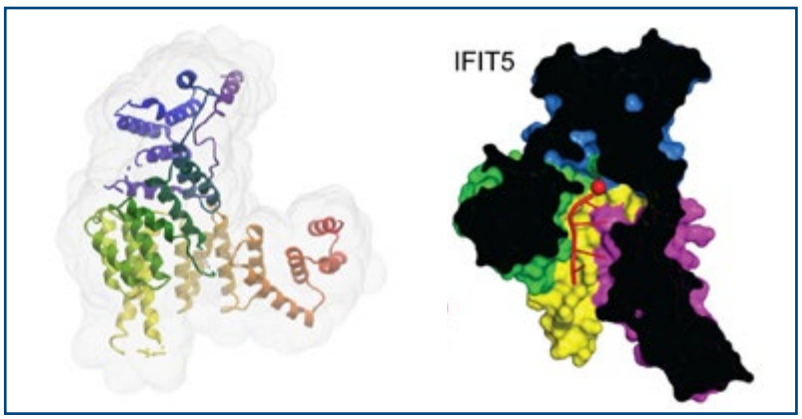

Fig. 1. Crystal structure of the human antiviral IFIT5 protein. Left, cartoon representation. Right, crosssection demonstrating that the dimensions of the pocket enable selectivity for single-stranded RNA [4].

SELECTED PUBLICATIONS:

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2. J. Kutner, I.G. Shabalin, D. Matelska, K.B. Handing, O. Gasiorowska, P. Sroka, M.W. Górna, K. Ginalski, K. Woźniak, W. Minor, Structural, Biochemical, and Evolutionary Characterizations of Glyoxylate/Hydroxypyruvate Reductases Show Their Division into Two Distinct Subfamilies, Biochemistry. 57(6) (2018) 963-977.
3. K. Byrgazov, R. Kastner, M. Górna, G. Hoermann, M. Koenig, M. Ulreich, M. Benesch, V. Strenger, H. Lackner, W. Schwinger, P. Sovinz, O.A. Haas, M. van den Heuvel-Eibrink, C.M. Niemeyer, O. Hantschel, P. Valent, G. Superti-Furga, C. Urban, M.N. Dworzak, T. Lion, NDEL1-PDGFRB fusion gene in a myeloid malignancy with eosinophilia associated with resistance to tyrosine kinase inhibitors, Leukemia. 31(1) (2017) 237-40.
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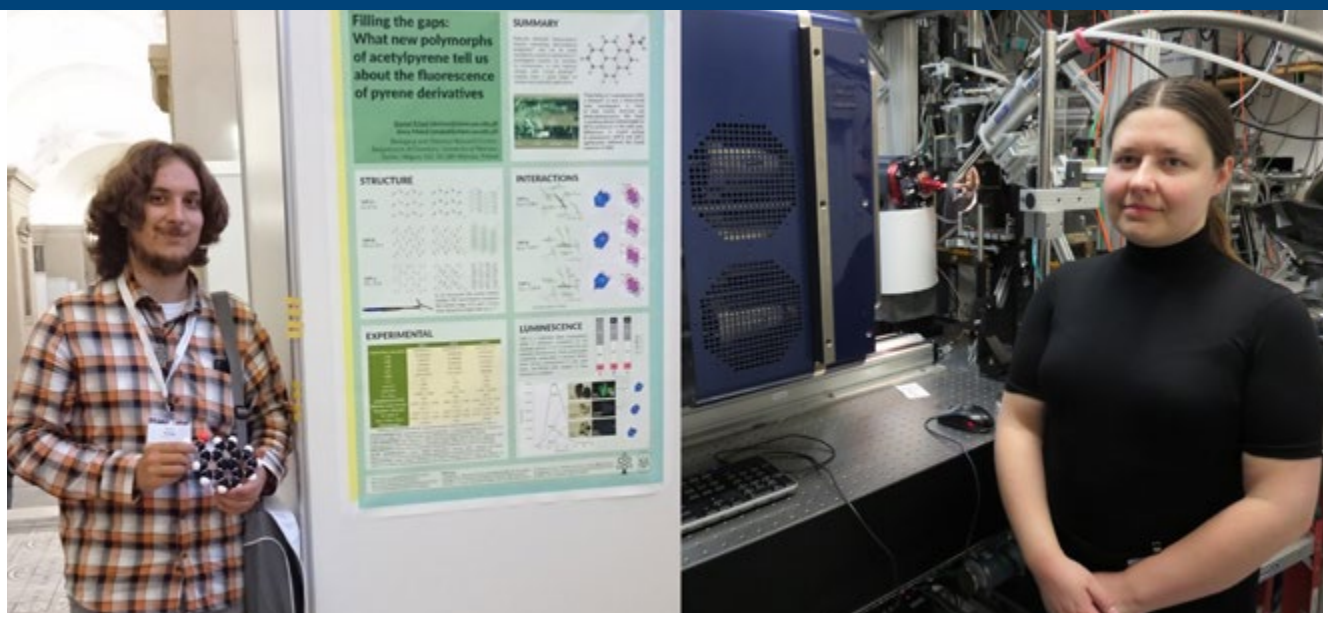
5. Y.M. Abbas, A. Pichlmair, M.W. Górna, G. Superti-Furga, B. Nagar, Structural basis for viral 5'-PPP-RNA recognition by human IFIT proteins, Nature. 494 (2013) 60-4.

Structure – Function Analysis Group



HEAD:

Anna Makal*, PhD DSc

GROUP MEMBERS:

Roman Gajda, PhD
PhD student: Daniel Tchoń
BSc student: Aleksandra Zwolenik

RESEARCH PROFILE:

Application of crystallographic methods to describe how macroscopic physicochemical properties of solid materials depend on their microscopic crystal structure; specifically molecular environment, degree of ordering, presence of modulations and other factors. The methods include X-ray and neutron diffraction (single crystal and powder) under ambient and non-ambient conditions, quantum crystallography tools and periodic DFT calculations.

CURRENT RESEARCH ACTIVITIES:

Our current research concentrates on model luminescent compounds such as pyrene derivatives and gold (I) complexes and how modification of their crystalline environment affects their luminescence by inducing color change, enhancing or quenching it. Investigation of the relationship between the crystal structure, electron density distribution and (photo) physical properties of such materials is achieved by means of X-ray diffraction experiments performed both *in-house* and at the synchrotron facilities, UV-VIS spectroscopy and theoretical calculations.
Modifications of crystalline surroundings are achieved by applying variable temperature or pressure on a crystal as well as by growing new polymorphs. Obtaining a broad spectrum of polymorphs and solvates of a given substrate means that we have to handle metastable or unstable crystal forms and often work with incomplete or otherwise challenging datasets. For instance, a vast majority of organic and metalorganic

***e-mail:** amakal@chem.uw.edu.pl

luminescent compounds crystallize in low-symmetry systems, which makes them particularly challenging when performing experiments at non-ambient conditions. Optimization of high pressure X-ray diffraction experiments for low symmetry systems and predicting attainable data completeness is one of our current objectives. Software package enabling it is in preparation.
Unlike in conventional crystal structure determination, we enjoy studying all cases of disorder, modulation or chemical short range ordering which manifest themselves in non-Bragg intensities.

Fig. 1. (left) Cover for "Crystal morphology fixed by interplay of π-stacking and hydrogen bonds – the case of 1-hydroxypyrene", CrystEngComm, 2019, 21, 1701–1717; (middle) Anna Makal, Daniel Tchoń and Roman Gajda at a manuscript writing bootcamp, Kruszyniany, July 2019; (right) Cover for "The Impact of Crystal Packing and Aurophilic Interactions on the Luminescence Properties in Polymorphs and Solvate of Aroylacetylide–Gold(I) Complexes", Chem. Eur. J. 2019, 25, 13131–13145

SELECTED PUBLICATIONS:

1. M. Głodek, S. Pawlędzio, A. Makal, D. Plażuk, The Impact of Crystal Packing and Aurophilic Interactions on the Luminescence Properties in Polymorphs and Solvate of Aroylacetylide–Gold(I) Complexes, Chem. Eur. J. 25 (2019) 13131–13145.
2. D. Tchoń, D. Trzybiński, A. Wrona-Piotrowicz, A. Makal, Polymorphism and resulting luminescence properties of 1-acetylpyrene, CrystEngComm. 21 (2019) 5845–5852.
3. D. Tchoń, A. Makal, Structure and piezochromism of pyrene-1-carbaldehyde at high pressure, Acta Cryst. B75 (2019) 343–353.
4. R. Gajda, M.A. Domański, M. Malińska, A. Makal, Crystal morphology fixed by interplay of π-stacking and hydrogen bonds – the case of 1-hydroxypyrene, CrystEngComm. 21 (2019) 1701–1717.
5. A. Makal, J. Krzeszczakowska, R. Gajda, Pressure-Dependent Structural and Luminescence Properties of 1-(Pyren-1-yl)but-2-yn-1-one, Molecules. 24 (2019) 1107.
6. M. Głodek, A. Makal, P. Paluch, M. Kądziołka-Gaweł, Y. Kobayashi, J. Zakrzewski, D. Plażuk, (Ar–CO–C≡C)(PEt3)Au and (Ar–C≡C)(PEt3)Au complexes bearing pyrenyl and ferrocenyl groups: synthesis, structure, and luminescence properties, Dalton Transactions. 47(19) (2018) 6702–6712.
7. R. Flamholc, A. Wrona-Piotrowicz, A. Makal, J. Zakrzewski, Pyrenylpyrazole-based donor/acceptor fluorescent dyes: Synthesis and photophysical properties, Dyes and Pigments. 154 (2018) 52–61.
8. A. Makal, Triethylphosphine as a molecular gear — phase transitions in ferrocenyl–acetylide–gold(I), Acta. Cryst. B74 (2018) 427–435.

Laboratory of Basic Aspects of Analytical Chemistry

UNIVERSITY OF WARSAW

WCh Faculty of Chemistry University of Warsaw

Analytical Spectrometry Research Group

HEAD:

Prof. Ewa Bulska*, PhD DSc;
DEPUTY: Barbara Wagner**, PhD DSc
(Archaeometry and Conservation Science)

GROUP MEMBERS:

Anna Konopka, PhD; Anna Ruszczyńska, PhD; Marcin Wojciechowski, PhD
Staff allocated at Biological and Chemical Research Center: Prof. Ludwik Halicz, PhD (Professor affiliated to the University of Warsaw); Prof. Katarzyna Wróbel, PhD DSc (Professor affiliated to the University of Warsaw); Jakub Karasiński, PhD; Eliza Kurek, PhD; Magdalena Michalska-Kacymirow, PhD; Julio C.E. Torres, PhD; Andrii Tupys, PhD
PhD students: Marta Bicka, Andrzej Gawor, Agata Jagielska, Adam Karpiński, Luiza Kępa, Cuc Thi Nguyen-Marcińczyk

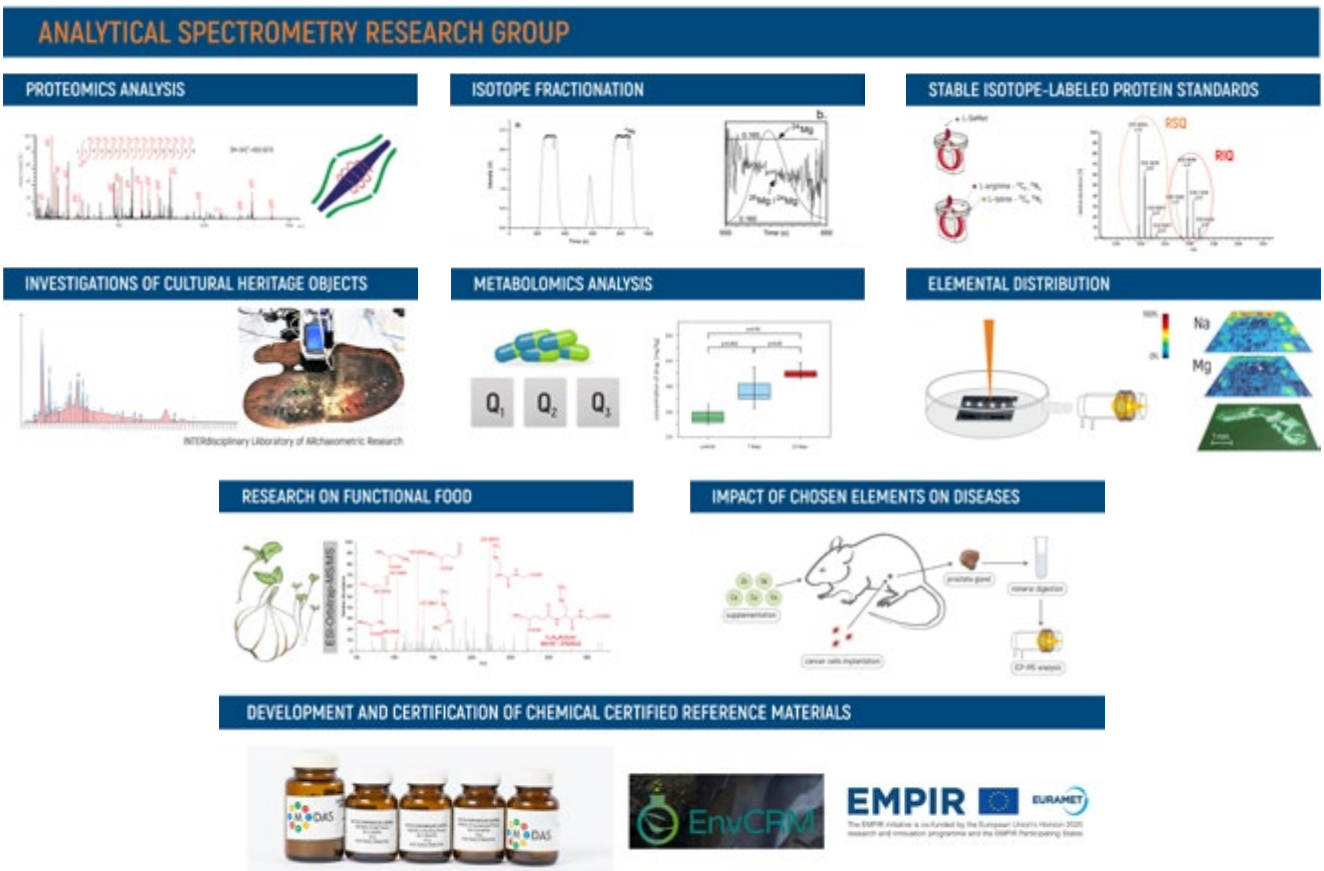
RESEARCH PROFILE:

Atomic and mass spectrometry for characterisation of matters (atomic and isotopic composition; molecular structure); Archaeometric investigation of historic objects; conservation science; Metrological principle in chemical measurements.

CURRENT RESEARCH ACTIVITIES:

Development of analytical procedures for the investigation of biotransformation and bio-metabolism of biologically active compounds; Trace analysis and chemical speciation in plants, food as well as clinical and environmentally relevant objects; stable isotopes and isotopic effects in nature; proteomic and metabolomics. Archaeometry; development of micro-invasive analytical scenarios for individual diagnosis of monuments, cultural heritage objects and works of art objects; investigation of surface and subsurface domains of solids. Analytical procedures for monitoring of industrial process. Physico-chemical processes of atomisation and ionisation in flame, graphite furnace as well as in plasmas. Development and certification of chemical certified reference materials.

***e-mail:** ebulska@chem.uw.edu.pl ****e-mail:** barbog@chem.uw.edu.pl



SELECTED PUBLICATIONS:

1. J. Karasiński, C. Nguyen-Marcińczyk, M. Wojciechowski, E. Bulska, L. Halicz, Determination isotope fractionation of Cr (III) during oxidation by LC/Low-Resolution MC-ICPMS, Journal of Analytical Atomic Spectrometry. 35 (2020) 560-566.
2. A. Bertran, D. Khomiak, A. Konopka, E. Rejmak, E. Bulska, J. Seco, L. Kaczmarek, L. Tarragó, R. Prades, Design and synthesis of selective and blood-brain barrier-permeable hydroxamate-based gelatinase inhibitors, Bioorganic Chemistry. 94 (2020) 103365.
3. A.A. Krata, M. Wojciechowski, E. Vassileva, E. Bulska, Reference measurements of mercury species in seafood using isotope dilution inductively coupled plasma mass spectrometry, Journal of Food Composition and Analysis. 86 (2020) 103381.
4. B. Wagner, L. Kępa, M. Donten, B. Wrzosek, G.Ż. Żukowska, A. Lewandowska, Laser ablation inductively coupled plasma mass spectrometry appointed to subserve pigment identification, Microchem J. 146 (2019) 279-285.
5. K. Grucza, K. Kowalczyk, M. Wicka, M. Szutowski, E. Bulska, D. Kwiatkowska, The use of a valid and straightforward method for the identification of higenamine in dietary supplements in view of anti-doping rule violation cases, Drug Test Anal. 11 (2019) 912-917.
6. O. Syta, B. Wagner, E. Bulska, D. Zielińska, G.Z. Żukowska, J. Gonzalez, R. Russo, Elemental imaging of heterogeneous inorganic archaeological samples by means of simultaneous laser induced breakdown spectroscopy and laser ablation inductively coupled plasma mass spectrometry measurements, Talanta. 179 (2018) 784-791.
7. J. Karasiński, E. Bulska, L. Halicz, M. Wojciechowski, A.A. Krata, Direct determination of δ44/42Ca isotope ratio by ion chromatography/low-resolution multicollector ICPMS, J Mass Spectrom. 53 (2018) 78-82.
8. A. Weremczuk, A. Ruszczyńska, E. Bulska, D.M. Antosiewicz, NO-Dependent programmed cell death is involved in the formation of Zn-related lesions in tobacco leaves, Metallomics. 9 (2017) 924-935.
9. J. Karasiński, K. Wróbel, A.R. Corrales Escobosa, A. Konopka, E. Bulska, K. Wróbel, Allium cepa L. Response to Sodium Selenite (Se(IV)) Studied in Plant Roots by a LC-MS-Based Proteomic Approach, Journal of Agricultural and Food Chemistry. 65 (2017) 3995-4004.
10. A. Ruszczyńska, A. Konopka, E. Kurek, J.C. Torres Elguera, E. Bulska, Investigation of biotransformation of selenium in plants using spectrometric methods, Spectrochimica Acta - Part B Atomic Spectroscopy. 130 (2017) 7-16.

Analytical Microsystems Research Group

HEAD:

Łukasz Tymecki*, PhD DSc

GROUP MEMBERS:

Michał Michalec, MSc
PhD students: Mateusz Granica, Izabela Lewińska

RESEARCH PROFILE:

Designing, optimization (miniaturization, maintenance free operation) and validation of analytical systems targeted towards various analytes relevant from clinical point of view and focused on practical use.

CURRENT RESEARCH ACTIVITIES:

Novel detection schemes, useful in clinical diagnostics. Optical and electrochemical sensors. Micro- and mesofluidic analytical systems. Mechanization and automation of analytical procedures. Lab-on-LED, Lab-on-Paper, Lab-on-Smarthone, Lab-on-Valve, Point-of-Care testing. Monitoring of hemodialysis. Rapid prototyping (3D printing) for analytical laboratory. Development of fit-to-purpose prototypes.

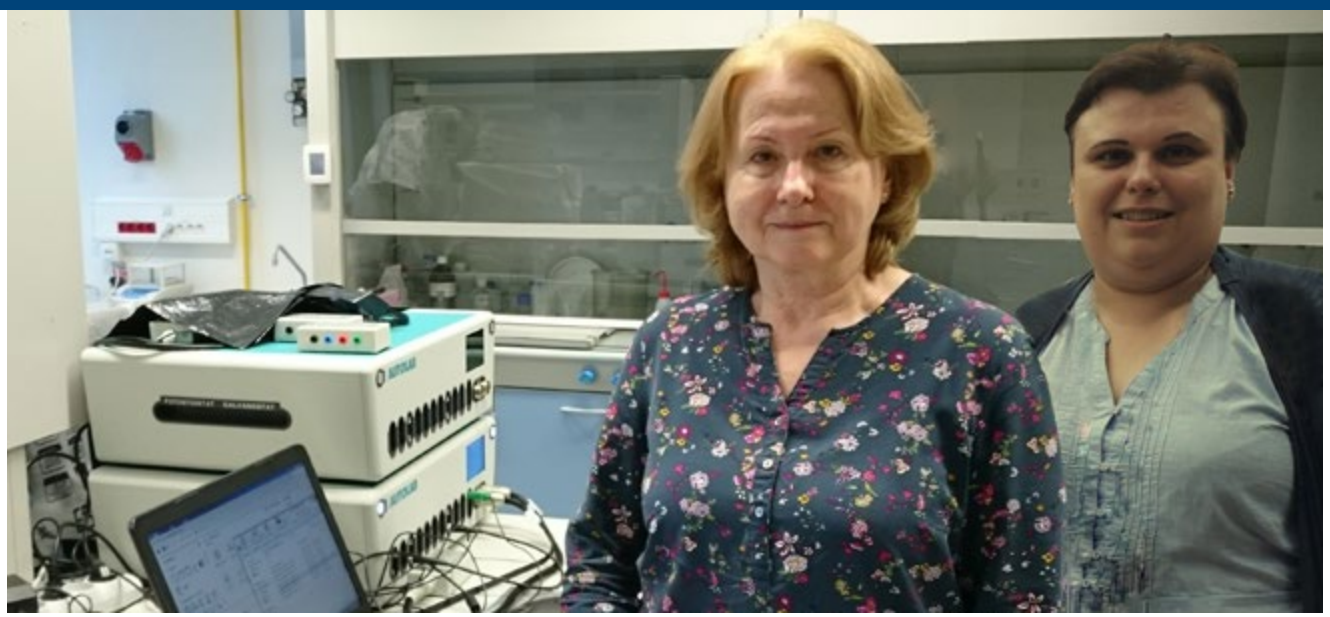
SELECTED PUBLICATIONS:

1. I. Lewińska, Ł. Tymecki, M. Michalec, An alternative, single-point method for creatinine determination in urine samples with optoelectronic detector. Critical comparison to Jaffé method, Talanta. 195 (2019) 865-869.
2. M. Granica, Ł. Tymecki, Analytical aspects of smart (phone) fluorometric measurements, Talanta. 197 (2019) 319-325.
3. D.J. Cocovi-Solberg, M. Rosende, M. Michalec, M. Miró, 3D Printing: The Second Dawn of Lab-On-Valve Fluidic Platforms for Automatic (Bio)Chemical Assays, Analytical Chemistry. 91 (2019) 1140-1149.
4. M. Michalec, Ł. Tymecki, 3D printed flow-through cuvette insert for UV–Vis spectrophotometric and fluorescence measurements, Talanta. 190 (2018) 423-428.
5. M. Granica, M. Fiedoruk-Pogrebniak, R. Koncki, Ł. Tymecki, Flow Injection Analysis in Lab-On-Paper format, Sensors and Actuators, B. Chemical. 257 (2018) 16-22.
6. M. Michalec, Ł. Tymecki, Multicommutated systems for analytical control of hemodialysis treatments (Book Chapter), in: Flow and Capillary Electrophoretic Analysis. (2018) 237-258.

*e-mail: l.tymecki@uw.edu.pl

7. M. Michalec, M. Granica, J. Bzura, R. Koncki, J. Matuszkiewicz-Rowińska, Ł. Tymecki, Optoelectronic detectors and flow analysis systems for determination of dialysate urea nitrogen, Sensors and Actuators, B: Chemical. 226 (2016) 563-56.
8. Ł. Tymecki, M. Pokrzywnicka, R. Koncki, Paired emitter detector diode (PEDD)-based photometry – An alternative approach, Analyst. 133 (2008) 1501-1504.
9. Ł. Tymecki, E. Zwierkowska, R. Koncki, Screen-printed reference electrodes for potentiometric measurements, Analytica Chimica Acta. 526 (2004) 3-11.

Bioanalytical Research Group



HEAD:

Prof. Magdalena Maj-Żurawska*, PhD DSc

GROUP MEMBERS:

Prof. Andrzej Lewenstam, PhD DSc (Professor affiliated to the University of Warsaw, allocated at Biological and Chemical Research Center); Adriana Palińska-Saadi, PhD (allocated at Biological and Chemical Research Center)

RESEARCH PROFILE:

Voltammetric and spectrometric analysis of interactions between nucleic acids and various substances.
Construction of chemical and biochemical sensors on screen-printed electrodes.
Construction of new ion-selective electrodes and optimizing their work conditions.
Potentiometric determination of the ions concentration in various samples.
Analyzes of biological and water samples by biochemical discrete analyzer.

CURRENT RESEARCH ACTIVITIES:

Our group conducts interdisciplinary research on the border of chemistry and biology. One of the areas of our research interest is the study of the interactions of nucleic acids with various chemical substances,

*e-mail: mmajzur@chem uw.edu.pl

e.g. therapeutic, toxic, antioxidant, using voltammetric and spectrometric methods. The aim of our study is to determine the affinity of different substances to nucleic acid chains and the nature of occurring interactions. We are especially interested in the interactions of deoxyribonucleic acid with chemical compounds with anticancer properties, including both drugs currently used in chemotherapy and new derivatives of these drugs. Our investigations allow to characterize the dependence of the interactions on the nucleotide sequence, the concentration of the chemical compound, as well as its structure.
The second area of our research interest includes ion-selective electrodes and determination of ion content in biological and environmental samples. We develop work on new ion-selective electrodes based on new ionophores and new materials, and on their application to various sample analyses.

The newest research field in our group is a determination of various substances, especially metals and ions, in water samples using a discrete analyzer. Actually, we are going to develop these activities, to optimize procedures of new substances determination and to enlarge the number of performed tests.
Our Laboratory is accredited by the Polish Centre for Accreditation (PCA) in accordance with the requirements specified in PN-EN ISO/IEC 17025:2018-02 General requirements for the competence of testing and calibration laboratories.

SELECTED PUBLICATIONS:

1. M. Zając, A. Lewenstam, P. Bednarczyk, K. Dołowy, Measurement of multi ion transport through human bronchial epithelial cell line provides an insight into the mechanism of defective water transport in cystic fibrosis, Membranes. 43(10) (2020) 1-13.
2. P. Piotrowska, M. Łazicka, A. Palińska-Saadi, B. Paterczyk, Ł. Kowalewska, J. Grzyb, M. Maj-Żurawska, M. Garstka, Electrochemical characterization of LHCII on graphite electrodes - Potential-dependent photoactivation and arrangement of complexes, Bioelectrochemistry. 127 (2019) 37–48.
3. M. Ordak, M. Maj-Żurawska, H. Matsumoto, M. Bujalska-Zadrożny, I. Kieres-Salomoński, T. Nasierowski, E. Muszyńska, M. Wojnar, Ionized magnesium in plasma and erythrocytes for the assessment of low magnesium status in alcohol dependent patients, Drug Alcohol Depend. 178 (2017) 271–276.
4. A. Palińska-Saadi, M. Łukasiewicz, J. Oszczapowicz, M. Łukawska, I. Oszczapowicz, E. Zwierkowska, S. Achmatowicz, M. Maj-Żurawska, Voltammetric and spectrophotometric studies on DNA interacting with daunorubicin and its amidino derivatives, Electroanalysis. 29(1) (2017) 172–181.
5. D. Janiszek, M.M. Karpińska, A. Niewiadomy, A. Girstun, H. Elżanowska, M. Maj-Żurawska, P.J. Kulesza, Phase transition detection in accumulation of a potential anticancer drug Cl-IPBD with DNA: supercoiled and linear pUC19 plasmids, Electrochim. Acta. 210 (2016) 422–434.
6. M. Ordak, H. Matsumoto, T. Nasierowski, E. Bulska, M. Maj-Żurawska, M. Wojnar, Role of selenium in pathology of alcohol dependence – indications for supplementation, J. Elementol. 18(4) (2013) 757–767.
7. A. Gniazdowska, A. Palińska-Saadi, E. Krawczyk, H. Elżanowska, M. Maj-Żurawska, Supercoiled and linear plasmid DNAs interactions with methylene blue, Bioelectrochemistry. 92 (2013) 32–41.
8. M. Maj-Żurawska, A. Lewenstam, Selectivity coefficients of ion-selective magnesium electrodes used for simultaneous determination of magnesium and calcium ions, Talanta. 87 (2011) 295–301.
9. Z. Mousavi, A. Teter, A. Lewenstam, M. Maj-Żurawska, A. Ivaska, J. Bobacka, Comparison of multi-walled carbon nanotubes and poly(3-octylthiophene) as ion-to-electron transducers in all-solid-state potassium ion-selective electrodes, Electroanalysis. 23(6) (2011) 1352–1358.
10. A. Palińska, A. Grodzka, H. Elżanowska, B. Kępska, E. Zwierkowska, S. Achmatowicz, M. Maj-Żurawska, Methylene blue interactions with chromosomal and plasmid DNA on screen-printed carbon electrodes, Electroanalysis. 22(12) (2010) 1306–1313.

BioAnalytics group

HEAD:

Prof. Robert Koncki*, PhD DSc

GROUP MEMBERS:

Marta Fiedoruk-Pogrebniak, PhD; Kamil Strzelak, PhD
PhD students: Justyna Bzura, Natalia Rybkowska, Justyna Skoczek

RESEARCH PROFILE:

Analytical methods, devices and systems for clinical and biomedical diagnostics.

CURRENT RESEARCH ACTIVITIES:

Mechanized flow bioanalytical systems and microfluidics (Lab on-Paper). Optoelectronic detectors, sensors and biosensors. 3D-printed analytical devices. Analysis of physiological fluids, Monitoring of biomedical processes, Hemodialysis, Iron metabolism. Target analytes: selected electrolytes, metabolites, toxins, vitamins, antibiotics and proteins. Enzyme activity assays and Immunoassays.

SELECTED PUBLICATIONS:

1. J. Bzura, M. Fiedoruk-Pogrebniak, R. Koncki, Photometric and fluorometric alkaline phosphatase assays using the simplest enzyme substrates, Talanta. 190 (2018) 193-198.
2. M. Granica, M. Fiedoruk-Pogrebniak, R. Koncki, Ł. Tymecki, Flow injection analysis in Lab on Paper format, Sens. Actuators B. 257 (2018) 16-22.
3. N. Rybkowska, K. Strzelak, R. Koncki, A comparison of photometric methods for serum iron determination under flow analysis conditions, Sens. Actuators B. 254 (2018) 307-313.
4. K. Strzelak, N. Rybkowska, A. Wiśniewska, R. Koncki, Photometric flow analysis system for biomedical investigations of transferrin speciation in human serum, Anal. Chim. Acta. 995 (2017) 43-51.
5. K. Strzelak, J. Misztal, Ł. Tymecki, R. Koncki, Bianalyte multicommutated flow analysis system for microproteinuria diagnostics, Talanta. 148 (2016) 707-711.
6. M. Michalec, Ł. Tymecki, R. Koncki, Biomedical analytical monitor of artificial kidney operation: monitoring of creatinine removal, J. Pharm. Biomed. Anal. 128 (2016) 28-34.

*e-mail: rkoncki@chem.uw.edu.pl

7. M. Michalec, M. Granica, J. Bzura, R. Koncki, J. Matuszkiewicz-Rowińska, Ł. Tymecki, Optoelectronic detectors and flow analysis systems for determination of dialysate urea nitrogen, Sens. Actuators B. 226 (2016) 563-569.
8. M. Pokrzywnicka, R. Koncki, Ł. Tymecki, Towards optoelectronic urea biosensors, Anal. Bioanal. Chem. 407 (2015) 1807-1812.
9. M. Fiedoruk-Pogrebniak, R. Koncki, Multicommutated flow analysis system based on fluorescence microdetectors for simultaneous determination of phosphate and calcium ions in human serum, Talanta. 144 (2015) 184-188.
10. K. Strzelak, R. Koncki, An immunoprecipitation assay in the multicommutated flow analysis format, Analyst. 140 (2015) 7271-7277.
and more: http://beta.chem.uw.edu.pl/people/RKoncki/publikacje.html

Sensors group

HEAD:

Prof. Agata Michalska*, PhD DSc (Laboratory of Basic Aspects of Analytical Chemistry) and
Prof. Krzysztof Maksymiuk*, PhD DSc (Laboratory of Electroanalytical Chemistry)

GROUP MEMBERS:

Anna Baranowska-Korczyc, PhD; Ewa Jaworska, PhD; Dawid Kałuża, PhD; Anna Kisiel, PhD; Emilia Stelmach, PhD

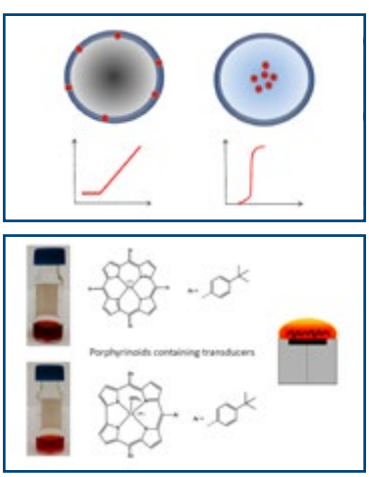
RESEARCH PROFILE:

The main research interest is in development of electrochemical and optical sensors – taking advantage of understanding mechanism underlying their operation and benefitting from novel materials, especially those in nanostructure format. The focus in sensors development is on modification by nanostructural materials.

CURRENT RESEARCH ACTIVITIES:

• Optical nanosensors - tailoring material to needs.

Micro and nano- spheres, capsules are prepared – tailoring of properties of the nanoprobe materials results in significant differences in analytical performance.



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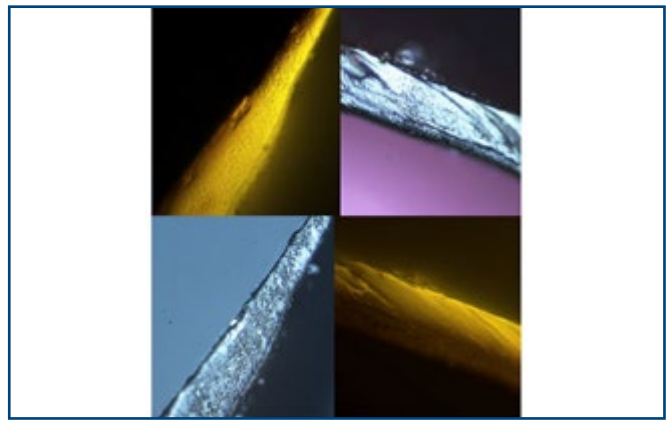
• Ion-selective electrodes and related sensors of improved performance.

The electrochemical sensors are well established group of sensors, however there is still a room for improvements of their performance or stability, extending the classical concepts taking advantage of e.g. novel materials.

*e-mail: agatam@chem.uw.edu.pl, kmaks@chem.uw.edu.pl

- Instrumental insight into ion-selective membranes and processes occurring within them.

Ion-selective membranes as receptor layers are important not only for electrochemical but also for optical sensors, detection based on these systems is ruled by processes occurring on and within the phase. Instrumental insight into ion-selective membrane is crucial to understand performance of sensors.



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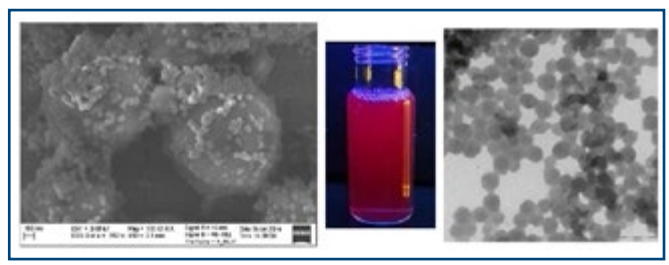
- Preparation and modification of nanostructural materials for sensor oriented purposes.

Tailored synthesis of nanostructural materials is important to obtain sensors of desired purposes. The spontaneous processes allows preparation of different structures useful to prepare improved optical or electrochemical sensors.



Reproduced from Chem. Commun. 51 (2015) 12645 – 12648 with permission from The Royal Society of Chemistry.

SELECTED PUBLICATIONS:

1. E. Jaworska, M. Mazur, K. Maksymiuk, A. Michalska, Fate of Poly(3-octylthiophene) Transducer in Solid Contact Ion-Selective Electrodes, Anal.Chem. 90 (2018) 2625–2630.
2. K. Kłucińska, E. Jaworska, K. Maksymiuk, A. Michalska, Fluorescent Polypyrrole Nanospheres – Synthesis and Properties of "Wireless" Redox Probes, Electroanalysis. 29 (2017) 2167-2176.
3. E. Jaworska, M.L. Naitana, E. Stelmach, G. Pomarico, M. Wojciechowski, E. Bulska, K. Maksymiuk, R. Paolesse, A. Michalska, Introducing Cobalt(II) Porphyrin / Cobalt(III) Corrole Containing Transducers for Improved Potential Reproducibility and Performance of All-Solid-State Ion-Selective Electrodes, Anal. Chem. 89 (2017) 7107-7114.
4. E. Stelmach, K. Maksymiuk, A. Michalska, Copolymeric Hexyl Acrylate – Methacrylic Acid Microspheres – Surface vs. Bulk Reactive Carboxyl Groups. Coulometric and Colorimetric Determination and Analytical Applications for Heterogeneous Microtitration, Talanta. 159 (2016) 248-254.
5. A. Kisiel, A. Michalska, K. Maksymiuk, Bilayer Membranes for Ion-Selective Electrodes, J.Electroanal.Chem. 766 (2016) 128-134.
6. K. Melzer, V.D. Bhatt, E. Jaworska, R. Mittermeier, K. Maksymiuk, A. Michalska, P. Lugli, Enzyme Assays Using Sensor Arrays Based on Ion-Selective Carbon Nanotube Field-Effect Transistors, Biosens. Bioelectron. 84 (2016) 7-14.
7. K. Kłucińska, E. Stelmach, A. Kisiel, K. Maksymiuk, A. Michalska, Nanoparticles of fluorescent conjugated polymers - novel ion-selective optodes, Anal. Chem. 88 (2016) 5644-5648.
8. K. Kłucińska, E. Jaworska, P. Gryczan, K. Maksymiuk, A. Michalska, Synthesis of conducting polymer nanospheres of high electrochemical activity, Chem. Commun. 51 (2015) 12645–12648.
9. K. Kłucińska, R. Jurczakowski, K. Maksymiuk, A. Michalska, Ultrasensitive 4-Methylumbelliferone Fluorimetric Determination of Water Contents in Aprotic Solvents, Talanta. 132 (2015) 392-397.
10. E. Woźnica, K. Maksymiuk, A. Michalska, Polyacrylate Microspheres for Tuneable Fluorimetric Zinc Ions Sensor, Anal. Chem. 86 (2014) 411–418.

Laboratory of Chromatography and Environmental Analysis

UNIVERSITY OF WARSAW

WCh Faculty of Chemistry University of Warsaw

Separation Techniques

HEAD:

Prof. Krystyna Pyrzyńska*, PhD DSc

GROUP MEMBERS:

Magdalena Biesaga, PhD DSc;
Ewa Poboży, PhD DSc
PhD students: Anna Kubiak, Joanna Mroczek, Maria Pęgier, Mateusz Pęgier, Małgorzata Rogozińska, Elżbieta Sobolewska

RESEARCH PROFILE:

- Mechanism of retention in liquid chromatography and capillary electrophoresis
- Modification of silica capillary for electrochromatography
- Polyphenolic compounds in food samples
- Antioxidant properties of food products
- Metabolism of polyphenolic compounds in vivo and in vitro
- Interactions between polyphenolic compounds and vitamins
- Sorbents modified with graphene and graphene oxide in solid phase extraction
- Molecularly imprinted sorbents for separation/preconcentration of biologically active compounds

CURRENT RESEARCH ACTIVITIES:

Investigation of basic factors affecting the separation efficiency of chromatographic separation in HPLC and electrophoretic separation. Optimization of chromatographic and electrophoretic separation of selected groups of proteins, pesticides and pharmaceutical residues, polyphenols and metabolites; their identification using LC/MS methods. Trace metal determinations in environmental samples. Development of new methods for sample processing with application of solid sorbents, carbon nanostructures and molecularly imprinted polymers. Application of HPLC in determination of polyphenols in food samples and investigation of antioxidant properties of different polyphenols occurring in foods using spectrophotometric and electrochemical methods.

*e-mail: kryspyrz@chem.uw.edu.pl

Application of capillary electrophoresis in determination of selected metabolites, neurotransmitters and proteins in physiological fluids. Application of HPLC in determination of natural dyes in archaeological samples.

SELECTED PUBLICATIONS:

1. A. Kubiak, A. Ciric, M. Biesaga, Dummy molecularly imprinted polymer (DMIP) as a sorbent for bisphenol S and bisphenol F extraction from food samples, Microchem. J. 156 (2020) 104836.
2. K. Pyrzyńska, Nanomaterials in speciation analysis of metals and metalloids, Talanta. 212 (2020) 120784.
3. K. Pyrzyńska, A. Sentkowska, Liquid chromatographic analysis of selenium species in plant materials, TrAC – Trends Anal. Chem. 111 (2019) 128-138.
4. M. Pęgier, K. Kilian, K. Pyrzyńska, Enrichment of scandium by carbon nanotubes in the presence of calcium matrix, Microchem. J. 137 (2018) 371–375.
5. B. Witkowski, M. Ganeczko, H. Hryszko, M. Stachurska, T. Gierczak, M. Biesaga, Identification of orcein and selected natural dyes in 14th and 15th century liturgical paraments with high-performance liquid chromatography coupled to the electrospray ionization tandem mass spectrometry (HPLC-ESI/MS/MS), Microchem. J. 133 (2017) 370-379.
6. K. Pyrzyńska, A. Kubiak, I. Wysocka, Application of solid phase extraction procedures for rare earth elements determination in environmental samples, Talanta. 15 (2016) 15-22.
7. K. Kilian, M. Pęgier, K. Pyrzyńska, The fast method of Cu-porphyrin complex synthesis for potential use in positron emission tomography imaging, Spectrochim. Acta Part A. 159 (2016) 123–127.
8. E. Poboży, A. Sentkowska, A. Piskór, Comparison of three modifications of fused-silica capillaries and untreated capillaries for protein profiling of maize extracts by capillary electrophoresis, J. Sep. Sci. 37 (2014) 2388-2394.
9. I. Sergiel, P. Pohl, M. Biesaga, A. Mirończyk, Suitability of three-dimensional synchronous fluorescence spectroscopy for fingerprint analysis of honey samples with reference to their phenolic profiles chromatography/tandem mass spectrometry, Food Chem. 145 (2014) 319-326.
10. A. Sentkowska, M. Biesaga, K. Pyrzyńska, Effects of the operation parameters on HILIC separation of flavonoids on zwitterionic column, Talanta. 115 (2013) 284-290.

Analytical chemistry in investigation and protection of the environment

HEAD:

Prof. Beata Krasnodębska-Ostręga*, PhD DSc

GROUP MEMBERS:

Ewa Biaduń, PhD; Katarzyna Kińska, PhD; Joanna Kowalska, PhD; Monika Sadowska, PhD
PhD students: Krzysztof Drwal, Alicja Kużelewska

RESEARCH PROFILE:

Analytical chemistry applied in environmental studies: environmental monitoring, evaluation of environmental pollution caused by human activity, fate of the pollutants in the environment, development of analytical tools dedicated for environmental analysis.

The main topics and analytical challenges that we meet are: determination of trace amounts of metals and metalloids in environmental samples (water, soil, sediments, plant and animal tissues, food), development of new methods of electrochemical determination of elements and their speciation in natural samples, phytoremediation processes, waste management and disposal, speciation analysis (chemical and physical speciation, fractionation), preparation of new control materials, biomonitoring and sample banking, methods of sample pretreatment (sampling, milling, homogenization), digestion/mineralization in open and closed systems (microwave assisted) and UV digestion (chemically or catalytically accelerated), application of solid phase extraction in trace speciation analysis (sample matrix simplification, separation and/or preconcentration of analytes).

CURRENT RESEARCH ACTIVITIES:

Recognition of defense mechanisms developed by plants, e.g. white mustard cultivated in the presence of high concentrations of As, Tl, Cd, Pt, Pd and Rh.

*e-mail: bekras@chem.uw.edu.pl


Reagent-free photodegradation of organic compounds used as a method of preparation of water samples for speciation analysis (HPLC with UV-Vis detection, ICP MS, voltammetry). Study of the stability of speciation (Tl, Cr, As) during sampling and sample pretreatment. Fractionation studies applied for evaluation of mobility and bioavailability of harmful and nutritious substances from soil.
Application of anodic and cathodic stripping voltammetry for trace analysis (below ppb level) of hazardous elements (Sn, Cd, Tl, Pb, Cr, As, Pt, Pd, Rh) in natural samples.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2. K. Kińska, J. Jimenez-Lamana, J. Kowalska, B. Krasnodębska-Ostręga, J. Szpunar, Study of the uptake and bioaccumulation of palladium nanoparticles by Sinapis alba using Single Particle ICP-MS, Sci. Total Environ. 615 (2018) 1078-1085.
3. J. Kowalska, K. Kińska, M. Biesaga, M. Asztemborska, Application of selective extraction and reverse phase chromatography with three detectors – PAD, FLD and ESI MS for characterization of platinum metabolites and identification of phytochelatins in Sinapis alba L. tissues, Microchem. J. 132 (2017) 198-204.
4. M. Sadowska, E. Biaduń, B. Krasnodębska-Ostręga, Stability of Tl(III) in the context of speciation analysis of thallium in plants, Chemosphere. 144 (2016) 1216-1223.
5. E. Biaduń, M. Sadowska, N. Ospina-Alvarez, B. Krasnodębska-Ostręga, Direct speciation analysis of thallium based on solid phase extraction and specific retention of a Tl(III) complex on alumina coated with sodium dodecyl sulfate, Microchim Acta. 183 (2016) 177–183.
6. J. Kowalska, K. Kińska, J. Pałdyna, M. Czyżewska, K. Boder, B. Krasnodębska-Ostręga, Determination of traces of Pt and Rh in soil and quartz samples contaminated by automobile exhaust after an ion-exchange matrix separation, Talanta. 127 (2014) 250–254.
7. B. Krasnodębska-Ostręga, M. Sadowska, K. Piotrowska, M. Wojda, Thallium (III) determination in the Baltic seawater samples by ICP MS after preconcentration on SGX C18 modified with DDTC, Talanta. 112 (2013) 73-79.
8. B. Krasnodębska-Ostręga, M. Sadowska, S. Ostrowska, Thallium speciation in plant tissues – Tl(III) found in Sinapis alba L. grown in soil polluted with tailing sediment containing thallium minerals, Talanta. 93 (2012) 326-329.
9. Ł. Jedynak, J. Kowalska, Stability of arsenic species in hydroponic medium and its influence on arsenic uptake and distribution in White mustard (Sinapis alba L.), Microchem. J. 98 (2011) 163-169.
10. B. Krasnodębska-Ostręga, J. Pałdyna, J. Kowalska, Ł. Jedynak, J. Golimowski, Fractionation study in bioleached metallurgy wastes using six-step sequential extraction, J. Hazard. Mater. 167 (2009) 128-135.

Laboratory of Dielectrics and Magnetics

UNIVERSITY OF WARSAW

WCh Faculty of Chemistry University of Warsaw

Liquid Crystals and Polymers

HEAD:

Prof. Ewa Górecka*, PhD DSc

GROUP MEMBERS:

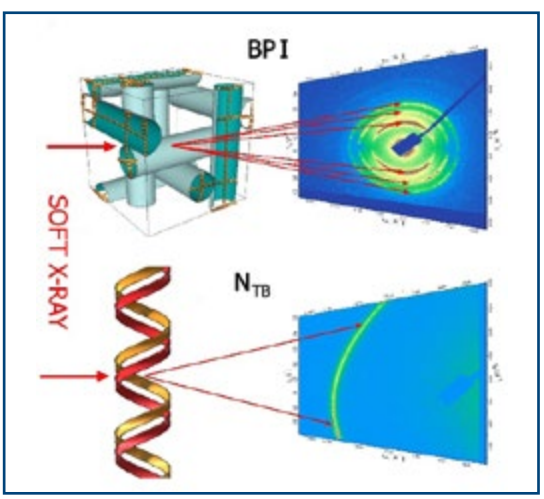
prof. Adam Krówczyński, PhD DSc (emeritus); Damian Pociecha, PhD DSc; Paweł Majewski, PhD; Jadwiga Szydłowska, PhD (emeritus)
PhD students: Muhammed Ali, Magdalena Fedorczyk, Arkadiusz Leniart, Andrzej Sitkiewicz

RESEARCH PROFILE:

liquid crystals, polymers, nanoparticles and generally soft matter science

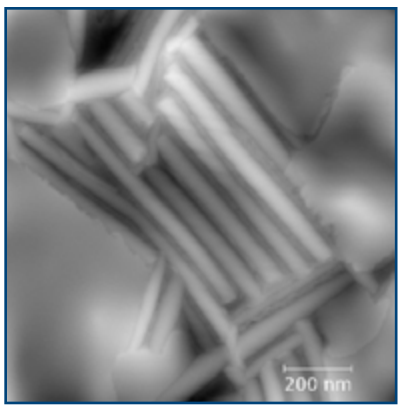
CURRENT RESEARCH ACTIVITIES:

- Chiral structures built form achiral/chiral molecules: chiral symmetry breaking in soft matter is a hot topic of current research. Recently, such a phenomenon was found in a fluidic phase showing orientational order of molecules - the nematic phase; although built of achiral molecules, the phase can exhibit structural chirality as molecules form a short-pitch helices. Recently, similar short-pitch helical structure was confirmed also in the smectic phases by resonant X-ray measurements. Resonant X-ray scattering was also applied to resolve the structure of complex liquid crystalline phases without positional order, e.g. blue phases.



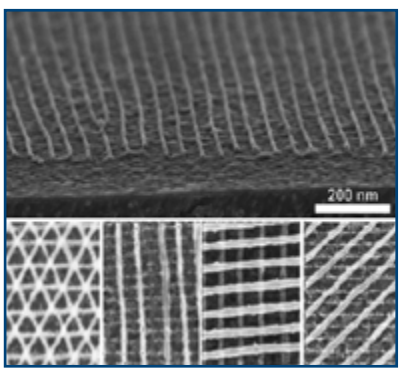
*e-mail: gorecka@chem.uw.edu.pl

- Complex morphology: nanotubes, nano-ribbons, sponges. The liquid crystalline or crystalline phases made of molecules with non-trivial geometry (e.g. bent-core, dimeric) might exhibits an unusual, highly porous sponge-like, twisted ribbon or tubular morphology. The morphology can be programmed by adsorption of low-weight mesogenic molecules on the crystal surface.



- Organic electronics: Liquid crystals as self-organizing and self-healing materials are often considered as an attractive alternative to solid state electronics and used to produce OLED, OFET and other-type photovoltaic devices. Pre-condition for electronic application of liquid crystalline materials is their fast, anisotropic charge mobility. Efficient charge transport is inherent to many materials forming columnar phases, as the columnar stacking of molecules allows charge hoping between neighboring molecules due to their strong orbitals overlapping.

- Block Co-Polymers: practical application of block co-polymers (BCP) and BCP-derived nanostructures in filtration membranes, transparent electrodes, light polarizers, anti-reflection layers, superhydrophobic coatings, chemical sensors and catalytic materials requires fast and efficient methods for polymer alignment. It was shown that by thermal gradients induced by localized laser heating and shear fields it is possible to align block-copolymer film in less than a second. Utilizing this method novel BCPs architectures can be obtained and further used as templates for the conversion to multi-layered inorganic (metallic or metal oxide) nanostructures with precise spatial control over their chemical composition.



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2. E. Górecka, N. Vaupotič, A. Zep, D. Pociecha, From sponges to nanotubes – a change of nano-crystal morphology for acute-angle bent-core molecules, Angew. Chem. Int. Ed. 55 (2016) 3468–3472.
3. E. Górecka, N. Vaupotic, A. Zep, D. Pociecha, J. Yoshioka, J. Yamamoto, H. Takezoe, A Twist-Bend Nematic (NTB) Phase of Chiral Materials, Angew. Chem. Int. Ed. 54 (2015) 10155–10159.
4. P.W. Majewski, A. Rahman, C.T. Black, K.G. Yager, Arbitrary lattice symmetries via block copolymer nanomeshe, Nat. Commun. 6 (2015) 7448.
5. P.W. Majewski, K.G. Yager, Latent Alignment in Pathway-Dependent Ordering of Block Copolymer Thin Films, Nano Lett. 15 (2015) 5221-5228.
6. A. Zep, M.M. Wójcik, W. Lewandowski, K. Sitkowska, A. Promiński, J. Mieczkowski, D. Pociecha, E. Górecka, Phototunable Liquid-Crystalline Phases Made of Nanoparticles, Angew. Chem. Int. Ed. 53 (2014) 13725-13728.

Laboratory of Electroanalytical Chemistry

UNIVERSITY OF WARSAW

WCh Faculty of Chemistry University of Warsaw

Highly Functionalized Materials for Electrochemical Science, Nanotechnology and Sustainable Energetics

HEAD:

Prof. Paweł J. Kulesza*, PhD DSc; Iwona A. Rutkowska*, PhD DSc

GROUP MEMBERS:

prof. Zbigniew Galus, PhD DSc (emeritus);
Beata Dembińska, PhD; Hanna Elżanowska, PhD;
Cezary Gumiński, PhD; Barbara Kowalewska, PhD;
Magdalena Skunik-Nuckowska, PhD;
Sylwia Żołądek, PhD
PhD students: Magdalena Blicharska-Sobolewska, Kamila Brzozowska, Katarzyna Jakubów-Piotrowska, Dominika Janiszek, Justyna Lubera, Weronika Łotowska, Justyna Makowska, Weronika Postek, Ewelina Seta, Ewelina Szaniawska, Anna Wadas, Katarzyna Węgrzyn

RESEARCH PROFILE:

Our interests concern various aspects of fundamental and applied electroanalytical chemistry related to materials chemistry as well as to kinetics and mechanism of electrode reactions. Our major research achievements are at the borderline of electrochemistry, inorganic chemistry and materials chemistry with special emphasis on elucidation of mechanisms of charge propagation in model mixed-valent polynuclear inorganic systems (polyoxometallates, Prussian Blue type metal hexacyanometallates, hybrids with organic conducting polymers) and, later, on the relation between the structure of novel materials and their electrocatalytic activity in electrochemical and photoelectrochemical energy conversion devices (e.g. P. J. Kulesza, I. A. Rutkowska). The advanced functional materials can find application in alternative energy sources such as fuel cells (e.g. B. Dembinska), biofuel cells and photoelectrochemical cells (e.g. dye-sensitized solar cells, electrolyzers for hydrogen generations). Furthermore, we are interested in fabrication, characterization and utilization of various functionalized and intentionally decorated noble metal nanoparticles (e.g. S. Żołądek). The feasibility of demonstrating possible analytical applications, such as determination of highly inert analytes, potential-controlled preconcentration of certain ions and reactants, amperometric sensing and biosensing should be mentioned here. We also concentrate on the description of mechanisms and dynamics of charge propagation of solid, crystalline or semi-liquid materials involving reversible redox transitions allowing for charge mediation and storage. Special attention is paid to the development and characterization of highly porous nanostructured carbons (including graphene nanoplatelets) for charge storage in supercapacitive type devices (e.g. M. Skunik-Nuckowska).

*e-mail: pkulesza@chem.uw.edu.pl, ilinek@chem.uw.edu.pl

Of particular interest is design and characterization of bioelectrocatalytic nanostructured systems with potential applications in biofuel cells and analytical biosensors (e.g. B. Kowalewska). In the research, enzymes from the oxidoreductase family are used as biocatalysts for the oxidation reaction of the fuel, i.e. glucose, lactates, ethanol. Finally, the biomedical aspects of electrochemical research are explored, e.g. to elucidate interactions of plazmid DNA with pentamidine in comparison to potential anticancer drug, Cl-IPBD (e.g. H. Elzanowska). Fundamental chemical properties of inorganic systems are of our concern as well (e.g. C. Gumiński).

CURRENT RESEARCH ACTIVITIES:

Our research aims at better understanding of the role of the metal oxide nanostructured additivities that affect the catalytic performance of noble metal nanoparticles with respect to adsorption, desorption and catalytic steps during oxidation of simple organic fuels (e.g. I. A. Rutkowska) or oxygen reduction (e.g. B. Dembińska, S. Żołądek). We demonstrate and emphasize the importance of interactions with the metal oxide support and emphasize its chemical state and activity toward removal of undesirable hydrogen peroxide intermediate during the oxygen reduction reaction. We also develop new catalytic systems permitting selective conversion (electrochemical, photoelectrochemical) of CO_2 to small organic molecules (e.g. I. A. Rutkowska, P. J. Kulesza). In bioelectrochemical research, carbon nanostructures (carbon nanotubes, graphene, fullerene) that are appropriately modified are utilized as highly conductive matrices, enabling effective electron transfer from the enzyme redox center to the electrode surface (e.g. B. Kowalewska). Finally, electrochemical studies aiming at elucidating interactions of plasmid DNA with antifungal and antibacterial compounds are also pursued (e.g. H. Elżanowska). High-power capacitor-like batteries are of our concern as well (e.g. M. Skunik-Nuckowska).

SELECTED PUBLICATIONS:

1. E. Szaniawska, K. Bieńkowski, I.A. Rutkowska, P.J. Kulesza, R. Solarska, Enhanced photoelectrochemical CO_2-reduction system based on mixed Cu_2O - nonstoichiometric TiO_2 photocathode. Catal. Today. 300 (2018) 145-151.
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7. D. Janiszek, M.M. Karpińska, A. Niewiadomy, A. Girstun, H. Elżanowska, M. Maj-Żurawska, P.J. Kulesza, Phase Transition Detection in Accumulation of a Potential Anticancer Drug Cl-IPBD with DNA: Supercoiled and Linear pUC19 Plasmids, Electrochimica Acta. 210 (2016) 422-431.
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Catalysis and Physicochemistry of Surface

HEAD:

Adam Lewera*, PhD DSc

GROUP MEMBERS:

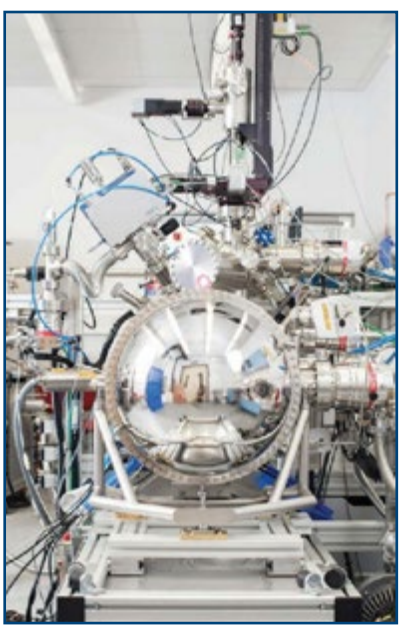
Maciej Gorzkowski, PhD
PhD students: Barbara Gralec, Justyna Piwowar, Paweł Wnuk

RESEARCH PROFILE:

Electronic origins of catalytic activity

CURRENT RESEARCH ACTIVITIES:

The aim of the research is to gain a better understanding of the mechanisms of catalytic reactions and the factors influencing the catalytic activity. Particular emphasis is put on the relationship between the surface electronic properties and the overall catalytic activity, and also how the change in electronic properties of a given surface change the mechanisms of catalytic reactions occurring at that surface. Combination of various methods, such as X-ray Photoelectron Spectroscopy, UV-photoelectron Spectroscopy, Differential Electrochemical Mass Spectrometry and electrochemical methods allows for a better insight especially on electrocatalytic reactions. This research is closely related to developing new materials for electrodes in new sources of electricity, e.g. for low temperature fuel cells, feed with liquid fuels. This promising energy sources are still economically unviable due to low activity or anode and cathode catalysts, and developing new, more active electrocatalysts is needed in order to make low temperature fuel cells widely used.



*e-mail: alewera@chem.uw.edu.pl

SELECTED PUBLICATIONS:

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5. J. Seweryn, A. Lewera, Electrooxidation of ethanol on carbon-supported Pt-Pd nanoparticles, Journal of Power Sources. 205 (2012) 264–271.
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9. Panakkattu K. Babu, A. Lewera, Jong Ho Chung, R. Hunger, W. Jaegermann, N. Alonso-Vante, A. Więckowski, E. Oldfield, Selenium Becomes Metallic in Ru-Se Fuel Cell Catalysts: An EC-NMR and XPS Investigation, Journal of the American Chemical Society. 129(49) (2007) 15140-15141.
10. A. Lewera, W.P. Zhou, R. Hunger, W. Jaegermann, A. Więckowski, S. Yockel, P. S. Bagus, Core-level Binding Energy Shifts in Pt-Ru nanoparticels: A puzzle resolved, Chemical Physics Letters. 447 (2007) 39-43.

Group of Nonlinear Dynamics in Chemical and Electrochemical systems

HEAD:

Prof. Marek Orlik*, PhD DSc

GROUP MEMBERS:

BSc student: Przemysław Oliwa

RESEARCH PROFILE

Studies of dynamic self-organization of matter in chemical and electrochemical systems exhibiting nonlinear dynamics. Such phenomena, occurring beyond the state of chemical equilibrium, comprise (i) spontaneous oscillatory variations of the systems' state and (ii) multistability, i.e. the coexistence of more than one stable steady-state for the same set of control parameters.

Moreover, the coupling of transport (e.g., diffusion) with nonlinear (electro)chemical reactions can give rise to the non-equilibrium (dissipative) patterns. All these kinds of phenomena occur in various chemical and physical systems, mimicking thus the self-organization and pattern formation in biological systems (e.g. Turing patterns, pulsatory heart dynamics, circadian rhythm. etc.). The universal characteristics of those phenomena is given by their mathematical analysis, leading to the schemes of bifurcations common for various dynamical systems [1, 2].

CURRENT RESEARCH ACTIVITIES:

Recent research activity of the group focusses on the oscillations and pattern formation in the chemical oscillators based on the oxidation of sulfur-containing compounds by hydrogen peroxide. For the H_2O_2–SCN^- – OH^- – Cu^{2+} oscillator, the most important achievements include the reduction of its complex reaction mechanism to the so-called "minimal oscillator", i.e. the core reaction steps which are necessary to induce the oscillatory instability (Fig. 1).
Moreover, it was discovered that this system, in the presence of luminol as an indicator, gives rise to luminescent dissipative patterns only under condition of the non-uniform distribution of temperature, which

*e-mail: morlik@chem.uw.edu.pl

causes the spatial distribution of the oscillatory reaction dynamics. Analogous experimental conditions applied to the H_2O_2 – $S_2O_3^{2-}$ – H^+ – Cu^{2+} system in the presence of the pH indicator caused the formation of travelling front of pH (Fig. 2).
Both latter results indicate the novel mechanism of pattern formation in aqueous media, complementing those proposed for the systems with uniform temperature distribution.

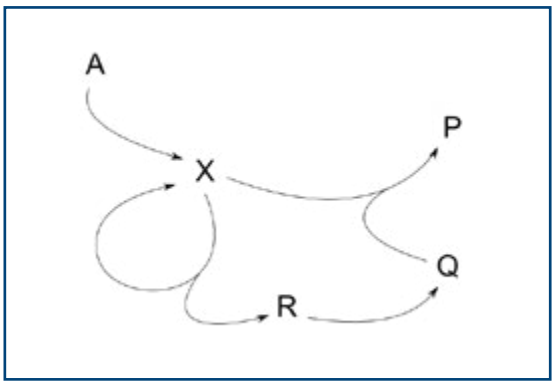

Fig. 1. Reaction network of the "minimal oscillator" of the H_2O_2 – SCN^- – OH^- - Cu^{2+} system in which X is autocatalytically produced from reactant A and then X is consumed by intermediate Q acting as a negative feedback species [4]. Reprinted from [4] with permission from John Wiley and Sons, Inc. © 2015.

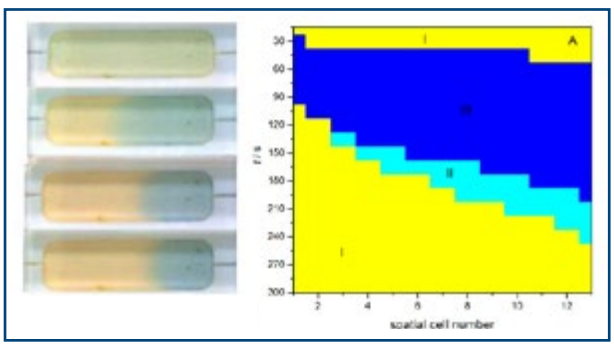

Fig. 2 (left) Experimentally reported color pH front moving in the H_2O_2 - $S_2O_3^{2-}$ - H+ - Cu^{2+} + thymol blue system subject to inhomogeneous temperature distribution; (right) mathematical model of this process [5]. Reprinted with permission from [5] Copyright 2016, American Chemical Society.

SELECTED PUBLICATIONS:

1. M. Jędrusiak, M. Orlik, The formation and spatiotemporal progress of the pH wave induced by the temperature gradient in the thin-layer H_2O_2 – $Na_2S_2O_3$ – H_2SO_4 – $CuSO_4$ dynamical system, J. Phys. Chem. B. 120 (2016) 3169-3177.
2. M. Jędrusiak, A. Wiśniewski, M. Orlik, The model of "minimal oscillator" derived from the kinetic mechanism of the H_2O_2 – NaSCN – NaOH – $CuSO_4$ dynamical system, Int. J. Chem. Kinet. 47 (2015) 791–802.
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4. M. Orlik, Self-Organization in electrochemical systems. II. Spatiotemporal patterns and control of chaos. In: Scholz F. (ed.) Monographs in Electrochemistry, Springer, Berlin-Heidelberg 2012.
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Hybrid Materials for Electrocatalysis and Photocatalysis

HEAD:

Krzysztof Miecznikowski*, PhD DSc

GROUP MEMBERS:

PhD student: Barbara Zakrzewska

RESEARCH PROFILE:

Our interests concern elaboration of materials and compounds of potential application in electrocatalysis, photocatalysis and various type of sensors.

CURRENT RESEARCH ACTIVITIES:

Preparation and electrochemical characterization of novel materials for electrooxidation of oxygen reduction reaction (ORR) based on platinum nanoparticles and nonprecious metal catalysts.
Development of novel integrated electrocatalyst sytems for electrooxidation of polyhydric and monohydric alcohols as alternative technologies to hydrogen based fuel cells.
The investigations focus principally on photoelectrochemical properties of hierarchical semiconducting oxide electrodes, such as tungsten trioxide (WO_3), ferric oxide (Fe_2O_3) and polyoxometalates that are employed to split water or photodecompose organic pollutants present in water.
Development of new colorimetric test for onsite preliminary drugs tests in illicit samples. These studies are conducted in cooperation with the Central Forensic Laboratory of the Police Research Institute in Warsaw.

SELECTED PUBLICATIONS:

1. E. Biaduń, N. Nowak, J. Kowalska, K. Miecznikowski, B. Krasnodębska-Ostręga, Organic matter decomposition before arsenic speciation analysis of water sample - "Soft decomposition" using nano-photocatalysts, Chemosphere. 207 (2018) 481.
2. W.H. Steinecker, K. Miecznikowski, P.J. Kulesza, Z.D. Sandlin, J.A. Cox, Amperometric detector for gas chromatography based on a silica sol-gel solid electrolyte, Talanta. 174 (2017) 1.
3. L. Adamczyk, J.A. Cox, K. Miecznikowski, Activation of a Pt-based alloy by a Keggin-type cesium salt of heteropolytungstate towards electrochemical oxidation of ethylene glycol in acidic medium, International Journal of Hydrogen Energy. 42 (2017) 5035.

*e-mail: kmiecz@chem.uw.edu.pl

4. B. Krasnodębska-Ostręga, A. Bielecka, E. Biaduń, K. Miecznikowski, Mesoporous film of WO3-the "sunlight" assisted decomposition of surfactant in wastewater for voltammetric determination of Pb, Applied Surface Science. 388 (2016) 746.
5. K. Miecznikowski, A. Ramírez, S. Fiechter, P. Bogdanoff, E. Szaniawska, A. Wadas, P.J. Kulesza, Development of Hybrid Tungsten Oxide Photoanodes Admixed with Borododecatungstate-Polyanion Modified-Hematite: Enhancement of Water Oxidation upon Irradiation with Visible Light, Electrochimica Acta. 179 (2015) 379.
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7. L. Adamczyk, K. Miecznikowski, Solid-state electrochemical behavior of Keggin-type borotungstic acid single crystal, Journal of Solid State Electrochemistry. 17 (2013) 1167.
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9. K. Miecznikowski, P.J. Kulesza, Activation of dispersed PtSn/C nanoparticles by tungsten oxide matrix towards more efficient oxidation of ethanol, Journal Power Sources. 196 (2011) 2595.

Laboratory of Electrochemistry

HEAD:

Rafał Jurczakowski*, PhD DSc

GROUP MEMBERS:

Piotr Połczyński, PhD
PhD students: Paweł Kulboka, Rafał Rutkowski, Maciej Słojewski
MSc students: Elwis Borecki, Agnieszka Prus

RESEARCH PROFILE:

Contributing to a better understanding of surfaces, interfaces, nanostructures and their applications. Development of synthesis methods of well-defined surfaces and nanostructured materials and investigations of processes at the interfaces by using electrochemical methods and impedance spectroscopy.

CURRENT RESEARCH ACTIVITIES:

Research covers surface/interface reactivity, ion transport, materials for heterogeneous catalysis, and electrochemical/photoelectrochemical energy conversion and storage. Our group is interested in the innovative use of the electrochemical methods in chemical science. Our work is also related to the theoretical development and the use of impedance spectroscopy for kinetic and thermodynamic studies of (electro)chemical systems under both supported and unsupported (solid state) conditions.
Impedance spectroscopy (IS) is a relatively new and powerful method allowing for the investigation of electrical properties of matter and relaxation phenomena with time constants ranging over nearly ten orders of magnitude. Electrochemical impedance spectroscopy (EIS), unlike any other electrochemical method, can provide a full insight into the mechanism and kinetics of electrode processes. We develop comprehensive explanations and theories describing different physicochemical systems allowing for a broader application of IS in material science and electrochemistry (EIS).
Our scientific research is also related to the hydrogen sorption phenomena and electrode reactions involving hydrogen adsorption and absorption in heterogeneous catalysis. Hydrogen can be considered as an ideal energy carrier, however, hydrogen storage is one of the most challenging problem to be solved

*e-mail: rafjur@chem.uw.edu.pl

toward the realization of the hydrogen economy. Metallic based hydrogen storage materials have an ability to reversibly absorb and release significant amount of hydrogen directly or under electrochemical conditions. Reversible hydride formation may be applied in many areas such as rechargeable batteries, hydrogen storage systems and cooling devices. Another potential application is related to hydrogen sensing. The mechanism of hydrogen absorption in metals remains still unresolved problem yet its understanding on the molecular level plays a key role during the design of novel materials of required absorption properties.

SELECTED PUBLICATIONS:

1. T. Pajkossy, R. Jurczakowski, Electrochemical impedance spectroscopy in interfacial studies. Current Opinion in Electrochemistry. 1(1) (2017) 53-58.
2. B. Łosiewicz, R. Jurczakowski, A. Lasia, Kinetics of hydrogen underpotential deposition at iridium in sulfuric and perchloric acids. Electrochim Acta. 225 (2017) 160-167.
3. P. Połczyński, R. Jurczakowski, Extremely fast hydrogen absorption/desorption through platinum overlayers, J Power Sources. 305 (2016) 233-239.
4. P. Połczyński, R. Jurczakowski, Impedance as a Tool for Rapid and Complete Characterization of Electrocatalytic Systems Involving Redox Mediators, Electrochim Acta. 188 (2016) 882-887.
5. A. Januszewska, G. Dercz, A. Lewera, R. Jurczakowski, Spontaneous Chemical Ordering in Bimetallic Nanoparticles, The Journal of Physical Chemistry C. 119(34) (2015) 19817-19825.
6. W. Adamczyk, P. Połczyński, A. Mika, T. Jaroń, Z. Mazej, K.J. Fijałkowski, R. Jurczakowski, W. Grochala, New Ag(F1-xClx) phases for energy storage applications, J Fluorine Chem. 174 (2015) 22-29.
7. R. Jurczakowski, P. Połczyński, Impedance of Mediated Electrochemical Processes. Novel Impedance Element for Unequal Diffusivities, J Phys Chem C. 118(15) (2014) 7980-7988.

Laboratory of Electrochmical Power Sources

UNIVERSITY OF WARSAW

WCh Faculty of Chemistry University of Warsaw

Radiochemistry for Medicine and Industry

HEAD:

Zbigniew Rogulski*, PhD DSc

GROUP MEMBERS:

prof. Andrzej Czerwiński, PhD DSc; Maciej Chotkowski, PhD DSc; Michał Grdeń, PhD DSc; Krzysztof Kilian, PhD DSc; Marek Pruszyński, PhD DSc; Paulina Hamankiewicz, PhD; PhD; Katarzyna Pałka, PhD; Elżbieta Winnicka, PhD
PhD students: Jakub Boratyński, Łukasz Cheda, Joanna Gaweł, Michał Jagodziński, Martyna Mieszkowska, Dawid Pogoda, Damian Połomski, Weronika Wargocka, Jakub Witkowski

RESEARCH PROFILE:

Our group's research interests lie in three main areas: 1. application of radioisotopes in medicine, in particular, studying the affinity of chemical substances to body tissues, 2. monitoring of radioactive wastes 3. Energy storage and transformation: batteries, fuel cells.

CURRENT RESEARCH ACTIVITIES:

We closely cooperate with industry therefore most of our inventions have multiple industrial applications. Our group members conduct pre-clinical research on pharmaceuticals and radiopharmaceuticals using PET/SPECT/CT techniques, they also modify and recycle electrochemical power sources and study the phenomena of oxidation of precious and base metals. The group has modern and unique equipment at its disposal which enables world-class research in the field of molecular imaging, synthesis of radioisotope-tagged compounds and studying materials used in electrochemical power sources. The equipment includes: three-module PET/CT/SPECT scanner, a system of individually ventilated cages (IVC) for mice and rats, hot cells, isotope generators and modules for the synthesis and portioning of radioisotope-labelled compounds (among others ^{18}F, ^{64}Cu, ^{68}Ga), a quality control system for radiopharmaceuticals, an EDXRF X-ray fluorescence spectrometer for quantitative and qualitative analysis of samples, equipment for spectroelectrochemical tests (UV-vis spectrometers, potentiostats), potentiostats, galvanostats and battery testers.

*e-mail: rogul@chem.uw.edu.pl

SELECTED PUBLICATIONS:

1. A. Wójtowicz, P. Krug, P. Głowala, A.B. Hungría, M. Chotkowski, K. Wiktorska, M. Mazur, Nano-radiogold-decorated composite bioparticles, Materials Science and Engineering C. 97 (2019) 768-775.
2. M. Grdeń, G. Jerkiewicz, Influence of Surface Treatment on the Kinetics of the Hydrogen Evolution Reaction on Bulk and Porous Nickel Materials, Electrocatalysis. 10 (2019) 173-183.
3. Ł. Kiraga, Ł. Cheda, B. Taciak, K. Różańska, K. Tonecka, A. Szulc, K. Kilian, E. Górka, Z. Rogulski, T. P. Rygiel, M. Król, Changes in hypoxia level of CT26 tumors during various stages of development and comparing different methods of hypoxia determination, PLoS ONE. 13 (2018).
4. M. Ciebiera, J. Szymańska-Majchrzak, A. Sentkowska, K. Kilian, Z. Rogulski, G. Nowicka, G. Jakiel, P. Tomaszewski, M Włodarczyk, Alpha-Tocopherol Serum Levels Are Increased in Caucasian Women with Uterine Fibroids: A Pilot Study, BioMed Research International. (2018) 6793726.
5. K. Kilian, Ł. Cheda, M. Sitarz, K. Szkliniarz, J. Choiński, A. Stolarz, Separation of ^{44}Sc from Natural Calcium Carbonate Targets for Synthesis of ^{44}Sc-DOTATATE, Molecules. 23 (2018) 1787.
6. M. Chotkowski, M. Grdeń, B. Wrzosek, Intermediate oxidation states of technetium in alkaline solutions, Journal of Electroanalytical Chemistry. 829 (2018) 148-156.
7. M. Pruszyński, M. D'Huyvetter, F. Bruchertseifer, A. Morgenstern, T. Lahoutte, Evaluation of an Anti-HER2 Nanobody Labeled with ^{225} Ac for Targeted α-Particle Therapy of Cancer, Molecular Pharmaceutics. 15 (2018) 1457-1466.
8. M. Chotkowski, D. Połomski, Extraction of pertechnetates from HNO_3 solutions into ionic liquids, Journal of Radioanalytical and Nuclear Chemistry. 314 (2017) 87-92.
9. M. Grdeń, Impedance study on the capacitance of silver electrode oxidised in alkaline electrolyte, Journal of Solid State Electrochemistry. 21 (2017) 3333-3344.
10. M. Grdeń, Platinum oxidation in alkaline electrolyte under potentiostatic conditions, Electrochemistry Communications. 61 (2015) 14-17.

Hydride Cells and Hydrides Research Group

HEAD:

Katarzyna Hubkowska-Kosińska*, PhD

GROUP MEMBERS:

prof. Andrzej Czerwiński, PhD DSc;
Michał Krajewski, PhD; Małgorzata Pająk, PhD;
Michał Symonowicz, MSc

RESEARCH PROFILE:

Our research is mainly focused on the development and improvement of hydrogen storage materials as well as their applications in the nickel-metal hydride batteries.

CURRENT RESEARCH ACTIVITIES:

Current studies of our research group are mainly focused on fundamental research on hydrogen electrosorption in model systems such as palladium and its alloys with ruthenium, rhodium and platinum in concentrated alkaline solutions and in protic ionic liquids (Fig. 1) as well as examination of sorption-desorption of hydrogen in transition metal alloys, type AB_5 and hybrid system: Pd alloys/AB_5 used as negative electrodes in nickel-metal hydride batteries. Moreover, we are also during research on AB_5 particles covered with palladium and other noble metal (alloys) nanoparticles to obtain high performance anode for Ni-MH battery.

*e-mail: khubkowska@chem.uw.edu.pl

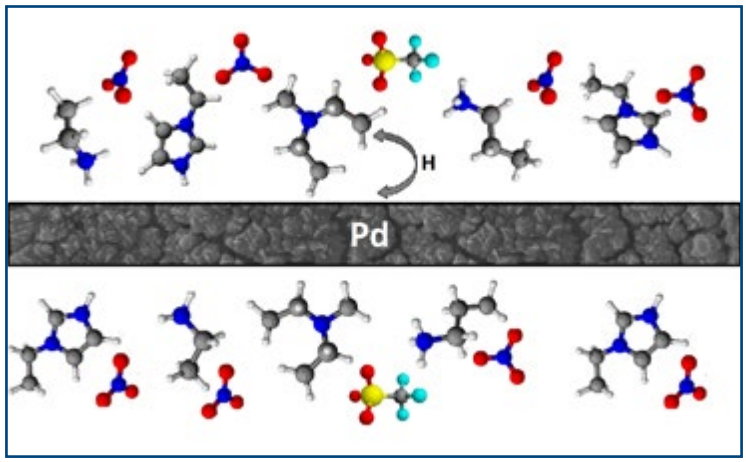


Fig. 1. The schematic illustration of hydrogen electrosorption into/from Pd thin layer electrode in the non-aqueous electrolytes – protic ionic liquids: diethylmethylammonium triflate (DEMA-TFO), ethylammonium nitrate (EAN), propylammonium nitrate (PAN) and 1-ethylimidazolium nitrate (C_2IMN).

SELECTED PUBLICATIONS:

1. K. Hubkowska, M. Soszko, M. Krajewski, A. Czerwiński, Enhanced kinetics of hydrogen electrosorption in AB5 hydrogen storage alloy decorated with Pd nanoparticles, Electrochemistry Communications. 100 (2019) 100.
2. M. Pająk, K. Hubkowska, A. Czerwiński, The study of hydrogen sorption in palladium limited volume electrode from DEMA-TFO ionic liquid, Journal of Electroanalytical Chemistry. 825 (2018) 73.
3. K. Hubkowska, M. Soszko, M. Symonowicz, M. Łukaszewski, A. Czerwiński, Electrochemical behavior of a Pd thin film electrode in concentrated alkaline media, Electrocatalysis. 8 (2017) 295.

Lithium-ion Battery Group

HEAD:

Bartosz Hamankiewicz*, PhD

GROUP MEMBERS:

prof. Andrzej Czerwiński, PhD DSc; Michał Krajewski, PhD; Małgorzata Pająk, PhD; Maciej Ratyński, PhD; Dominika Ziółkowska, PhD Eng
PhD students: Maciej Boczar, Hermes Llain Jimenez

RESEARCH PROFILE:

Principal investigations of electrochemical phenomenon in intercalated compounds. Synhesis, construction and electrochemical analysis of lithium and sodium ion battery materials. Electrochemistry of intercalation compounds in non-aqueous media.

CURRENT RESEARCH ACTIVITIES:

Synthesis and determination of physicochemical and electrochemical properties of lithium-manganese orthosilicate as a cathode material in lithium-ion battery (NCN OPUS Project). Development of new synthetic route of lithium nickel-manganese-cobalt oxide as a positive electrode material. Development of lithium titanate oxide as a negative electrode in lithium-ion battery. Construction and determination of electrochemical parameters of lithium-ion battery in Swagelok and coin-cell type cells based on developed materials. Construction and electrochemical properties of lithium-ion batteries in new electrolytes (PolStorEn Consortium). Construction of lithium-ion battery prototype in cylindrical standard 18650 (TECHMATSTRATEG Project). Determination of electrochemical parameters of commertial lithium-ion electrodes (VARTA) for electrochemical model predicting battery performance and cycle life (H2020 Project). Preparation of copper oxide electrode for primary lithium-ion cells.

*e-mail: bhamankiewicz@chem.uw.edu.pl

SELECTED PUBLICATIONS:

1. M. Krajewski, B. Hamankiewicz, A. Czerwiński, Voltammetric and impedance characterization of $Li_4Ti_5O_{12}$/n-Ag composite for lithium-ion batteries, Electrochim. Acta. 219 (2016) 277–283.
2. B. Hamankiewicz, M. Michalska, M. Krajewski, D. Ziółkowska, L. Lipińska, K. Korona, M. Kamińska, A. Czerwiński, The effect of electrode thickness on electrochemical performance of $LiMn_2O_4$ cathode synthesized by modified sol-gel method, Solid State Ionics. 262 (2014) 9-13.
3. M. Michalska, B. Hamankiewicz, D. Ziółkowska, M. Krajewski, L. Lipińska, M. Andrzejczuk, K. Korona, A. Czerwiński, Influence of $LiMn_2O_4$ modification with CeO_2 on electrode performance, Electrochim. Acta. 136 (2014) 286-291.
4. M. Krajewski, M. Michalska, B. Hamankiewicz, D. Ziółkowska, K.P. Korona, J.B. Jasiński, M. Kamińska, L. Lipińska, A. Czerwiński, $Li_4Ti_5O_{12}$ modified with Ag nanoparticles as an advanced anode material in lithium-ion batteries, J. Power Sources. 245 (2014) 764-771.
5. D. Ziółkowska, K.P. Korona, B. Hamankiewicz, S.-H. Wu, M.-S. Chen, J.B. Jasiński, M. Kamińska, A. Czerwiński, The Role of SnO_2 Surface Coating on the Electrochemical Performance of $LiFePO_4$ Cathode Materials, Electrochim. Acta. 108 (2013) 532-539.
6. B. Hamankiewicz, A. Czerwiński, M. Krajewski, M. Michalska, L. Lipińska, J. Kozakiewicz, J. Przybylski, K. Sylwestrzak, W. Sarna, Lithium-ion battery, Polish Patent Pending P.416704.

Laboratory of Electrochemistry

UNIVERSITY OF WARSAW

WCh Faculty of Chemistry University of Warsaw

Composite nanomaterials for photocatalysis and solar cells

HEAD:

Prof. Magdalena Skompska*, PhD DSc

GROUP MEMBERS:

Iraida Demchenko, PhD DSc;
Agata Fedorczyk, PhD;
Maciej Kwiatkowski, PhD;
Kamila Zarębska, PhD
PhD student: Tomasz Łęcki
MSc student: Ewelina Kwiatkowska

RESEARCH PROFILE:

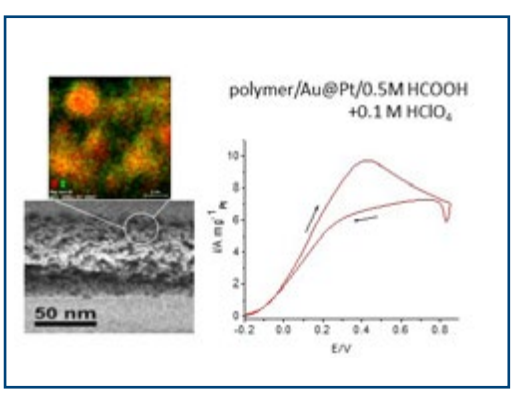
The scientific interest of the group is focused on elaboration of hybrid materials based on conducting polymers, metal nanoparticles, nanostructural semiconductors, and metal oxides, investigation of their electronic structure and applications in photocatalysis, electrocatalysis and solar cells.

Conducting polymers

- Electrosynthesis and characterization of conducting polymers: (poly(3-alkylthiophenes), poly(3,4-dialkoxythiophenes), polypyrrole derivatives, poly(N-vinylcarbazole), poly(1,8-diaminocarbazole), etc. Correlation of synthesis conditions with electrochemical properties of the polymer films in p- and n-doping ranges, polymer conductivity, morphology and molecular structure.

Nanostructural hybrid materials

- Elaboration of the composites: conducting polymer/semiconductor nanoparticles or fullerenes for application in the solar cells.
- Synthesis of metal nanoparticles (Au, Ag, Au@Pt) in the polymer matrices and investigation of their catalytic and electrocatalytic activity.
- Hydrothermal and electrochemical synthesis of ZnO nanorods and nanoplates on transparent conducting substrates (ITO, FTO). Sensitization of ZnO nanorods with CdS and CdSe nanocrystals for solar cells application.
- Elaboration of core-shell composites for photocatalysis

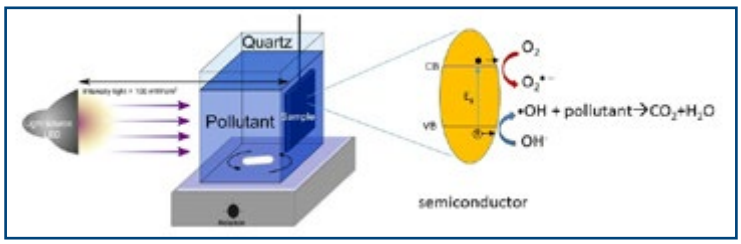


*e-mail: mskomps@chem.uw.edu.pl

(ZnO/TiO_2, TiO_2/CdS/polymer) and photoelectrocatalysis (ZnO/TiO_2 decorated with Au nanoparticles) in UV and visible light.

Employed techniques:

- "wet chemistry" methods for synthesis of nanomaterials: high pressure and microwave-assisted hydrothermal methods, sol-gel, etc.
- electrochemical methods (classical and electrochemical quartz microbalance – EQCM), spectroscopies (UV/vis and FTIR in transmission and reflection modes, Raman), X-ray spectroscopies, scaterring and corresponding computational modelling, XRD, microscopic techniques: AFM/STM, SEM, HR-TEM.



CURRENT RESEARCH ACTIVITIES:

1. Synthesis and characterization of new composite materials of the type: Fe_3O_4/TiO_2, $ZnO/BiVO_4$ for photocatalysis under visible light.
2. Preparation of visible-light driven photocatalysts by activation of the wide band-gap semiconductors ($SrTiO_3$, ZnO and $TiO_2/SrTiO_3$ composites) with plasmonic metal nanoparticles or by metal or non-metal doping.
3. Application of the elaborated materials in potential-assisted solar water splitting and photodegradation of organic water pollutants.
4. Organic/inorganic hybrid solar cells. The research group is involved in realization of the joint project "Efficient and light photo-rechargeable electric energy storage systems based on solar cell-lithium ion battery or solar cell-supercapacitor structures for special applications" within TECHMATSTRATEG (realized by consortium of 8 research groups).

SELECTED PUBLICATIONS:

1. I.N. Demchenko "Analytical Techniques for Characterization of Oxide-based Materials" Chap. 4 in "Oxide-based Materials and Structures: Fundamentals and Applications", Taylor & Francis Ltd, London, UK. ISBN 10 0367252392 (2020).
2. I.N. Demchenko, R. Ratajczak, Y. Melikhov et al., Valence band of ZnO:Yb probed by resonant photoemission spectroscopy, Materials science in semiconductor processing. 91 (2019) 306.
3. T. Łęcki, K. Zarębska, K. Sobczak, M. Skompska, Photocatalytic degradation of 4-chlorophenol with the use of FTO/TiO_2/$SrTiO_3$ composite prepared by microwave-assisted hydrothermal method, Appl. Surf. Sci. 470 (2019) 991.
4. K. Zarębska, T. Łęcki, M. Skompska, Synthesis of CdSe on ZnO nanorods by SILAR and electrochemical methods and comparison of photoelectrochemical properties of the FTO/ZnO/CdSe electrodes, J. Electroanal. Chem. 819 (2018) 459-468.
5. M. Kwiatkowski, R. Chassagnon, O. Heintz, N. Geoffroy, M. Skompska, I. Bezverkhyy, Improvement of Photocatalytic and Photoelectrochemical Activity of ZnO/TiO_2 Core/Shell System through Additional Calcination: Insight into the Mechanism, Applied Catalysis B: Environmental. 204 (2017) 200-208.
6. A. Fedorczyk , R. Pomorski, M. Chmielewski, J. Ratajczak, Z. Kaszkur, M. Skompska, Bimetallic Au@Pt nanoparticles dispersed in conducting polymer – A catalyst of enhanced activity towards formic acid electrooxidation, Electrochimica Acta. 246 (2017) 1029-1041.
7. A. Fedorczyk, J. Ratajczak, O. Kuzmych, M. Skompska, Kinetic studies of catalytic reduction of 4-nitrophenol with $NaBH_4$ by means of Au nanoparticles dispersed in a conducting polymer matrix, J. Solid State Electrochemistry. 19 (2015) 2849–2858.
8. M. Kwiatkowski, I. Bezverkhyy, M. Skompska, ZnO nanorods covered with TiO_2 layer: simple sol-gel preparation, optical, photocatalytic and photoelectrochemical properties, Journal of Materials Chemistry A. 24 (2015) 12748-12760.
9. M. Skompska, K. Zarębska, Electrodeposition of ZnO Nanorod Arrays on Transparent Conducting Substrates – a Review, Electrochimica Acta. 127 (2014) 467-488.
10. K. Zarębska, M. Kwiatkowski, M. Gniadek, M. Skompska, Electrodeposition of $Zn(OH)_2$, ZnO thin films and nanosheet-like Zn seed layers and influence of their morphology on growth of ZnO nanorods, Electrochimica Acta. 98 (2013) 255-262.

BioNanoLab

HEAD:

Maciej Mazur*, PhD DSc

GROUP MEMBERS:

PhD students: Paulina Głowala, Marta Bartel, Barbara Wysocka, Ilona Mojzych, Marta Kwiatkowska, Jarosław Wojciechowski

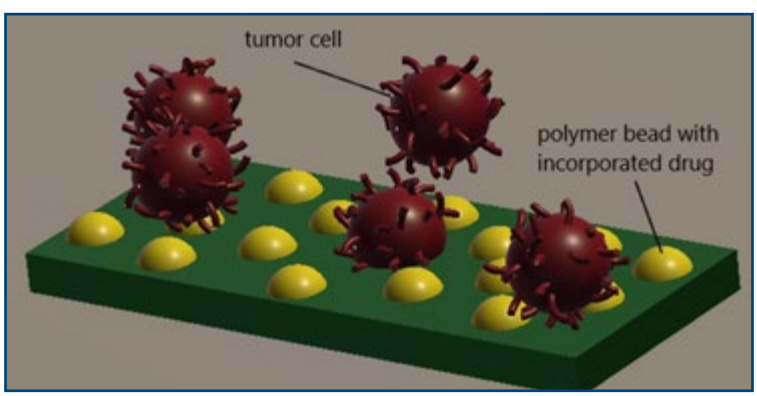
RESEARCH PROFILE:

Synthesis and physicochemical characterization of bionanomaterials, drug nanocarriers and contrast agents for medical imaging, hybrid organic-inorganic particles, biomineralization phenomena in invertebrates, new methods for the diagnosis of kidney diseases.

CURRENT RESEARCH ACTIVITIES:

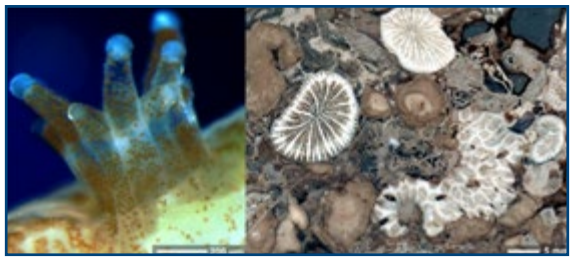
The research interests of the group focus on several main topics.

The first one is synthesis of nanoparticulate species prepared from organic (polymers) and inorganic (metals, non-metals, oxides, hydroxides) materials. These structures are next investigated with a range of



*e-mail: mmazur@chem.uw.edu.pl

physicochemical techniques including microscopy (SEM, TEM, AFM, optical microscopy, Raman mapping), spectroscopy (vibrational spectroscopy, absorption and emission in UV-VIS range, XPS, TOF-SIMS), electrochemistry, etc. The focus is on medical applications where the particles act as drug carriers or contrast agents in 3D imaging methods (CT, MRI, SPECT and PET).



The second research path is being developed in cooperation with the PAS Institute of Paleobiology and is devoted to investigations of biomineralization and diagenetic processes in invertebrates like corals, sponges, arthropods, etc. These studies are conducted using spectroscopic (Raman) and microscopic techniques (SEM, TEM, AFM).

The third area of research is the development of new analytical tools for the diagnosis of kidney diseases, e.g. nephrotic syndrome. These studies are conducted in cooperation with the Warsaw Medical University.

SELECTED PUBLICATIONS:

1. J. Stolarski, F.R. Bosellini, C.C. Wallace, A.M. Gothmann, M. Mazur, I. Domart-Coulon, E. Gutner-Hoch, R.D. Neuser, O. Levy, A. Shemesh, A. Meibom, A unique coral biomineralization pattern has resisted 40 million years of major ocean chemistry change. Scientific Reports. 6 (2016).
2. K. Frankowiak, X.T. Wang, D.M. Sigman, A.M. Gothmann, M.V. Kitahara, M. Mazur, A. Meibom, J. Stolarski, Photosymbiosis and the expansion of shallow-water corals. Science Advances. 2 (2016).
3. K. Kijewska, A. Jarzębińska, J. Kowalska, J. Jemielity, D. Kępińska, J. Szczytko, M. Pisarek, K. Wiktorska, J. Stolarski, P. Krysiński, A. Twardowski, M. Mazur, Magnetic-Nanoparticle-Decorated Polypyrrole Microvessels: Toward Encapsulation of mRNA Cap Analogues, Biomacromolecules. 14 (2013) 1867-1876.
4. K. Kijewska, G.J. Blanchard, J. Szlachetko, J. Stolarski, A. Kisiel, A. Michalska, K. Maksymiuk, M. Pisarek, P. Majewski, P. Krysiński, M. Mazur, Photopolymerized polypyrrole microvessels. Chemistry: A European Journal. 18 (2012) 310-320.
5. J. Stolarski, A. Meibom, R. Przeniosło, M. Mazur, A Cretaceous scleractinian coral with a calcitic skeleton, Science. 318 (2007) 92-94.

Laboratory of Biomolecular Structures

HEAD:

Prof. Paweł Krysiński*, PhD DSc

GROUP MEMBERS:

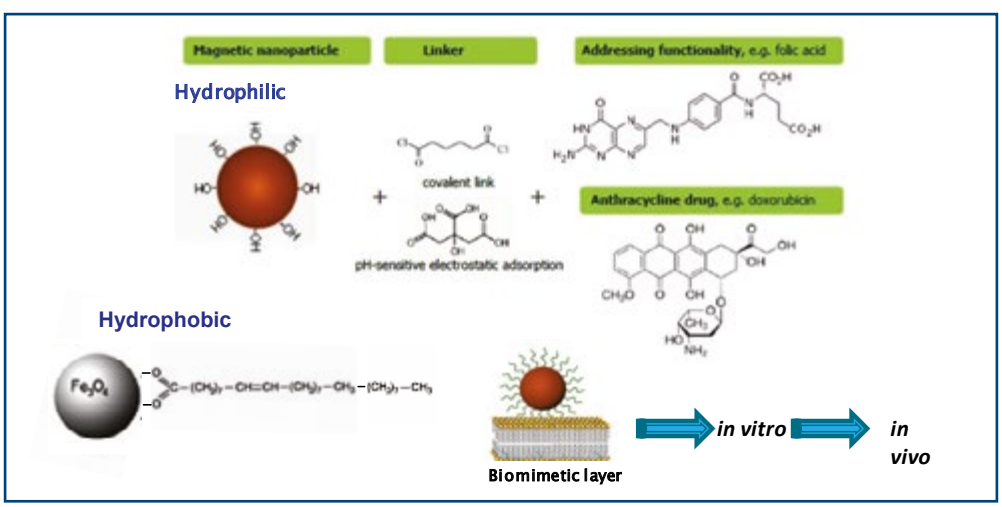
Dorota Nieciecka, PhD;
Magdalena Osial, PhD
PhD student: Aleksandra Rękorajska

RESEARCH PROFILE:

Electrochemistry and spectroscopy of magnetic nanoparticle interactions with organized biomimetic systems.

CURRENT RESEARCH ACTIVITIES:

Synthesis of magnetic nanoparticles NP) for drug delivery; electrochemical analysis of their interactions with biomimetic membranes; Langmuir and Langmuir-Blodgett layers; core and surface tailoring of NPs for multitasking purposes. Magnetothermal effect of hybrid nanostructures.



*e-mail: pakrys@chem.uw.edu.pl

SELECTED PUBLICATIONS:

1. M. Osial, P. Rybicka, M. Pękała, G. Cichowicz, M. Cyrański, P. Krysiński, Easy Synthesis and Characterization of Holmium-Doped SPIONs, Nanomaterials. 8 (2018) 430.
2. A. Rękorajska, G. Cichowicz, M. Cyrański, M. Grdeń, M. Pękała, G.J. Blanchard, Synthesis and Characterization of Tb-Doped Nanoferrites, ChemNanoMat. 4 (2018) 231-242.
3. M. Szlęzak, D. Nieciecka, A. Joniec, M. Pękała, E. Górecka, M. Emo, M.J. Stebe, P. Krysiński, R. Bilewicz, Monoolein Cubic Phase Gels and Cubosomes Doped with Magnetic Nanoparticles-Hybrid Materials for Controlled Drug Release, ACS Applied Mat.& Interf. 9 (2017) 2796-2805.
4. A. Joniec, S. Sęk, P. Krysiński, Magnetoliposomes as Potential Carries of Doxorubicin to Tumours, Chem.-A Europ.J. 22 (2016) 17715-17724.
5. D. Nieciecka, A. Królikowska, K. Kijewska, G.J. Blanchard, Hydrophilic iron oxide nanoparticles probe the organization of biomimetic layers: electrochemical and spectroscopic evidence, Electrochim. Acta. 209 (2016) 671-681.

Surface electrochemistry of semiconductors and polymers research group

HEAD:

Paweł Oracz*, PhD DSc

GROUP MEMBERS:

prof. Krystyna Jackowska, PhD DSc (emeritus);
prof. Marek Szklarczyk, PhD DSc; Marcin Strawski, PhD;
PhD student: Bartosz Czerwieniec

RESEARCH PROFILE:

The scientific interest of the group is focused on three fields of research. The studies of physico-chemical processes and material science tied with electrodeposition of semiconductive materials, deposition of polyelectrolytes and calculation of thermodynamic properties of halogenated hydrocarbons in IUPAC-NIST standard.

We apply electrochemical methods for direct deposition of semiconductor electrodes. The goal is to optimize deposition processes to obtain an easy and cheap method for the production of materials applied in photo-electrochemical processes (water splitting, photocatalysis). In the case of deposition of polyelectrolytes we endeavor to the preparation of layers that will exhibit proper permeability properties for the application of these materials for encapsulation of biological cells. The goal is also to use these systems as scaffolds for hybrid organic-inorganic composites.

CURRENT RESEARCH ACTIVITIES:

1. Electrodeposition of SiOx based electrodes for photoelectrochemical application
2. Electrodeposition of CdSe, Se based electrodes for photoelectrochemical application
3. Calculation of solubility of halogenated hydrocarbons in IUPAC-NIST standard
4. Preparation of polyelectrolytes multilayers (PEM) systems, studies focused on composition-properties dependencies
5. Structural interaction studies in PEM systems
6. Application of PEM as scaffolds for inorganic nanostructures.

*e-mail: poracz@chem.uw.edu.pl

SELECTED PUBLICATIONS:

1. B. Czerwieniec, M. Strawski, L.H. Granicka, M. Szklarczyk, AFM study of adhesion and interactions between polyelectrolyte bilayers assembly, Colloids and Surfaces A: Physicochemical and Engineering Aspects. 555 (2018) 465-472.
2. M. Strawski, L.H. Granicka, M. Szklarczyk, Redox properties of polyelectrolyte multilayer modified electrodes: a significant effect of the interactions between the polyelectrolyte layers in the films, Electrochimica Acta. 226 (2017) 121-131.
3. A. Krywko-Cendrowska, L. Marot, L. Philippe, M. Strawski, E. Meyer, M. Szklarczyk, Spectroscopic characterization and photoactivity of SiOx-based films electrochemically grown on Cu surfaces, Journal of Applied Electrochemistry. 47 (2017) 917–930.
4. P. Oracz, M. Góral, B. Wiśniewska-Gocłowska, D.G. Shaw, A. Mączyński, IUPAC-NIST Solubility Data Series. 101. Alcohols + Hydrocarbons + Water. Part 2. C1–C3 Alcohols + Aliphatic Hydrocarbons, Journal of Physical and Chemical Reference Data. 45 (2016) 033102.
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Laboratory of Molecular Modeling

UNIVERSITY OF WARSAW

WCh Faculty of Chemistry University of Warsaw

Biomodellab in Biological and Chemical Research Centre

HEAD:

Prof. Sławomir Filipek*, PhD DSc

GROUP MEMBERS:

Pakhuri Mehta, PhD; Przemysław Miszta, PhD; Szymon Niewieczerzał, PhD; Elżbieta Wagner, PhD
PhD students: Aleksander Dębiński, Jakub Jakowiecki, Krzysztof Młynarczyk, Mariusz Możajew, Aleksandra Szczęsny
MSc students: Maciej Iżyk, Urszula Orzeł
IT specialist: Paweł Pasznik, MSc

RESEARCH PROFILE:

- Investigations of drugs and proteins especially in biological membrane environments
- molecular dynamics simulations of biological systems
- study of activation processes in G-protein-coupled receptors (GPCRs)
- ligand docking to proteins and use of other methods for drug design
- interactions of proteins with graphene, carbon nanotubes and lipid cubic phases

CURRENT RESEARCH ACTIVITIES:

- Research on rhodopsin and other proteins involved in vision processes. Oligomerization of rhodopsin as a universal feature for other G-protein-coupled receptors (GPCRs). Large biological complexes of oligomeric rhodopsin with G protein and arrestin (publications 1-3)
- Study of activation processes of GPCRs (opioid receptors, adenosine receptors, serotonin receptors, and others) (publications 4-6)
- Homology modeling of GPCRs – construction of web service GPCRM (publications 7-8)
- Interactions of proteins with graphene and lipid cubic phases (publications 9-10)

*e-mail: sfilipek@chem.uw.edu.pl

SELECTED PUBLICATIONS:

1. S. Gulati, B. Jastrzębska, S. Banerjee, A. Placeres, P. Miszta, S. Gao, K. Gunderson, G. Tochtrop, S. Filipek, K. Katayama, P.D. Kiser, M. Mogi, P.L. Stewart, K. Palczewski, Photocyclic behavior of rhodopsin induced by a novel isomerization mechanism, Proc. Natl. Acad. Sci. USA. 114 (2017) E2608-E2615.
2. S. Filipek, K.A. Krzyśko, D. Fotiadis, Y. Liang, D.A. Saperstein, A. Engel, K. Palczewski, A concept for G protein activation by G protein-coupled receptor dimers: the transducin/ rhodopsin interface, Photochem. Photobiol. Sci. 3 (2004) 628-638.
3. D. Fotiadis, Y. Liang, S. Filipek, D.A. Saperstein, A. Engel, K. Palczewski, Atomic force microscopy: Rhodopsin dimers in native disc membranes, Nature. 421 (2003) 127-128.
4. S. Yuan, Q. Peng, K. Palczewski, H. Vogel, S. Filipek, Mechanistic studies on the stereoselectivity of the serotonin 5-HT1A receptor, Angew. Chem. Int. Ed. 55 (2016) 8661-8665.
5. S. Yuan, H.C.S. Chan, H. Vogel, S. Filipek, R.C. Stevens, K. Palczewski, The molecular mechanism of P2Y1 receptor activation, Angew. Chem. Int. Ed. 55 (2016) 10331-10335.
6. S. Yuan, K. Palczewski, Q. Peng, M. Koliński, H. Vogel, S. Filipek, The mechanism of ligand-induced activation or inhibition of mu- and kappa-opioid receptors, Angew. Chem. Int. Ed. 54 (2015) 7560-7563.
7. P. Miszta, P. Pasznik, J. Jakowiecki, A. Sztyler, D. Latek, S. Filipek, GPCRM: a homology modeling web service with triple membrane-fitted quality assessment of GPCR models, Nucleic Acids Research. 46 (2018) W387-W395.
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10. S. Viswanathan, T.N. Narayanan, K. Aran, K.D. Fink, J. Paredes, P.M. Ajayan, S. Filipek, P. Miszta, H.C. Tekin, F. Inci, U. Demirci, P. Li, K.I. Bolotin, D. Liepmann, V. Renugopalakrishnan, Graphene–protein field effect biosensors: glucose sensing, Mater. Today. 18 (2015) 513-522.

Laboratory of Natural Products Chemistry

UNIVERSITY OF WARSAW

WCh Faculty of Chemistry University of Warsaw

Laboratory of Natural Products Chemistry

HEAD:

Prof. Zbigniew Czarnocki*, PhD DSc

GROUP MEMBERS:

Piotr Roszkowski, PhD DSc; Zuzanna Molęda, PhD; Joanna Szawkało, PhD; Anna Zawadzka, PhD
PhD students: Anna Kończyk, Karolina Staniak

RESEARCH PROFILE:

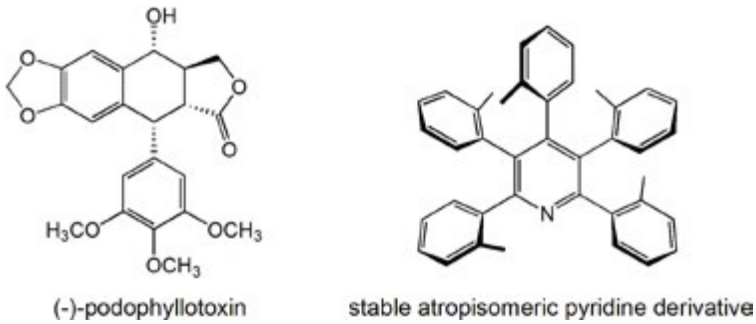
Asymmetric catalysis, stereoselective organic synthesis, medicinal chemistry

CURRENT RESEARCH ACTIVITIES:

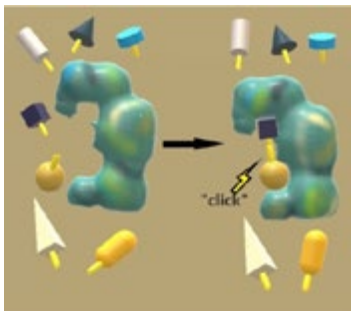
Our main research areas are connected with the chemistry of natural products. In particular, we are interested in the stereoselective organic synthesis, often choosing natural compounds as our synthetic goals (alkaloids, lignans) or as chiral auxiliaries in various kinds of stereoselective synthesis, like asymmetric transfer hydrogenation (ATH).
Also, different heterocycles of pharmacological relevance are the subject of our study, together with the estimation of their biological activity. We were able to complete the synthesis of several natural products (cryspine A, podophyllotoxin, trypargine) and some heterocycles of pharmacological importance (aptazepine, praziquantel).
We are also interested in atropisomerism, which is a type of stereochemistry being a consequence of the hindered rotational barrier in suitably substituted biaryls and analogous compounds. Many biologically active compounds exist in the form of pure atropisomers and this phenomenon has important implications for medicinal chemistry.
We also work on the development of new multipotent cholinesterase inhibitors, designing and synthesizing hybrids of melatonin, tacrine and galantamine. The new hybrid cholinesterases inhibitors are protected by patents and can be used in relief and/or treatment of the neurodegenerative disorders, among them the Alzheimer's disease.

*e-mail: czarnoz@chem.uw.edu.pll

For an effective screening of biologically active compounds, we are using target-guided synthesis approach, in which the target enzyme synthesizes its own inhibitors, selecting from a combinatorial library pairs of building blocks, which form together the best final ligands.



(-)-podophyllotoxin stable atropisomeric pyridine derivative



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2. P. Pomarański, P. Roszkowski, J.K. Maurin, A. Budzianowski, Z. Czarnocki, Some mechanistic aspects regarding the Suzuki–Miyaura reaction between selected ortho-substituted phenylboronic acids and 3,4,5-tribromo-2,6-dimethylpyridine, Beilstein Journal of Organic Chemistry. 14 (2018) 2384–2393.
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5. K. Lisiecki, P. Roszkowski, K.K. Krawczyk, J.K. Maurin, Z. Czarnocki, Unexpected regioselectivity in the photocyclization of a chiral 2,3-bisbenzylidenesuccinate, leading to a podophyllotoxin related cyclolignan, Journal of Photochemistry and Photobiology A: Chemistry. 364 (2018) 297–302.
6. K. Kucharewicz, M. Dudkowska, A. Zawadzka, M. Ogrodnik, A.A. Szczepankiewicz, Z. Czarnocki, E. Sikora, Simultaneous induction and blockade of autophagy by a single agent, Cell Death and Disease. 9(3) (2018) 353.
7. K. Lisiecki, K.K. Krawczyk, P. Roszkowski, J.K. Maurin, A. Budzianowski, Z. Czarnocki, Unusual visible-light photolytic cleavage of tertiary amides during the synthesis of cyclolignans related to podophyllotoxin, Tetrahedron. 73(44) (2017) 6316-6328.
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Laboratory of Nuclear Magnetic Resonance Spectroscopy

UNIVERSITY OF WARSAW

Faculty of Chemistry
University of Warsaw

Laboratory of Nuclear Magnetic Resonance Spectroscopy

HEAD:

Piotr Garbacz*, PhD DSc

GROUP MEMBERS:

prof. Karol Jackowski, PhD DSc (emeritus); Włodzimierz Makulski, PhD DSc; Bożena Adrjan, PhD; Marcin Wilczek, PhD
PhD students: Artur Brzezicki, Mateusz Słowiński

RESEARCH PROFILE:

Experimental and theoretical magnetic resonance studies of fundamental interactions between the electromagnetic field and nuclear magnetic moments are aimed at the determination of the interaction parameters with ultra-high precision and the search for new and not observed yet effects.

CURRENT RESEARCH ACTIVITIES:

Experimental studies of nuclear magnetic resonance in the gas and liquid phase combined with quantum chemical computations focus on the determination of nuclear magnetic shielding, nuclear magnetic dipole moments, and indirect spin-spin coupling in small and medium-size molecules including water, molecular hydrogen, and components of the Earth's atmosphere. The goals of these studies are to examine (i) nuclear magnetic parameters of the isolated molecule and (ii) the influence of intermolecular interactions, isotopic substitution and the application of external fields on these parameters. For instance, it is anticipated that the application of the electric field induces several new magnetic resonance effects that permit to determine directly the absolute configuration of the molecule. In order to find these new effects, we study spin dynamics using quantum information processing methods and design, model, and fabricate dedicated resonance circuits.

SELECTED PUBLICATIONS:

1. W. Makulski, M. Wilczek, K. Jackowski, ^{17}O and ^{1}H NMR spectral parameters in isolated water molecules, Phys. Chem. Chem. Phys. 20 (2018) 22468-22476.

*e-mail: pgarbacz@chem.uw.edu.pl

2. P. Garbacz, W. Makulski, W-183 nuclear dipole moment determined by gas-phase NMR spectroscopy, Chem. Phys. 498 (2017) 7-11.
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5. P. Garbacz, Nuclear relaxation in an electric field enables the determination of isotropic magnetic shielding, J. Chem. Phys. 145 (2016) 064202-1 – 064202-10.
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8. W. Makulski, ^{83}Kr nuclear magnetic moment in terms of that of ^{3}He, Magn. Reson. Chem. 52 (2014) 430-434.
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Laboratory of Organic Nanomaterials and Biomolecules Synthesis

UNIVERSITY OF WARSAW

WCh Faculty of Chemistry University of Warsaw

Laboratory of organic nanomaterials synthesis

HEAD:

Prof. Józef Mieczkowski*, PhD DSc

GROUP MEMBERS:

Wiktor Lewandowski, PhD DSc; Monika Góra, PhD; Joanna Matraszek, PhD; Joanna Wolska, PhD; Michał Wójcik, PhD
PhD students: Maciej Bagiński, Sylwia Parzyszek, Sylwia Polakiewicz, Piotr Szustakiewicz, Ewelina Tomczyk, Jarosław Wróbel

RESEARCH PROFILE:

Organic nanomaterials, organic derivatization of nanomaterials, organic semiconductors. The first two rely on using organic chemistry techniques in nanotechnology. The purpose is to prepare nanomaterials with prospective applications in optoelectronics and medicine as well as study the relation between molecular structure and self-assembled state. We work with metallic, semiconductor and ferrite nanoparticles, as well as with graphene derivatives. By grafting surface of these nanomaterials with organic compounds designed in our laboratory we have the capability to control stability, spatial arrangement, solubility and biological activity of nanocomponents. In the field of semiconductors we give new life to old organic dyes by preparing their new derivatives with the view on using them in photonic technologies.

CURRENT RESEARCH ACTIVITIES:

Currently we are actively working in few different directions. All of them concern organic synthesis (liquid-crystals, organic semiconductors) and often synthesis of nanoparticles. By careful choice of the building blocks we can prepare a variety of nanomaterials with different applicative potential.
In one branch of projects we are aiming at the synthesis of reconfigurable assemblies of nanoparticles

*e-mail: mieczkow@chem.uw.edu.pl

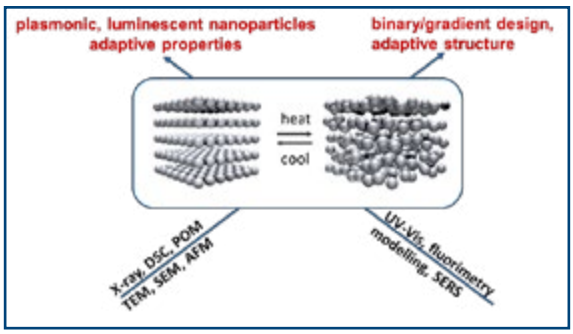

Fig. 1. Key tools and goals of achieving reconfigurable assemblies of nanoparticles.

(NPs). We are interested in such materials since it has been shown that in future they can solve a variety of technological problems of modern optoelectronic devices (low efficiency of light emitting diodes and solar panels, or assure access to optical computers). One of the very few methods that allows to achieve reconfigurabile nanoparticle assemblies is covering NPs with liquid crystals (LCs). Thus, in our work we synthesize various types of NPs (PbS, Au, Ag, Fe_3O_4 and other), design and synthesize liquid crystalline compounds and finally combine these building blocks. We have already prepared thermo-, light- and magneto-sensitive materials in which nanoparticle arrangement (thus properties of such materials) can be precisely controlled with external stimuli.

In another set of projects we seek for efficient drug delivery carriers based on nanoparticles. This work requires the synthesis of water-soluble nanoparticles and combining these materials with drugs. By assuring high stability and compatibility with biological media we allow the NPs to circulate in living organisms, while clever organic reactions program the carried drug to be released preferentially in the cancer cells.

Apart from the utilization of organic molecules to modification of the surface of the large variety of nanoparticles our research efforts are dedicated to organic semiconductors. We design and synthesize new derivatives of organic dyes which are known for a long time (such as diketopyrrolopyrrole or perinone). In the next step we characterize their optical, electrochemical and structural properties. The compounds of the best physicochemical properties are applied in test devices (OLED, OFET, OPVC).

Self-assembled and self-organized liquid crystals are function materials in many fields of advanced technologies. It is well established that the type of the mesophase, and thus material properties, are determined to large extent by the shape of mesogenic molecule and various non-covalent, intra- and intermolecular interactions. It is very important to find the connection between architecture of soft matter and nanostructures they create.

To face these needs, we synthesize a number of mesogens and investigate the molecular systems they form. All of the obtained compounds are physicochemically tested using a wide number of complementary methods such as: polarizing microscopy, microcalorimetry, X-ray techniques (SAXS, GADDS), as well as AFM and STM measurements.

SELECTED PUBLICATIONS:

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5. W. Lewandowski, M. Fruhnert, J. Mieczkowski et al., Dynamically self-assembled silver nanoparticles as a thermally tunable metamaterial, Nature Communications. 6 (2015) 6590.

6. J. Matraszek, J. Zapała, J. Mieczkowski et al., 1D, 2D and 3D liquid crystalline phases formed by bent-core mesogens, Chemical Communications. 51(24) (2015) 5048-5051.
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10. E. Górecka, D. Pociecha, J. Mieczkowski et al., Axially polar columnar phase made of polycatenar bent-shaped molecules, Journal of the American Chemical Society. 126(49) (2004) 15946-15947.

Chemistry and Biochemistry of Nucleic Acids Components

HEAD:

Marzena Jankowska-Anyszka*, PhD DSc

GROUP MEMBERS:

Karolina Piecyk, PhD
PhD student: Paulina Pietrow

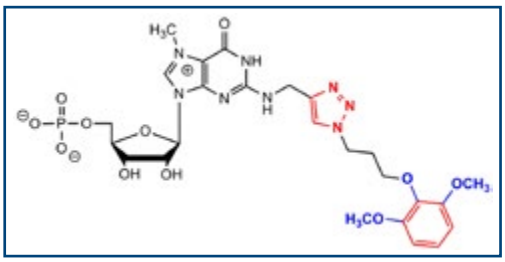
RESEARCH PROFILE:

- Synthesis of 5' end mRNA (cap) analogues and their usage in biochemical and biophysical studies on translation initiation, splicing, intracelullar transport and stability of mRNA in eukaryotic cells;
- Synthesis and biochemical investigation of translation inhibitors with potential therapeutical application as anti-cancer drugs;
- Synthesis of nucleotides conjugates capable to penetratrate cell membrane;
- Design and synthesis of tools for examinations of gene expression in parasitic nematodes;
- Chemistry and biochemistry of nucleosides and nucleotides.

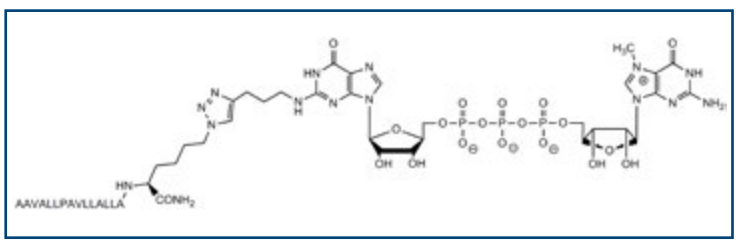
CURRENT RESEARCH ACTIVITIES:

(A) Design and synthesis of new cap analogs as translation inhibitors with potential therapeutic application. To date numerous modified cap analogues have been synthesized in our laboratory and tested as translation inhibitors of cap-dependent translation *in vitro* that compete with mRNA for the binding site of eIF4E (eukaryotic initiation factor 4E). One of the most interesting and promising group of compounds, which synthesis have been developed in our group, contains N2-modified 7-methylguanosine (the best of them is shown in the figure). Currently, we are working on an introduction of different types of aromatic groups (such as oxazole, thiazole) into this position and on the synthesis of cap analogues possessing double modifications (e.g. in N2 and N7 positions).

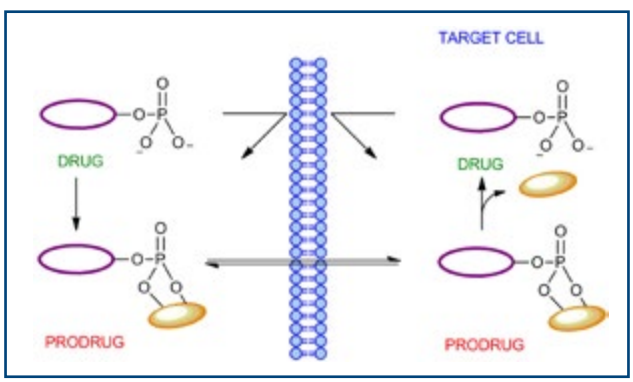
*e-mail: marzena@chem.uw.edu.pl



(B) Synthesis, biological and biophysical evaluation of mRNA cap-peptide conjugates for targeted delivery of cap analogues to cancer cells. All cap analogues obtained so far, unfortunately, have not been used in in vivo studies because they are unable to pass through the cell membrane due to the presence of electrical charge. The development of a system for the delivery of analogues to cancer cells would open the possibility of practical use of such cap analogs with excellent inhibitory properties. Currently we are testing two ways for such a delivery: conjugation of analogs with cell-penetrating peptides (CPP) and masking the charge of nucleotides. The first idea is based on the exceptional property of CPP to carry into cells a wide variety of cargoes. Our project comprise of the design and synthesis of conjugates consisting of a cap analog and a cell-penetrating peptide (such as MPS shown in the figure, TAT) and/or a cell-targeting peptide (such as iRGD) that are connected through enzyme degradable various types of bonds. The resulting constructs are subjected to *in vitro* and *in vivo* biological and biophysical studies.

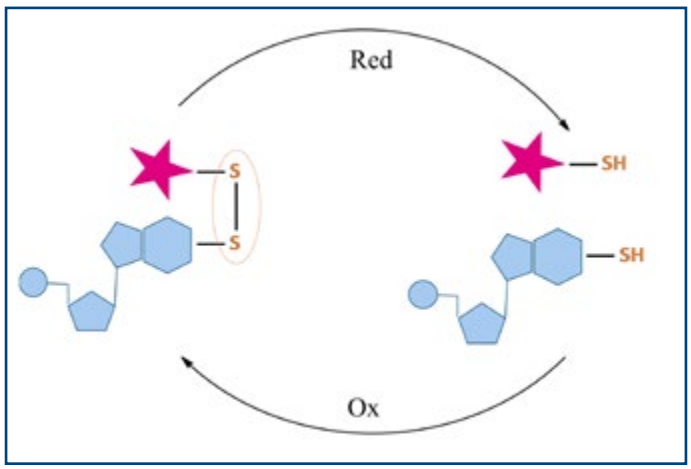


(C) Pro-nucleotides based on mRNA cap structures – synthesis, biological and biophysical evaluation. Prodrugs are bioreversible derivatives of drug molecules that undergo an enzymatic and/or chemical transformation in vivo to release the active drug. We'd like to implement this idea to 5'-monophosphate cap analogs and convert them to prodrug forms by derivatization of the phosphorus-coupled oxygen(s) to form neutral phospho di- or triester(s) or amidophospho mono-, di- or tiesters.



(D) Synthesis of dinucleotide cap analogs for RNA-based biopharmaceuticals.
RNA-based biopharmaceuticals, which include therapeutics and vaccines, are a relatively new way of treatment for a number of chronic and rare diseases. Application of 5'-capped RNA requires synthesis of RNA terminated with cap that most often are accomplish by the use of a cap dinucleotide such as m7GpppG. Our group is focused on the synthesis of new dinucleotide cap analogs that allow proper incorporation of dinucleotide cap analog during *in vitro* transcription and improve an effectiveness of translation and stability of transcripts.

(E) Synthesis of mono- and dinucleotide disulfide derivatives.
Compounds containing a thiol group in their structure (thiols) play a fundamental role in many biochemical and pharmacological processes due to the redox properties of function group (-SH). In our group, we develop methods for the synthesis of disulfide bridge between nucleotides and compounds performing a specific function i.e. fluorescent marker, cell penetrating peptides, compounds increasing solubility or affinity for a particular protein.



SELECTED PUBLICATIONS:

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2. K. Piecyk, M. Łukaszewicz, K. Kamel, M. Janowska, P. Pietrow, S. Kmiecik, M. Jankowska-Anyszka, Isoxazole-containing 5′ mRNA cap analogues as inhibitors of the translation initiation proces, Bioorganic Chemistry. 96 (2020) 103583.
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4. K. Piecyk, P. Kryńska, J. Kałużna, M. Jankowska-Anyszka, Synthesis of the first double-functionalized dinucleotide mRNA cap analogue for its specific labeling, Tetrahedron Letters. 58 (2017) 3037-3040.
5. R. Worch, K. Piecyk, A.B. Kolasa, M. Jankowska-Anyszka, Translocation of 5′ mRNA cap analogue — peptide conjugates across the membranes of giant unilamellar vesicles, Biochimica et Biophysica Acta (BBA) – Biomembranes. 1858 (2016) 311-317.
6. K. Piecyk, A. Niedźwiecka, A. Ferenc-Mrozek, M. Łukaszewicz, E. Darżynkiewicz, M. Jankowska-Anyszka, How to find the optimal partner—studies of snurportin 1 interactions with U snRNA 5' TMG-cap analogues containing modified 2-amino group of 7-methylguanosine, Bioorganic & Medicinal Chemistry. 23 (2015) 4660-4668.
7. K. Piecyk, M. Łukaszewicz, E. Darżynkiewicz, M. Jankowska-Anyszka, Triazole-containing monophosphate mRNA cap analogs as effective translation inhibitors, RNA. 20 (2014) 1539-1547.
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10. W.Z. Liu, M. Jankowska-Anyszka, K. Piecyk, L. Dickson, A. Wallace, A. Niedźwiecka, J. Stępiński, R. Stolarski, E. Darżynkiewicz, J. Kieft, R. Zhao, D.N.M. Jones, R.E. Davis, Structural basis for nematode eIF4E binding an m(2,2,7)G-Cap and its implications for translation initiation, Nucleic Acids Research. 39 (2011) 8820-8832.

Laboratory of Organometallic Synthesis

UNIVERSITY OF WARSAW

WCh Faculty of Chemistry University of Warsaw

Laboratory of Organometallic Synthesis

HEAD:

Prof. Karol Grela*, PhD DSc Eng

GROUP MEMBERS:

Anna Kajetanowicz, PhD Eng;
Louis Monsigny, PhD; Adrian Sytniczuk, PhD;
Magdalena Walczak, MSc Eng;
Anna Mączka, MSc; Marcin Gołębicki, MSc;
Łukasz Szczuciński, MSc
PhD students: Mariusz Milewski,
Michał Patrzałek, Michał Dąbrowski, Wojciech Nogaś, Paweł Małecki, Sebastian Planer,
Anna Marczyk, Katarzyna Gajda,
Marta Czarnota-Bojarska, Paweł Krzesiński,
Tomasz Nienałtowski, Magdalena Drzazga,
Kamil Kosik

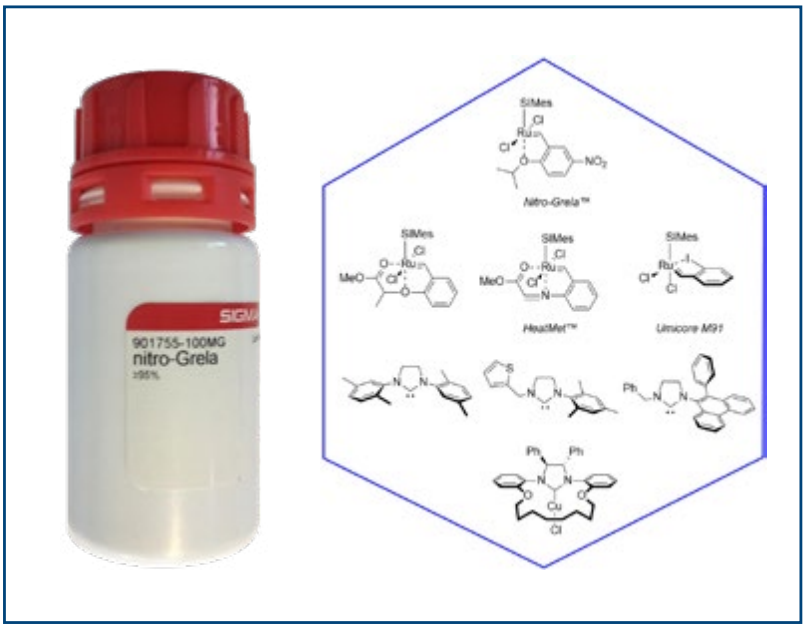
RESEARCH PROFILE:

Research carried out by this group concerns application of different catalytic reactions in organic synthesis, especially in synthesis of natural products, polymers and pharmaceuticals. Currently, work of the group is focused on organic synthesis by means of transition metals, with emphasis on metathesis of alkenes and alkynes, and on chemistry of renewable resources.
Such research must be conducted under the atmosphere of an inert gas, by use of the Schlenk technique, that allows work under anhydrous and anaerobic conditions.
http://www.karolgrela.eu/

CURRENT RESEARCH ACTIVITIES:

The main research areas of the group are designing new, user-friendly catalysts that enable easier purification of reaction products, analyzing the possibilities of the reuse of catalysts, and expanding the application range of metathesis in organic synthesis. The research laboratories of the group are fully equipped with modern instruments, including dry-boxes, GC, GC/MS and HPLC chromatographs, and NMR 400 MHz spectrometer with autosampler.

*e-mail: karol.grela@gmail.com



SELECTED PUBLICATIONS:

1. P. Małecki, K. Gajda, R. Gajda, K. Woźniak, B. Trzaskowski, A. Kajetanowicz, K. Grela, Specialized Ruthenium Olefin Metathesis Catalysts Bearing Bulky Unsymmetrical NHC Ligands: Computations, Synthesis, and Application, ACS Catal. 9 (2019) 587–598.
2. A. Sytniczuk, M. Dąbrowski, Ł. Banach, M. Urban, S. Czarnocka-Śniadała, M. Milewski, A. Kajetanowicz, K. Grela, At Long Last: Olefin Metathesis Macrocyclization at High Concentration, J. Am. Chem. Soc. 140 (2018) 8895-8901.
3. G. Szczepaniak, A. Ruszczyńska, K. Kosiński, E. Bulska, K. Grela, Highly efficient and time economical purification of olefin metathesis products from metal residues using an isocyanide scavenger, Green Chem. 20 (2018) 1280-1289.
4. A. Sytniczuk, A. Leszczyńska, A. Kajetanowicz, K. Grela, Preparation of Musk-Smelling Macrocyclic Lactones from Biomass: Looking for the Optimal Substrate Combination, ChemSusChem. 18 (2018) 3157-3166.
5. M. Michalska, K. Grudzień, P. Małecki, K. Grela, Gold(I)-Catalyzed Formation of Naphthalene/Acenaphthene Heterocyclic Acetals, Org. Lett. 20 (2018) 954–957.
6. V. Cesar, Y. Zhang, W. Kośnik, A. Zieliński, A.A. Rajkiewicz, M. Ruamps, S. Bastin, N. Lugan, G. Lavigne, K. Grela, Ruthenium Catalysts Supported by Amino-Substituted N-Heterocyclic Carbene Ligands for Olefin Metathesis of Challenging Substrates, Chem. Eur. J. 23 (2017) 1950-1955.
7. A. Jana, K. Grela, Mild Functionalization of Tetraoxane Derivatives via Olefin Metathesis: Compatibility of Ruthenium Alkylidene Catalysts with Peroxides, Org. Lett. 19 (2017) 520-523.
8. S.J. Czarnocki, I. Czeluśniak, T.K. Olszewski, M. Malińska, K. Woźniak, K. Grela, Rational and Then Serendipitous Formation of Aza Analogues of Hoveyda-Type Catalysts Containing a Chelating Ester Group Leading to a Polymerization Catalyst Family, ACS Catal. 7 (2017) 4115-4121.
9. A. Jana, K. Woźniak, D. Trzybiński, K. Grela, Well-Defined Chiral Copper NHC Complex in Asymmetric Conjugated β-Borylation and One-Pot Metathesis-Asymmetric β-Borylation, Chem. Eur. J. 24 (2017) 891-897.
10. A. Jana, K. Grela, Forged and Fashioned for Faithfulness—Ruthenium Olefin Metathesis Catalysts Bearing Ammonium Tags, Chem. Commun. 54 (2017) 122-139.

Research Group of Methods of Organic Synthesis

HEAD:

Michał Barbasiewicz*, PhD DSc

GROUP MEMBERS:

Dariusz Basiak, PhD
PhD student: Damian Antoniak
MSc student: Michał Tryniszewski
BSc students: Jan Dudziński, Bartosz Pałuba

RESEARCH PROFILE:

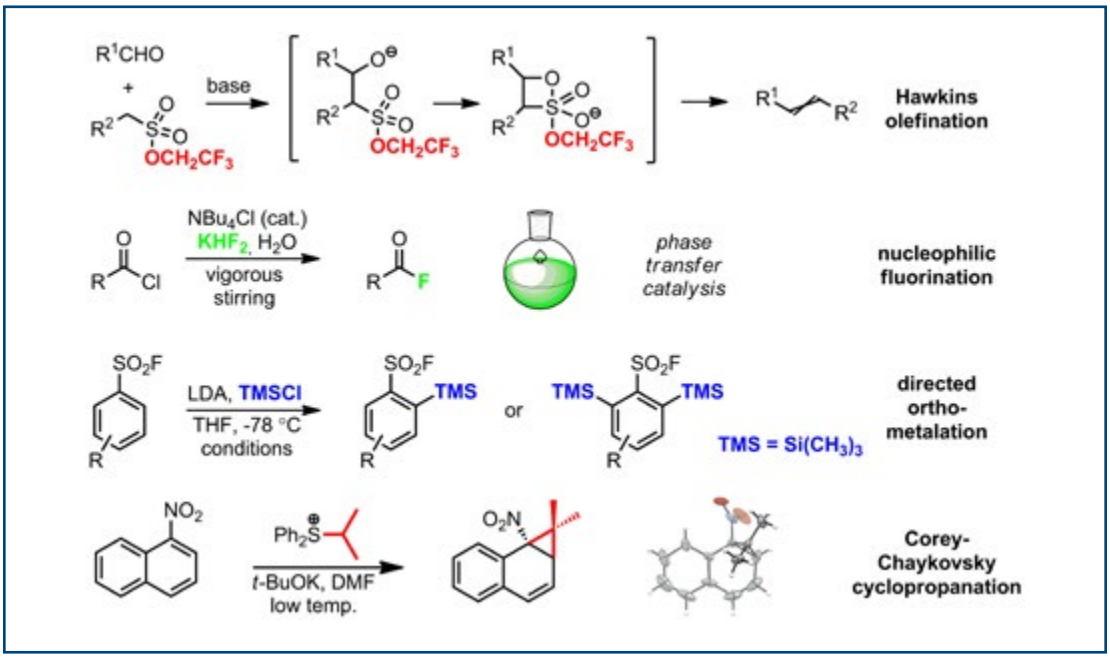
Development of new methodologies in synthetic organic chemistry

CURRENT RESEARCH ACTIVITIES:

We are interested in design and development of new organic transformations, based on fundamental reactivities of simple molecules and a canon of named reactions reported in the literature over decades. Examples of our studies are, e.g.: (1) Hawkins olefination with activated alkanesulfonates, which mimics mechanistic scheme of the Wittig reaction (cyclization and fragmentation of four-membered ring intermediate), (2) nucleophilic fluorination with aqueous bifluoride solution under phase-transfer catalyzed conditions, which enables efficient synthesis of acyl fluorides, (3) functionalization of arenesulfonyl fluorides by directed ortho-metalation with in situ electrophile trapping, and (4) Corey-Chaykovsky dearomatization of nitronaphthalene derivatives.

Our research concerns mainly classical methods of organic synthesis, based on unique features offered by organic derivatives of main group elements of the Periodic Table.

*e-mail: barbasiewicz@chem.uw.edu.pl



SELECTED PUBLICATIONS:

1. D. Antoniak, M. Barbasiewicz, Corey–Chaykovsky Cyclopropanation of Nitronaphthalenes: Access to Benzonorcaradienes and Related Systems, Org. Lett. 21 (2019) 9320–9325.
2. A. Talko, D. Antoniak, M. Barbasiewicz, Directed ortho-Metalation of Arenesulfonyl Fluorides and Aryl Fluorosulfates, Synthesis. 51 (2019) 2278–2286.
3. A. Talko, M. Barbasiewicz, Nucleophilic Fluorination with Aqueous Bifluoride Solution: Effect of the Phase-Transfer Catalyst, ACS Sustainable Chem. Eng. 6 (2018) 6693–6701.
4. B. Górski, A. Talko, T. Basak, M. Barbasiewicz, Olefination with Sulfonyl Halides and Esters: Scope, Limitations, and Mechanistic Studies of the Hawkins Reaction, Org. Lett. 19 (2017) 1756–1759.

Laboratory of Peptides

UNIVERSITY
OF WARSAW

WCh
Faculty of Chemistry
University of Warsaw

Laboratory of Peptides

HEAD:

Prof. Aleksandra Misicka-Kęsik*, PhD DSc

GROUP MEMBERS:

Karolina Pułka-Ziach, PhD DSc;
Kacper Błaziak, PhD; Bartłomiej Fedorczyk PhD, Naveen Gupta PhD; Anna Puszko, PhD; Dagmara Tymecka, PhD; Rafał Wieczorek, PhD; Beata Wileńska, PhD; Ewa Witkowska, PhD
PhD students: Paulina Bachurska, Katarzyna Kędzia, Katarzyna Masłowska, Radosław Piast

RESEARCH PROFILE:

Laboratory of Peptides is a research group focused on the development of structure activity relationship of novel peptides and peptidomimetics with desired biological activity. In this frame we possess vast expertise in design, synthesis and analysis of novel molecules with agonistic and antagonistic properties, which might be used in future therapeutic purposes. We have successfully designed potent peptidomimetics with antiangiogenic/antitumor activity and bifunctional peptides with antinociceptive activity as potential drug for the use in neuropathic pain.

The group is also actively working in the field of foldamers, developing their synthesis and performing the structural studies. Foldamers mimic the secondary structure of peptides, but the backbone is fully artificial. Our attention is focused on helical oligoureas and their analogues. We have successfully applied those compounds as mediators of electron transfer, what opens a possibility for the wider use of oligoureas in materials science or nanoelectronics.

*e-mail: misicka@chem.uw.edu.pl

CURRENT RESEARCH ACTIVITIES:

- Design, synthesis and conformation studies of peptidomimetics with antiangiogenic properties
- Synthesis of bifunctional peptides with analgesic activity
- Synthesis and conformation studies of oligourea foldamers and their analogues
- Application of helical foldamers as mediators of a long-distance transport of electrons
- HPLC-MS stability studies of peptidomimetics in physiological fluids
- Immunoenzymatic and in vitro studies of potential antiangiogenic compounds
- Mass spectrometry based search for biomarkers of pathological states
- Synthesis of lipopeptides
- Catalytic peptides in prebiotic reactions
- Antiangiogenic peptidomimetics for the use as radiopharmaceuticals

SELECTED PUBLICATIONS:

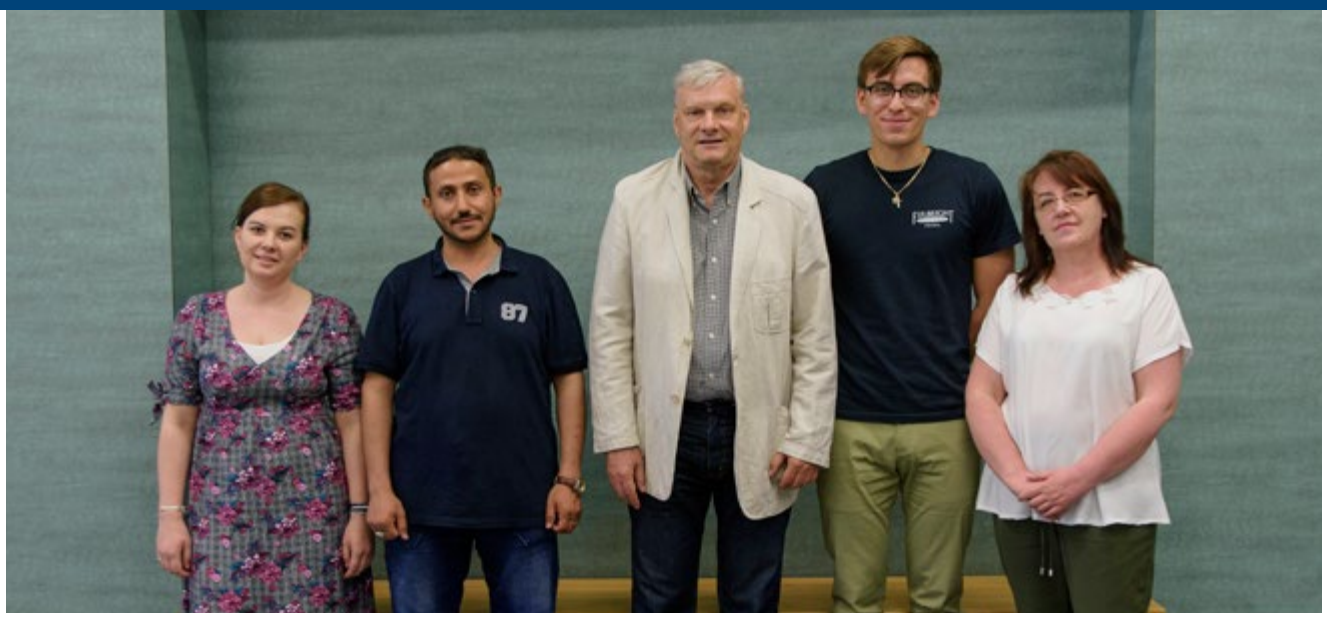
1. A.K. Puszko, P. Sosnowski, F. Raynaud, O. Hermine, G. Hopfgaftner, Y. Lepelletier, A. Misicka, Does Cysteine rule (CysR) complete the CendR principle? Increase in affinity of peptide ligands for NRP-1 through the presence of N-terminal cysteine, Biomolecules. 10 (2020) 448.
2. A. Królikowska, J. Cukras, M. Witkowski, D. Tymecka, A. Hernik-Magoń, A. Misicka, W. Dzwolak, SERS and DFT Study of Noble Metal-Anchored Cys-Trp/Trp-Cys Dipeptides: Influence of Main-Chain Direction and Terminal Modifications, Journal of Physical Chemistry C. 124 (2020) 7097-7116.
3. K. Pułka-Ziach, A.K. Puszko, J. Juhaniewicz-Dębińska, S. Sęk, Electron Transport and a Rectifying Effect of Oligourea Foldamer Films Entrapped within Nanoscale Junctions, Journal of Physical Chemistry C. 123 (2019) 1136–1141.
4. A.K. Puszko, P. Sosnowski, D. Tymecka, F. Raynaud, O. Hermine, Y. Lepelletier, A. Misicka, Neuropilin-1 peptide-like ligands with proline mimetics, tested using the improved chemiluminescence affinity detection method, MedChemComm. 10 (2019) 332-340.
5. J. Juhaniewicz-Dębińska, D. Tymecka, S. Sęk, Diverse effect of cationic lipopeptide on negatively charged and neutral lipid bilayers supported on gold electrodes, Electrochimica Acta. 298 (2019) 735-744.
6. B. Fedorczyk, P.F.J. Lipiński, A.K. Puszko, D. Tymecka, B. Wileńska, W. Dutka, G.Y. Perret, R. Wieczorek, A. Misicka, Triazolopeptides inhibiting the interaction between Neuropilin-1 and Vascular Endothelial Growth Factor 165, Molecules. 24 (2019) 1756.
7. A.K. Puszko, P. Sosnowski, K. Pułka-Ziach, O. Hermine, G. Hopfgaftner, Y. Lepelletier, A. Misicka, Urea moiety as amide bond mimetic in peptide-like inhibitors of VEGF-A165/NRP-1 complex, Bioorg Med Chem Lett. 29 (2019) 2493-2497.
8. B. Wileńska, D. Tymecka, M. Włodarczyk, A.Sobolewska-Włodarczyk, M. Wiśniewska-Jarosińska, J. Dyniewicz, A. Somogyi, J. Fichna, A. Misicka, Enkephalin degradation in serum of patients with inflammatory bowel diseases, Pharmacological Reports. 71 (2019) 42-47.
9. D. Tymecka, A.K. Puszko, P.F.J. Lipiński, B. Fedorczyk, B. Wileńska, K. Sura, G.Y. Perret, A. Misicka, Branched pentapeptides as potent inhibitors of the Vascular Endothelial Growth Factor 165 binding to Neuropilin-1, Eur J Med Chem. 158 (2018) 453-462.
10. K. Pułka-Ziach, S. Sęk, α-Helicomimetic foldamers as electron transfer mediators, Nanoscale. 9 (2017) 14913-14920.

Laboratory of Radiochemistry and Atmospheric Chemistry

UNIVERSITY OF WARSAW

WCh Faculty of Chemistry University of Warsaw

Laboratory of Radiochemistry and Atmospheric Chemistry



HEAD:

Prof. Tomasz Gierczak*, PhD DSc

GROUP MEMBERS:

Anna Makowska, PhD; Bartłomiej Witkowski, PhD
PhD students: Mohammed Al-sharafi, Monika Ganeczko

RESEARCH PROFILE:

- Analytical methods development for the determination of organic compounds in complex matrices using capillary gas chromatography coupled with mass spectrometry (GC/MS) and high-performance liquid chromatography coupled with tandem mass spectrometry HPLC/MS /MS.
- Investigation of the chemical processes taking place in the atmosphere; studying the mechanism of formation and transformation of secondary organic aerosols (SOAs) in the troposphere; investigation of kinetics and mechanism of organic compounds oxidation in atmospheric water.
- Analysis of organic compounds in archaeological samples of high historical value.

CURRENT RESEARCH ACTIVITIES:

At the moment, we are conducting a study of the composition of organic aerosol (SOA) resulting from the ozonolysis reaction of sesquiterpenes. Ozone reacts with β-caryophyllene in the gas phase in a flow reactor, without the presence of a scavenger. The resulting oxidized products condensed in the form of an aerosol. The aerosol is collected on the filter and the filter extract is analyzed by HPLC/MS/MS. A number of ozonolysis products have been identified and pathways of their formation have been proposed.

*e-mail: gierczak@chem.uw.edu.pl

SELECTED PUBLICATIONS:

1. B. Witkowski, A. Duchnowicz, M. Ganeczko, A. Laudy, T. Gierczak, M. Biesaga, Identification of proteins, drying oils, waxes and resins in the works of art micro-samples by chromatographic and mass spectrometric techniques, Journal of Separation Science. 41(3) (2018) 630-638.
2. B. Witkowski, S. Jurdana, T. Gierczak, Limononic acid oxidation by hydroxyl radicals and ozone in the aqueous phase, Environ. Sci. Technol. 52(6) (2018) 3402-3411.
3. B. Witkowski, M. Ganeczko, H. Hryszko, M. Stachurska, T. Gierczak, M. Biesaga, Identification of orcein and selected natural dyes in 14th and 15th century liturgical paraments with high-performance liquid chromatography coupled to the electrospray ionization tandem mass spectrometry (HPLC-ESI/MS/MS), Microchemical Journal. 133 (2017) 370-379.
4. B. Witkowski, T. Gierczak, Characterization of the limonene oxidation products with liquid chromatography coupled to the tandem mass spectrometry, Atmospheric Environment. 154 (2017) 297-307.

Laboratory of Spectroscopy and Intermolecular Interactions

UNIVERSITY OF WARSAW

WCh Faculty of Chemistry University of Warsaw

New Methods of NMR Spectroscopy

HEAD:

Prof. Wiktor Koźmiński*, PhD DSc

GROUP MEMBERS:

Rafał Augustyniak, PhD; Michał Nowakowski, PhD; Piotr Paluch, PhD; Alexandra Shchukina, PhD; Jan Stanek, PhD; Anna Zawadzka-Kazimierczuk, PhD; Szymon Żerko, PhD
PhD students: Dariusz Gołowicz, Michał Górka, Katarzyna Grudziąż

RESEARCH PROFILE:

Our group works mostly on methodological aspects of NMR spectroscopy. The aim of this work is faster and more accurate determination of structurally important NMR parameters, and their application in chemistry and biochemistry. Recently we focus on the development of new approaches for acquisition of multidimensional NMR spectra necessary in the studies of biomolecules.

Most important topics include: development of new pulse sequences for faster or more accurate determination of spectral parameters, methods of fast acquisition of multidimensional spectra, determination of scalar and residual dipolar couplings, chiral recognition.
Currently our work focuses on the following tasks:

- Acquisition of high dimensional NMR spectra (4-7D) and new strategies of resonance assignment in biomolecules.
- Application of new methods for the studies of intrinsically disordered proteins (IDP).
- Development of methods for cleaning spectra from artefacts which are result of sparse sampling. This would allow analysis of spectra featuring high dynamic range of peak amplitudes, as for example heteronuclear edited 4D NOESY.
- Development of NMR methods exploring the new possibilities of random sampling for the accurate and precise determination of scalar and residual dipolar couplings from 3 and 4D NMR spectra.
- Protein structure elucidation and protein interaction studies.
- Peptide structure elucidation.
- NMR resonance assignment, structure determination and dynamics of biomolecules in the solid-state.

*e-mail: kozmin@chem.uw.edu.pl

CURRENT RESEARCH ACTIVITIES:

Creating and developing new methods for measuring and processing multidimensional NMR spectra and their application in the study of semi- unstructured proteins. These achievements represent a breakthrough in NMR multidimensional spectroscopy and its applications, especially in biomolecule research.

SELECTED PUBLICATIONS:

1. K. Grudziąż, A. Zawadzka-Kazimierczuk, W. Koźmiński, High-dimensional NMR methods for intrinsically disordered proteins studies, Methods. 148 (2018) 81-87.
2. M. Baias, P.E.S. Smith, K. Shen, L.A. Joachimiak, S. Żerko, W. Koźmiński, J. Frydman, L. Frydman, Structure and dynamics of the Huntingtin exon-1 N-terminus: A solution NMR perspective, J. Am. Chem. Soc. 139 (2017) 1168–1176.
3. M. Nowakowski, S. Saxena, J. Stanek, S. Żerko, W. Koźmiński, Applications of high dimensional experiments in biomolecular NMR, Prog. Nucl. Mag. Res. Sp. 90-91 (2015) 49-73.
4. M. Urbańczyk, W. Koźmiński, K. Kazimierczuk, Accelerating Diffusion-Ordered NMR Spectroscopy by Joint Sparse Sampling of Diffusion and Time Dimensions, Angewandte Chemie Int. Ed. Engl. 53 (2014) 6464–6467.
5. J. Stanek, S. Saxena, L. Geist, R. Konrat, W. Koźmiński, Probing of Local Backbone Geometries in Intrinsically Disordered Proteins by Cross-Correlated NMR Relaxation, Angewandte Chemie Int. Ed. Engl. 52 (2013) 4604–4606.
6. K. Kazimierczuk, J. Stanek, A. Zawadzka-Kazimierczuk, W. Koźmiński, High-dimensional NMR spectra for structural studies of biomolecules, ChemPhysChem. 14 (2013) 3015–3025.
7. K. Kazimierczuk, M. Misiak, J. Stanek, A. Zawadzka-Kazimierczuk, W. Koźmiński, Generalized Fourier transform for non-uniform sampled data, Topics in Current Chemistry. 316 (2012) 79–124.
8. K. Kazimierczuk, J. Stanek, A. Zawadzka-Kazimierczuk, W. Koźmiński, Random sampling in multidimensional NMR spectroscopy, Prog. Nucl. Mag. Res. Sp. 57 (2010) 420–434.
9. K. Kazimierczuk, A. Zawadzka, W. Koźmiński, I. Zhukov, Determination of spin-spin couplings from ultrahigh resolution 3D NMR spectra obtained by optimized random sampling and Multidimensional Fourier ransformation, J. Am. Chem. Soc. 130 (2008) 5404-5405.
10. K. Kazimierczuk, W. Koźmiński, I. Zhukov, Two-dimensional Fourier transform of arbitrarily sampled NMR data sets, J. Magn. Reson. 179 (2006) 323-328.

Biophysical Chemistry Group

HEAD:

Prof. Wojciech Dzwolak*, PhD DSc

GROUP MEMBERS:

PhD students: Robert Dec, Marcin Guza, Bartosz Niżyński, Matylda Wacławska, Marcin Witkowski
MSc students: Mateusz Fortunka, Małgorzata Jabłońska

RESEARCH PROFILE:

Our research is focused on biological soft matter: its dynamics, conformational transitions, and processes leading to the hierarchical self-assembly of biopolymers and biomembranes. We are particularly interested in:

- mechanisms of protein aggregation,
- borderlines between determinism and randomness in conformational transitions of proteins,
- thermodynamics of protein folding and misfolding,
- applications of the biological self-organization in nanotechnology,
- biological applications of optical spectroscopy.

CURRENT RESEARCH ACTIVITIES:

1. Biophysical experimental and theoretical studies on the H-fragment of insulin – the newly identified highly amyloidogenic two-chain fragment of the hormone (Piejko M et al J. Biol. Chem. 290 (2015) 5947):

2. A multidisciplinary approach to the self-assembly of nanofibrils from short synthetic peptides: from the identification of fundamental driving forces of the phenomenon to future applications in material sciences and clinical diagnostics.

*e-mail: wdzwolak@chem.uw.edu.pl

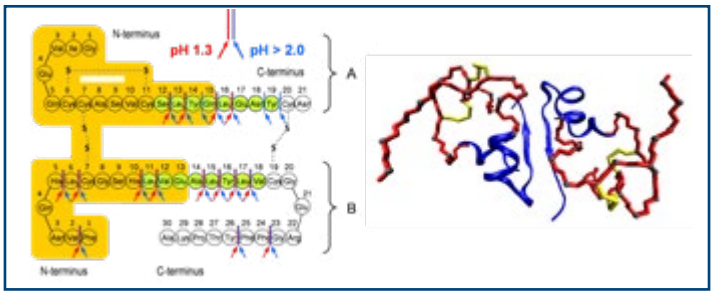


Fig. 1. The orange-marked covalent structure of the H-fragment is indicated within the primary sequence of bovine insulin monomer (left panel) and 3D-structure of the dimer (right side – red tubes).

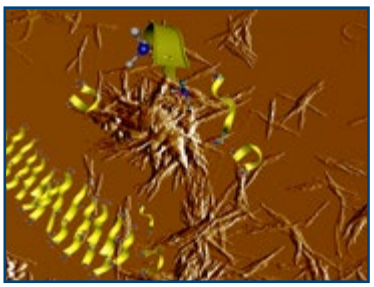


Fig. 2. AFM amplitude image of beta2-type fibrils self-assembled from short oligomers of L-glutamic acid (according to Hernik-Magoń A et al, *Colloid. Surface. B* 159 (2017) 861).

SELECTED PUBLICATIONS:

1. A. Hernik-Magoń, W. Puławski, B. Fedorczyk, D. Tymecka, A. Misicka, P. Szymczak, W. Dzwolak, Beware of cocktails: Chain-length bidispersity triggers explosive self-assembly of poly-L-glutamic acid β2-fibrils, Biomacromolecules. 17 (2016) 1376–1382.
2. M. Piejko, R. Dec, V. Babenko, A. Hoang, M. Szewczyk, P. Mak, W. Dzwolak, Highly amyloidogenic two-chain peptide fragments are released upon partial digestion of insulin with pepsin, J. Biol. Chem. 290 (2015) 5947–5958.
3. W. Surmacz-Chwedoruk, H. Nieznańska, S. Wójcik, W. Dzwolak, Cross-seeding of fibrils from two types of insulin induces new amyloid strains, Biochemistry. 51 (2012) 9460–9469.
4. V. Babenko, W. Dzwolak, Thioflavin T forms a non-fluorescent complex with α-helical poly-L-glutamic acid, Chem. Commun. 47 (2011) 10686–10688.
5. A. Fulara, A. Lakhani, S. Wójcik, H. Nieznańska, T.A. Keiderling, W. Dzwolak, Spiral superstructures of amyloid-like fibrils of polyglutamic acid: An infrared absorption and vibrational circular dichroism study, J. Phys. Chem. B. 115 (2011) 11010–11016.
6. A. Loksztejn, W. Dzwolak, Vortex-induced formation of insulin amyloid superstructures probed by time-lapse atomic force microscopy and circular dichroism spectroscopy, J. Mol. Biol. 395 (2010) 643–655.
7. W. Dzwolak, A. Loksztejn, A. Galińska-Rakoczy, R. Adachi, Y. Goto, L. Rupnicki, Conformational indeterminism in protein misfolding: chiral amplification on amyloidogenic pathway of insulin, J. Amer. Chem. Soc. 129 (2007) 7517-7522.
8. W. Dzwolak, R. Ravindra, C. Nicolini, R. Jansen, R. Winter, The diastereomeric assembly of polylysine is the low-volume pathway for preferential formation of beta-sheet aggregates, J. Amer. Chem. Soc. 126 (2004) 3762-3768.
9. W. Dzwolak, T. Muraki, M. Kato, Y. Taniguchi, Chain-length dependence of alpha-helix to beta-sheet transition in polylysine: model of protein aggregation studied by temperature-tuned FTIR spectroscopy, Biopolymers. 73 (2004) 463-469.

InFemto Research Group

HEAD:

Prof. Wojciech Gadomski*, PhD DSc

GROUP MEMBERS:

Bożena Ratajska-Gadomska, PhD DSc;
Piotr Piątkowski, PhD; Kamil Polok, PhD
PhD students: Nishith Maity (visiting from University of Lille), Adam Świątek
MSc student: Marzena Kaliszewska
BSc student: Jakub Pawlak

RESEARCH PROFILE:

Ultrafast dynamics and local structure in molecular systems by femtosecond pump-probe spectroscopy, molecular dynamics simulations, spontaneous Raman scattering, photoactive materials.

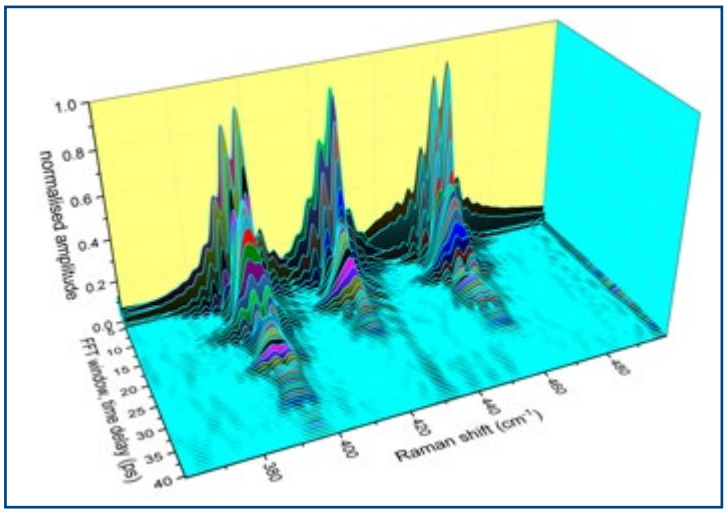
CURRENT RESEARCH ACTIVITIES:

Investigation of coherent response of the medium in femtosecond time resolved spectroscopy. Three time resolved techniques are applied: transient transmission spectroscopy, optical Kerr effect spectroscopy and transient absorption spectroscopy. The first two techniques provide the information on the vibrational dynamics of molecules composing the medium. Applying femtosecond pump pulses we can detect vibrations of frequencies up to 1000 cm^{-1}, which means also low frequency intermolecular vibrations. The third technique detects the dynamics of electronic transitions in molecules.

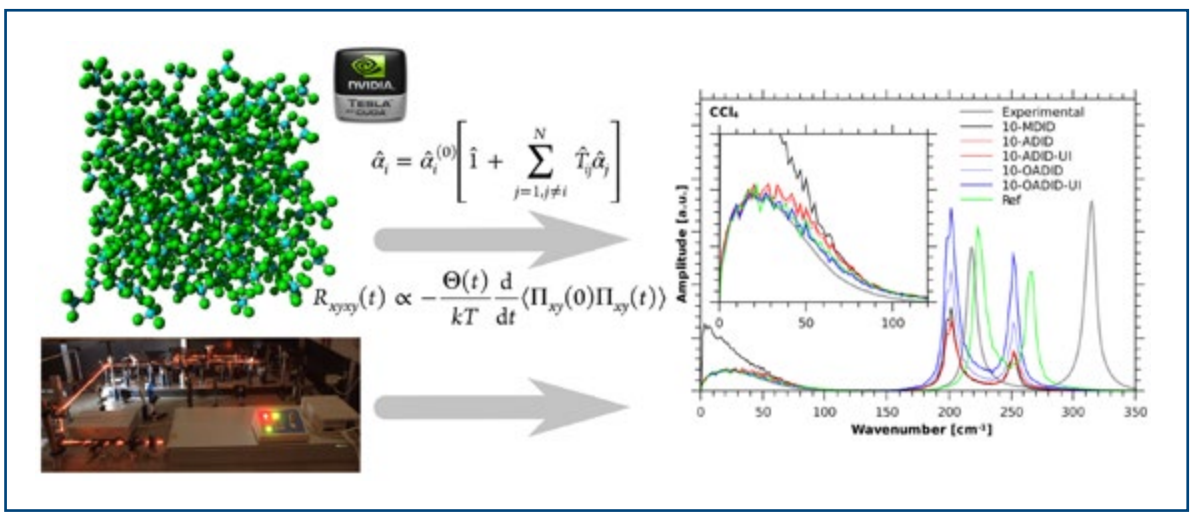
Our research has recently concentrated on the study of liquid tetrachlorides and trichlorides, their local structures and dynamics. We also build theoretical models describing our experimental results, which allow us to find important molecular parameters responsible for the dynamics of local order in liquids. Below there are some examples of our recent results.

We are developing scientific software for investigation of the local structure and ultrafast dynamics in liquids, based on molecular dynamics simulations. Our software involves calculation of various correlation functions, statistical analysis of hydrogen bond network and several methods of calculating the femtosecond optical Kerr effect signal. The simulations are made in parallel with experiments. Other investigated systems involve for example the methanol-chloroform mixture, which shows an enhanced

*e-mail: gado@chem.uw.edu.pl



Time evolution of transient transmission spectra of the symmetric stretching vibration in three tetrachlorides. Spectra have been obtained as fast Fourier transforms of time resolved signals. Fine structure of the spectra is connected with the natural abundance of chlorine isotopes ^{35}Cl and ^{37}Cl. It can be well seen due to very high resolution of the spectra.



The femtosecond optical Kerr effect signal is obtained from molecular dynamics simulations and from experiment. Multiple models are validated against the experimental signal to select the best one. The comparison is shown for the Fourier transformed signals. Further analysis of MD trajectoriy allows to distinguish different contributions to the signal.

polarity compared to its components in pure state. This results in a considerably increased solvatochromic effect for some dyes dissolved in this mixture, which is described in terms of synergistic solvation. We are using the same techniques for the mixtures of ionic liquids with simple solvents. These are of great interest due to their potential application as electrolytes in photovoltaic devices. In this study we want to understand the molecular origins of the macroscopic and solvation properties of those mixtures. Recently, the application of organic-inorganic lead trihalide perovskite semiconductors in solar cells gave rise to a new class of solar cells that achieved a power conversion efficiency of over 20%. Many important processes which shape the optical properties of nanostructured semiconductors occur on a femtosecond to nanosecond timescale. To research such fast evolution of photoexcited charge carriers we are using pump-probe transient absorption (TA) and terahertz (THz) spectroscopies with femtosecond resolution. The results of our experiments allow us to decipher the mechanisms behind high overall efficiency of perovskite-based solar cells.

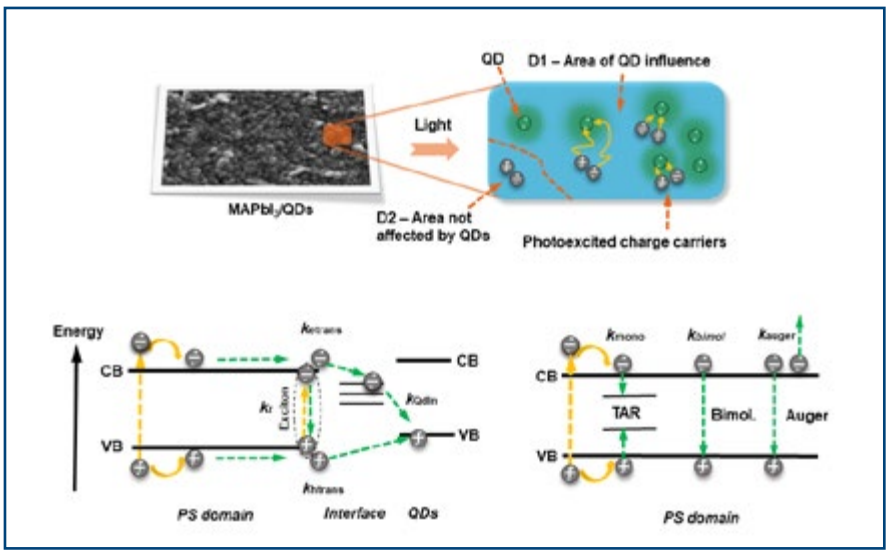


Diagram showing charge carriers migration in MAPbI3/PbS QDs system.

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1. N. Subba, K. Polok, P. Piątkowski, B. Ratajska-Gadomska, R. Biswas, W. Gadomski, P. Sen, Temperature Dependent Ultrafast Solvation Response and Solute Diffusion in Acetamide–Urea Deep Eutectic Solvent, J. Phys. Chem. B. 123(43) (2019) 9212-9221.
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4. K. Polok, Simulations of the OKE Response in Simple Liquids Using a Polarizable and a Non-Polarizable Force Field, J. Phys. Chem. B. 122 (2018) 1638.
5. P. Piątkowski, B. Cohen, S. Kazim, S. Ahmad, A. Douhal, How photon pump fluence changes the charge carrier relaxation mechanism in an organic–inorganic hybrid lead triiodide perovskite. Phys. Chem. Chem. Phys. 18 (2016) 27090-27101.
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10. B. Ratajska-Gadomska, W. Gadomski, Influence of confinement on solvation of ethanol in water studied by Raman spectroscopy, J. Chem. Phys. 133 (2010) 234505.

Materials for Biosensors

HEAD:

Barbara Pałys*, PhD DSc

GROUP MEMBERS:

Agnieszka Dąbrowska, PhD; Anna Jabłońska, PhD; Piotr Olejnik, PhD
PhD student: Sylwia Berbeć
MSc students: Dominik Cieśliński, Klaudia Karolak, Mateusz Kasztelan, Maria Królak, Sylwia Kot, Paweł Wasilewski

RESEARCH PROFILE:

Optical and electrocatalytic applications of graphene oxide and metallic nanostructures, nanostructures of conducting polymers as support for enzymes, controlled orientation of enzymes, PM-IRRAS and Raman studies of surfaces, infrared and Raman mapping of samples

CURRENT RESEARCH ACTIVITIES:

Currently we investigate applications of graphene oxide combined with metallic nanoparticles as possible fluorescence quenchers and enhancers of Raman and infrared spectra. We study also intrinsic electrocatalytic properties of reduced graphene oxide, composites with metallic nanoparticles and enzymes immobilized on such composites. Our interest includes also conducting polymers – in particular hydrogels composed of conducting polymers as supports for enzymes and/or other catalysts. Another research activity are studies of microplastics by infrared and Raman microscopy.

*e-mail: bpalys@chem.uw.edu.pl

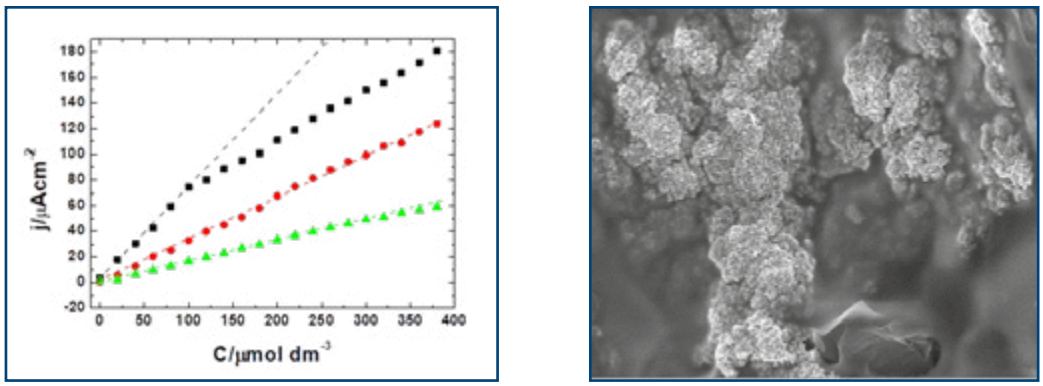

Fig. 1 Electrocatalytic reduction of H_2O_2 on electrochemically reduced graphene oxide on gold nanoparticles

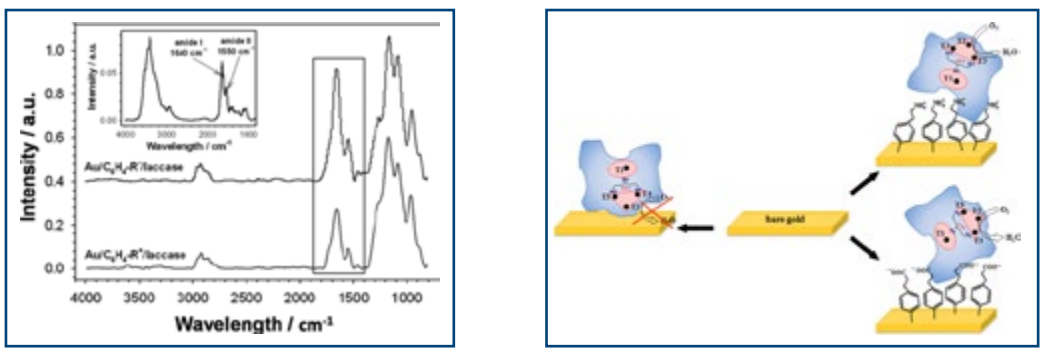

Fig. 2 PM-IRRAS spectra of laccase on variously charged surfaces[5] (reprinted with permission of ACS)

SELECTED PUBLICATIONS:

1. S. Berbeć, S. Żołądek, A. Jabłońska, B. Pałys, Electrochemically reduced graphene oxide on gold nanoparticles modified with a polyoxomolybdate film. Highly sensitive non-enzymatic electrochemical detection of H_2O_2, Sensors and Actuators B: Chemical. 258 (2018) 745–756.
2. A. Jabłońska, B. Pałys, Effect of the polymerization bath on structure and electrochemical properties of polyaniline-poly(styrene sulfonate) hydrogels, Journal of Electroanalytical Chemistry. 784 (2017) 115–123.
3. A. Jabłońska, M. Gniadek, B. Pałys, Enhancement of direct electrocatalytic activity of horseradish peroxidase on polyaniline nanotubes, J. Phys. Chem. C. 119 (2015) 12514–12522.
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Physico-chemistry of Materials („Szosz-lab”)

HEAD:

Robert Szoszkiewicz*, PhD DSc

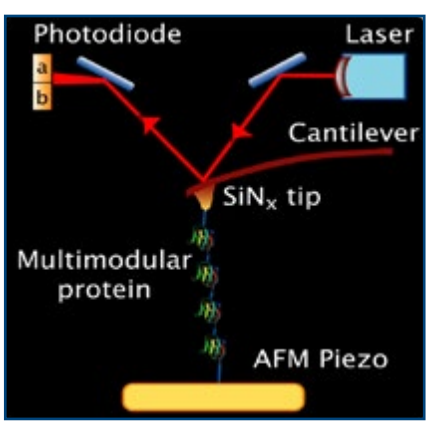
GROUP MEMBERS:

Katarzyna Wybrańska, PhD
PhD student: Saeed Sovizi
MSc students: Karolina Jaszczerska, Stanisław Sokołowski, Aleksandra Wosztyl
BSc students: Anna Kowalczyk, Aneta Mierzwa

RESEARCH PROFILE:

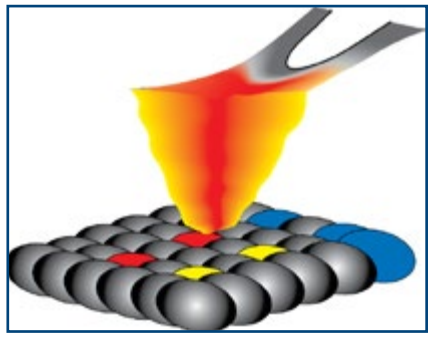
Our current research focuses on physico-chemical properties of various engineering surfaces and single-molecule biophysics of proteins and peptides.

• We measure nano-mechanical properties of nano- and micro-objects such as single proteins, as well as



*e-mail: rszoszkiewicz@chem.uw.edu.pl

- We modify the physico-chemical surface properties of 2D materials such as MoS_2 using heat and the thermochemical nanolithography (TCNL) method.



For our research we use modern methods of studying materials at local scales, including atomic force microscopy, selected lithography methods, methods of electron microscopy (SEM, TEM), methods of chemical composition analysis, such as X-ray photoelectron spectroscopy (XPS) and energy-dispersive X- ray spectroscopy (EDS), local Raman spectroscopy, and other methods.

SELECTED PUBLICATIONS:

1. U. Ukegbu, R. Szoszkiewicz, Microscopic kinetics of heat-induced oxidative etching of thick MoS2 crystals, Journal of Physical Chemistry C. 123 (2019) 22123-22129.
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3. A. Avila-Flores, L.R.M.M. Aps, N. Ploscariu, P. Sukthankar, R. Guo, K.E. Wilkinson, P. Games, R. Szoszkiewicz, R.P.S. Alves, M.O. Diniz, Y. Fang, L.C.S. Ferreira, J.M. Tomich, Gene Delivery and Immunomodulatory Effects of Plasmid DNA Associated with Branched Amphiphilic Peptide Capsules, Journal of Controlled Release. 241 (2016) 15-24.
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6. R. Szoszkiewicz, E. Riedo, Sliding charges, Nature Materials (News and Views). 13 (2014) 666-668.
7. E. Gnecco, E. Riedo, W.P. King, S.R. Marder, R. Szoszkiewicz, Linear ripples and traveling circular ripples produced on polymers by thermal AFM probes, Physical Review B. 79 (2009) 235421.
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Raman Spectroscopy Group

HEAD:

Prof. Andrzej Kudelski*, PhD DSc

GROUP MEMBERS:

Aleksandra Jaworska, PhD; Jan Krajczewski, PhD; Agata Królikowska, PhD; Beata Wrzosek, PhD
PhD students: Robert Ambroziak, Edyta Pyrak, Maria Żygieło

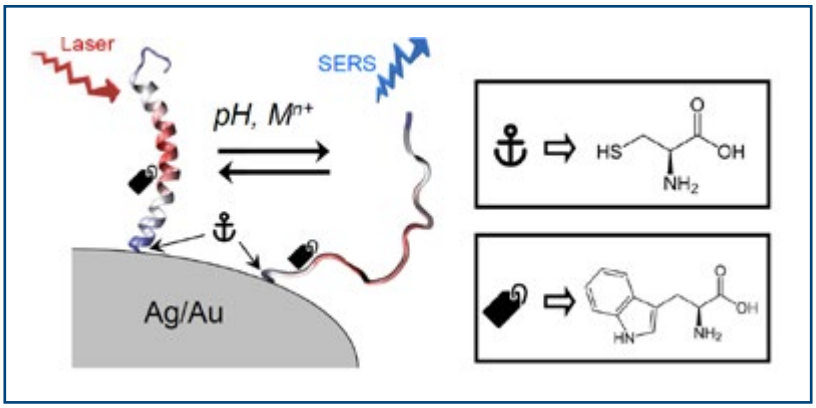
RESEARCH PROFILE:

Our research focuses on various applications of Raman spectroscopy, especially surface-enhanced Raman scattering (SERS).

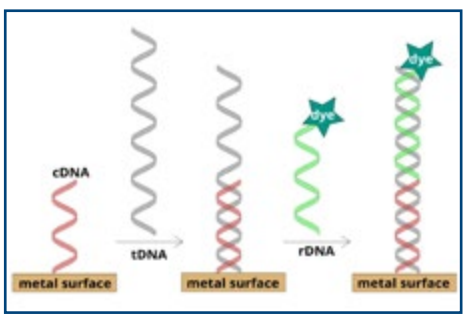
CURRENT RESEARCH ACTIVITIES:

- Hybrid nanostructures combining plasmonic and magnetic properties and their application for SERS detection and recovery/removal of the target analyte.
- SERS blinking on anisotropic silver nanoparticles.
- Theoretical modelling of vibrational spectra.
- Synthesis of system for controlled transport of biomolecules. Fabrication of SERS substrates with limited areas of appropriately selected monolayers and developing conditions for the control of their properties, and in consequence – monolayer structures, enabling efficient transport of adsorbed biomolecules over the entire SERS substrate.
- SERS studies of oligopeptides containing cysteine and tryptophan adsorbed on Ag and Au as models for biomolecular receptors with external stimuli-responsive conformations.
- In situ multi-spectroscopic molecular characterisation of DNA films on metal surfaces in aqueous environment.
- Application of SERS for detection of BRAF mutation in melanoma.
- Analysis of surfaces of various materials (especially in situ) using shell-isolated nanoparticle-enhanced Raman spectroscopy (SHINERS).

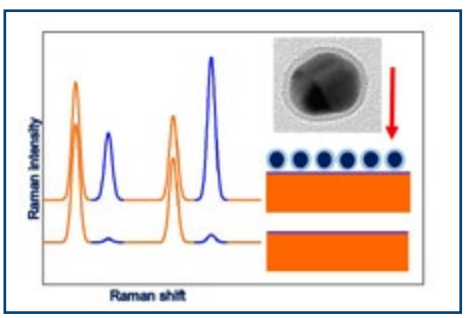
*e-mail: akudel@chem.uw.edu.pl



Scheme showing the idea of a SERS-based sensor, exploiting a protein-derived peptide fragment anchored to metal by Cys residue and labeled with Trp, responding with a conformational transition to external stimuli (e.g. pH or biologically relevant metal cation concentration).



The principles of detecting of DNA using SERS spectroscopy.



The principles of SHINERS measurements.

SELECTED PUBLICATIONS:

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Structural Dynamics Research Group

HEAD:

Katarzyna N. Jarzembska*, PhD DSc

GROUP MEMBERS:

Radosław Kamiński, PhD Eng
PhD student: Sylwia E. Kutniewska
MSc students: Krystyna Deresz, Piotr Łaski, Dariusz Szarejko
BSc student: Patryk Borowski

RESEARCH PROFILE:

Our research interests oscillate between Chemistry, Physics and Materials Science. They include: photocrystallography and solid-state structural dynamics, solid-state spectroscopy, chemical and physical crystallography for materials science, accurate crystallography under ambient and extreme conditions, computational chemistry, instrumentation and software development, crystal engineering.

CURRENT RESEARCH ACTIVITIES:

- Tracing of excited-state species in crystals and solution

Polynuclear transition-metal complexes often exhibit interesting optoelectronic or magnetic properties. The aim of our research is to deeply investigate the dynamics of light-induced processes, which occur both in crystals and in solutions. We focus our attention on charge transfer processes taking place in chemical systems containing multicentre coinage metal complexes and also in bridged transition metal complexes L_nM_1–bridge–M_2L_m (M_1, M_2 = Fe, Co, Cu, *etc*., bridge = CN, SCN, *etc*.; L_n, L_m = ligands). We are interested in finding relationships between molecular structure of such compounds, their configuration and charge distribution, metal-metal interactions and metal centre's communication through different linking groups, *etc*., and the macroscopic properties of the respective substances.

- Synthesis and characterisation of new photoswitchable materials

Currently, one of the main goals of chemistry and physics is to develop new materials that are able to respond rapidly and reliably to changes in local environment, and send out signals which let us know what is happening. Consequently, our research is dedicated to thorough and systematic investigations of the

*e-mail: katarzyna.jarzembska@uw.edu.pl

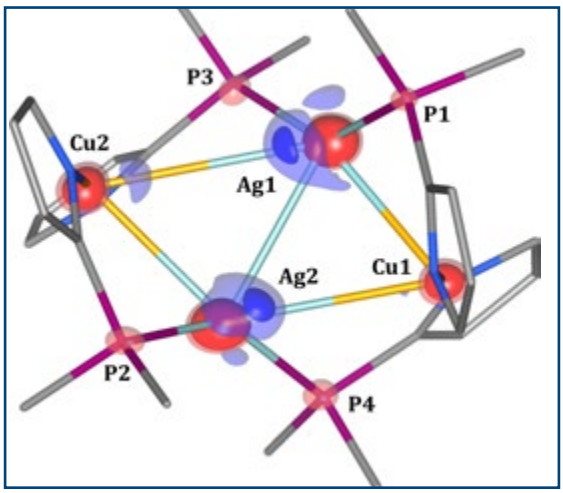
dynamics and nature of light-induced nitro group isomerisation reaction occurring in crystals of Ni, Cu or Co coordination compounds. We aim at designing promising photoswitchable materials characterised by desired reversibility, conversion percentage and stability.

- Crystal engineering

Crystal engineering methods are useful when analysing molecular motifs, relative crystal stabilities and origins of different properties of crystalline materials. We apply these tools to supplement our photocrystallographic studies and also to investigate crystals and cocrystals of boron-based compounds, pharmaceuticals and luminescent complexes, which have been of our interest for several years now.

- Method development and non-standard crystallography

Our scientific interests also cover preparation of useful tools (computer -codes, computational methods) and construction of devices for various crystallographic applications, including photocrystallography, experimental charge density studies and high-pressure crystallography. More details can be found on our website: **www.photocrystallography.eu**.



Photodifference map showing light-induced structural changes in a model silver(I)-copper(I) tetranuclear complex (reproduced from Inorg. Chem. 53 (2014) 10594).

SELECTED PUBLICATIONS:

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2. S.E. Kutniewska, R. Kamiński, W. Buchowicz, K.N. Jarzembska, Photo- and thermoswitchable half-sandwich nickel(II) complex: [Ni(η^5-C_5H_5)(IMes)(η^1-NO_2)], Inorg. Chem. (2019) 16712.
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5. K.N. Jarzembska, R. Kamiński. K. Durka, M. Kubsik, K. Nawara, E. Witkowska, M. Wiloch, S. Luliński, J. Waluk, I. Głowacki, K. Woźniak, New class of easily-synthesisable and modifiable organic materials for applications in luminescent devices, Dyes Pigm. 138 (2017) 267.
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7. C.F.A. Negre, K.J. Young, M. Belén Oviedo, L.J. Allen, C.G. Sánchez, K.N. Jarzembska, J.B. Benedict, R.H. Crabtree, P. Coppens, G.W. Brudvig, V.S. Batista, Photoelectrochemical hole injection revealed in polyoxotitanate nanocrystals functionalized with organic adsorbates, J. Am. Chem. Soc. 136 (2014) 16420.
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Theoretical Chemistry Team

HEAD:

Magdalena Pecul-Kudelska*, PhD DSc

GROUP MEMBERS:

Prof. Joanna Sadlej, PhD DSc (emeritus);
Janusz Cukras, PhD; Joanna Jankowska, PhD
PhD students: Katarzyna Jakubowska,
Maciej Kamiński

RESEARCH PROFILE:

Our research focuses on different aspects of light-molecules interactions. In particular, we apply and develop methods of quantum chemistry to study stability, spectroscopic properties, and photoreaction mechanisms of molecular and supramolecular systems. Our special focus is also set on Nuclear Magnetic Resonance and chiralooptical spectroscopic parameters. For up-to-date information, please visit our webpages: *tct.chem.uw.edu.pl* and *psiom.chem.uw.edu.pl/j_sadlej.html*

CURRENT RESEARCH ACTIVITIES:

MPK: Theory and modeling of Nuclear Magnetic Resonance and chiralooptical spectroscopic parameters:

- relativistic effects in NMR spectra;
- polarized-luminescence calculations;
- chiral recognition by molecular spectroscopy.

JC: Quantum-chemical spectroscopic calculations for molecules and supra-molecular complexes:

- circular- and axial-dichroism optical spectra, applications and methods development,
- high-quality vibrational spectra calculations,
- intermolecular interactions,
- noble-gas molecular systems,

***e-mail:** mpecul@chem.uw.edu.pl

- quantum chemistry software development (DALTON, Dalton Project)

JJ: Theoretical photochemistry studies aided with nonadiabatic molecular dynamics simulations:

- fundamental photochemical processes (excited state proton transfer, photostability of proto-biological molecular systems),
- modern materials for photovoltaics (hybrid perovskites, highly-polarized molecular wires)
- molecular photoswitching (biased photoswitching of diarylethenes, complex molecular photo-devices)
- nonadiabatic molecular dynamics methods development for modeling processes in highly-excited electronic states.

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2. J. Cukras, J.M.E. Ahokas, J. Lundell, Vibrational spectrum of HXeSH revisited: Combined computational and experimental study, Chem. Phys. Lett. 741 (2020) 137083.
3. A. Królikowska, J. Cukras, M. Witkowski, D. Tymecka, A. Hernik-Magoń, A. Misicka, W. Dzwolak, SERS and DFT Study of Noble-Metal-Anchored Cys-Trp/Trp-Cys Dipeptides: Influence of Main-Chain Direction and Terminal Modifications, J. Phys. Chem. C. 124 (2020) 7097–7116.
4. K. Jakubowska, M. Pecul, Nuclear Magnetic Resonance parameters of mercury atom and water molecule complex: Relativistic calculations, Chem. Phys. Lett. 736 (2019) 136775.
5. J. Jankowska, A.L. Sobolewski, Efficient Separation of Photogenerated Charges in a Ferroelectric Molecular Wire: Nonadiabatic Dynamics Study on 3, 5-Dicyano-1, 7-dimethylopyrrolo [3, 2-f] indole Trimer, ChemPhotoChem. 3 (2019) 187-192.
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7. K. Jakubowska, M. Pecul, M. Jaszuński, Spin-spin coupling constants in HC=CXH3 molecules; X=C, Si, Ge, Sn and Pb, Theor. Chem. Acc. 137 (2018) 41.
8. J. Jankowska, M. Barbatti, J. Sadlej, A.L. Sobolewski, Tailoring the Schiff base photoswitching–a non-adiabatic molecular dynamics study of substituent effect on excited state proton transfer, Phys. Chem. Chem. Phys. 19 (2017) 5318-5325.
9. J. Cukras, J. Kauczor, P. Norman, A. Rizzo, G.L.J.A. Rikken, S. Coriani, A complex-polarization-propagator protocol for magneto-chiral axial dichroism and birefringence dispersion, Phys. Chem. Chem. Phys. 18 (2016) 13267–13279.
10. M. Kamiński, J. Cukras, M. Pecul, A. Rizzo, S. Coriani, A computational protocol for the study of circularly polarized phosphorescence and circular dichroism in spin-forbidden absorption, Phys. Chem. Chem. Phys. 29 (2015) 19079–19086.

Laboratory of Stereocontrolled Organic Synthesis

UNIVERSITY OF WARSAW

WCh Faculty of Chemistry University of Warsaw

Laboratory of Stereocontrolled Organic Synthesis

HEAD:

Prof. Rafał Siciński*, PhD DSc

GROUP MEMBERS:

prof. Tomasz Bauer, PhD DSc;
prof. Janusz Jurczak, PhD DSc (emeritus);
Piotr Kwiatkowski, PhD DSc; Anna Piątek, PhD DSc; Piotr Piątek, PhD DSc; Jan Romański, PhD DSc; Katarzyna Sęktas, PhD; Krzysztof Ziach, PhD

RESEARCH PROFILE:

Academic staff in our Laboratory are engaged in a broad array of research activities, primarily in the field of stereocontrolled organic synthesis. Our studies cover a variety of research fields, such as multi-step target synthesis of biologically active compounds of potential therapeutic application, design and preparation of molecular receptors, high pressure organic synthesis or investigation of supramolecular and dynamic combinatorial chemistry. We also engage in the development of asymmetric catalytic methods, especially based on metal-free organic molecules and Lewis acids as chiral catalysts. Since many of our research projects are motivated by the biological functions and medicinal relevance of the developed compounds, we use molecular modeling and docking experiments to design promising drug candidates. We closely collaborate with Polish and foreign scientific institutions to perform biological testing of the synthesized compounds.

*e-mail: rasici@chem.uw.edu.pl

CURRENT RESEARCH ACTIVITIES:

1. Synthesis of steroid hormones agonists and antagonists
2. Design, synthesis and evaluation of cytotoxic properties of structurally modified vitamin D compounds
3. Synthesis of steroid transition metal complexes as potential anticancer drugs
4. Design, synthesis and binding studies of heteroditopic receptors capable of simultaneous binding of cations and anions (salts)
5. Design, synthesis and investigation of binding properties of ion pair sensors and supramolecular polymers
6. Synthesis and application of new chiral Lewis acids
7. High-pressure activation of enantioselective organocatalytic reactions
8. Asymmetric synthesis of fluoroorganic compounds
9. Development of enantioselective methods for the construction of quaternary stereogenic center
10. Asymmetric hydrogenation and tetrasubstituted alkenes synthesis as tools in preparation of biologically active compounds
11. Achmatowicz rearrangement of optically active α,β-unsaturated alcohols and amines as a tool in the synthesis of biologically active compounds
12. Dynamic combinatorial chemistry of imines
13. Supramolecular systems of “molecular walkers”
14. Photochemistry of polyenes
15. Spontaneous emergence of solid state chirality in achiral systems

SELECTED PUBLICATIONS:

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3. M. Biedrzycki, A. Kasztelan, P. Kwiatkowski, High-pressure accelerated enantioselective addition of indoles to trifluoromethyl ketones with low-loading of chiral BINOL-derived phosphoric acid, ChemCatChem. 9 (2017) 2453-2456.
4. M. Karbarz, J. Romański, Dual sensing by simple heteroditopic salt receptors containing an anthraquinone unit, Inorg. Chem. 55 (2016) 3616-3623.
5. A. Piątek, Ch. Chapuis, Grignard 1,4-additions to para-substituted (2R)-N-cinnamoylbornane-10,2-sultam derivatives: Revised configuration for the N,OAc-keteneacetal formation in the presence of Cu(I), Helv. Chim. Acta. 99 (2016) 573-582.
6. U. Kulesza, L.A. Plum, H.F. DeLuca, A. Mouriño, R.R. Siciński, A new suprasterol by photochemical reaction of 1α,25-dihydroxy-9-methylene-19-norvitamin D_3, Org. Biomol. Chem. 14 (2016) 1646-1652.
7. U. Kulesza, L.A. Plum, H.F. DeLuca, A. Mouriño, R.R. Siciński, Novel 9-alkyl- and 9-alkylidene-substituted 1α,25-dihydroxyvitamin D_3 analogues: Synthesis and biological examinations, J. Med. Chem. 58 (2015) 6237-6247.
8. M. Majdecki, J. Jurczak, T. Bauer, Palladium-catalyzed enantioselective allylic substitution in the presence of monodentate furanoside phosphoramidites, ChemCatChem. 7 (2015) 799-807.
9. T. Bauer, Enantioselective dialkylzinc-mediated alkynylation, arylation and alkenylation of carbonyl groups, Coor. Chem. Rev. 299 (2015) 83-150.
10. K. Ziach, J. Jurczak, Mirror symmetry breaking upon spontaneous crystallization from a dynamic combinatorial library of macrocyclic imines, Chem. Commun. 51 (2015) 4306-4309.

Supramolecular Chemistry Laboratory

HEAD:

Michał Chmielewski*, PhD DSc

GROUP MEMBERS:

Artur Chołuj, PhD
PhD student: Krystyna Maslowska
MSc students: Maria Korczak,
Marcin Wiszniewski, Kamil Ziemkiewicz

RESEARCH PROFILE:

1. metal-organic frameworks (MOFs)
2. supramolecular chemistry of anions

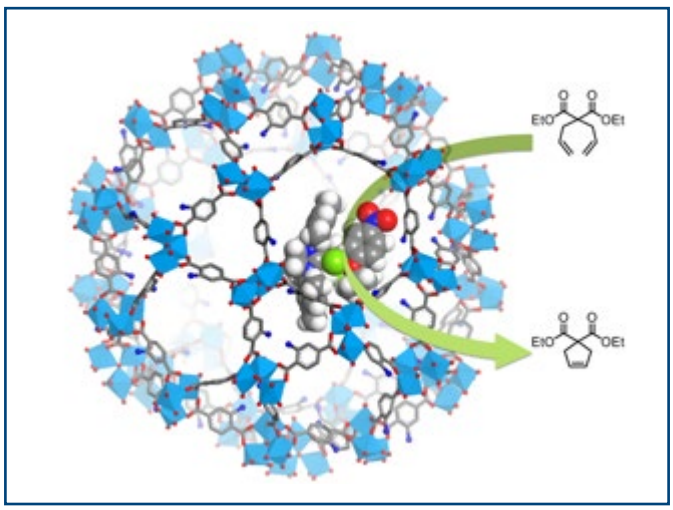
CURRENT RESEARCH ACTIVITIES:

Supramolecular chemistry – 'chemistry beyond molecule' – is an interdisciplinary field of research focusing mainly on self-organisation of molecules into well-defined chemical structures by reversible intermolecular interactions, such as coordination and hydrogen bonds, pi-stacking and others.

Our core specialties are 1) metal-organic frameworks and 2) supramolecular chemistry of anions.

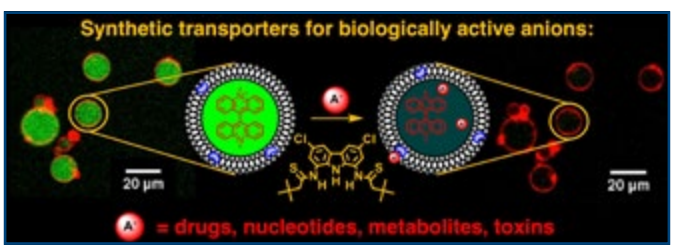
Metal-organic frameworks (MOFs) are crystalline coordination compounds with regular arrays of nanoscopic voids (such as cavities, channels, etc.) in their crystal structures. The porosities and functionalities of MOFs can be easily fine-tuned for multiple applications, such as gas storage (especially H_2, CH_4, and CO_2), separation processes, drug delivery, ion exchange, sensor technology, non-linear optics, magnetism, luminescence, and many others. We are particularly interested in developing conducting MOFs (in collaboration with researchers from MIT) for a wide variety of applications, including fuel cells, batteries, supercapacitors, catalysts, sensors, thermoelectrics, etc. In another line of research, we are also interested in catalytic processes inside the nanoscopic voids of MOFs. Our recent accomplishments in this field include the first successful immobilisation of olefin metathesis catalysts inside MOFs (in collaboration with the group of prof. K. Grela), the first incorporation of enantioselective hydrogenation catalysts into MOFs as well as the development of exquisite MOF catalysts for aerobic oxidation of alcohols to aldehydes.

*e-mail: mchmielewski@chem.uw.edu.pl



On the other hand, the development of molecules that are able to strongly and selectively bind anionic species is also of great importance in various fields, due to a range of important roles anions play in many chemical, biological, medicinal and environmental processes. Such molecules (receptors) could be useful as sensors and transporters able to facilitate anion transport through biological membranes. We also exploit anions as templates for the construction of complex, topologically non-trivial nanostructures, such as catenanes, rotaxanes, helicates, and grids.

For example, we have recently discovered a family of simple, easy-to-make and remarkably active anion transporters. In a major methodological contribution, we have developed the first direct method to study the transport of a variety of biologically relevant anions through lipid bilayers. Using this method, we have discovered the first artificial receptors able to transport amino acids through biological membranes. In another recent project, we have constructed the first photoswitchable ion-pair receptor. This major accomplishment has been published in the prestigious 'Journal of the American Chemical Society'. For the most recent accomplishments, follow our webpage: www.mchmielewski.pl



SELECTED PUBLICATIONS:

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2. K.M. Bąk, B. van Kolck, K. Maslowska-Jarzyna, P. Papadopoulou, A. Kros, M.J. Chmielewski, Oxyanion Transport across Lipid Bilayers: Direct Measurements in Large and Giant Unilamellar Vesicles, Chemical Communications. 56 (2020) 4910-4913.

3. Z. Kokan, M.J. Chmielewski, A Photoswitchable Heteroditopic Ion-Pair Receptor, J. Am. Chem. Soc. 140 (2018) 16010-16014.

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5. A. Chołuj, N. Nikishkin, M.J. Chmielewski, Facile post-synthetic deamination of MOFs and the synthesis of the missing parent compound of the MIL-101 family, Chem. Commun. 53 (2017) 10196-10199.

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9. K.M. Bąk, M.J. Chmielewski, Sulfate templated assembly of neutral receptors in aqueous DMSO – orthogonal versus biplane structures, Chem. Commun. 50 (2014) 1305-1308.
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Laboratory of Technology of Organic Functional Materials

UNIVERSITY OF WARSAW

WCh Faculty of Chemistry University of Warsaw

Laboratory of Technology of Organic Functional Materials

HEAD:

Prof. Grzegorz Litwinienko*, PhD DSc

GROUP MEMBERS:

Andrzej Kaim, PhD DSc; Elżbieta Megiel, PhD DSc;
Katarzyna Jodko-Piórecka, PhD Eng;
Agnieszka Krogul-Sobczak, PhD;
Piotr Piotrowski, PhD;
Hanna Wilczura-Wachnik, PhD
MSc: Adam Myśliński
PhD students: Jakub Cędrowski, Adrian Konopko, Jarosław Kusio, Paweł Przybylski
Technical Staff: Artur Gajda

RESEARCH PROFILE:

- chemistry of radicals and antioxidants,
- thermal analysis,
- carbonylation processes catalysed by palladium compounds.
- nitroxide-stabilized metallic nanoparticles for biomedical applications
- bimetallic nanostructures as catalysts and active supports for organocatalysts
- preparation of smart polymeric materials using Controlled Radical Polymerization
- egzohedral functionalization of fullerenes using cycloaddition reactions
- synthesis of metal nanoparticles (Au, FexOy) with unique catalytic properties.

CURRENT RESEARCH ACTIVITIES:

Studies on the rate of initiation of lipid peroxidation. A knowledge about the initiation rate has a capital importance during the studies of mechanism and kinetics of autoxidation and autoxidation inhibited by antioxidants. The studies are performed in emulsions and suspensions of liposomes.

Antioxidant activity of polyphenols in homo- and heterogeneous systems. The aim of this thematic line of our research is to determine the impact of acid-base equilibria on the antioxidant activity of phenols, to obtain the structure-activity relationship for mono- and polyphenolic antioxidants.

*e-mail: litwin@chem.uw.edu.pl

Studies on the antioxidant activity of catecholamines. Neurodegenerative diseases, such as amyotrophic lateral sclerosis, Alzheimer's disease, and Parkinson's disease, are characterized by a progressive degeneration and death of neurons associated with the overproduction of the Reactive Oxygen Species (the oxidative stress). Our goal is to get insights into protecting activity of catecholamine neurotransmitters in lipid systems exposed to Reactive Oxygen Species.

Application of thermal analysis techniques for studies of lipid oxidation. In our research we compare the standard analytical techniques (like Rancimat) with the results obtained by using thermal analysis (Differential Scanning Calorimetry, DSC).

Studies on carbonylation processes catalysed by palladium compounds. Our studies are aimed at developing new, environmentally safe, selective and active catalysts for carbonylation of aromatic nitrocompounds and amines as alternative, waste- and fosgene-free method of production of aromatic isocyanates, carbamates, and ureas.

SELECTED PUBLICATIONS:

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2. A. Konopko, J. Kusio, G. Litwinienko, Antioxidant Activity of Metal Nanoparticles Coated with Tocopherol-Like Residues — The Importance of Studies in Homo- and Heterogeneous Systems, Antioxidants. 9 (2020) 5, doi:10.3390/antiox9010005
3. A. Lewińska, J. Adamczyk-Grochala, D. Błoniarz, J. Olszówka, M. Kulpa-Greszta, G. Litwinienko, A. Tomaszewska, M. Wnuk, R. Pązik, AMPK-mediated senolytic and senostatic activity of quercetin surface functionalized Fe_3O_4 nanoparticles during oxidant-induced senescence in human fibroblasts, Redox Biology. 28 (2020) 101337.
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5. A. Krogul-Sobczak, P. Kasperska, G. Litwinienko, N-heterocyclic monodentate ligands as stabilizing agents for catalytically active Pd-nanoparticles, Catalysis Communications. 104 (2018) 86-90.
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9. P. Piotrowski, P. Pawłowska, R. Bilewicz, A. Kaim, Selective and reversible self-assembly of C60 fullerene on a 9,10-bis(S-acetylthiomethyl) anthracene modified gold surface, RSC Advances. 6 (2016) 53101-53106.
10. M. Goździewska, G. Cichowicz, K. Markowska, K. Zawada, E. Megiel, Nitroxide-coated silver nanoparticles: synthesis, surface physicochemistry and antibacterial activity, RSC Advances. 5 (2015) 58403-58415.

Laboratory of Theory and Applications of Electrodes

UNIVERSITY OF WARSAW

WCh Faculty of Chemistry University of Warsaw

Laboratory of Bionanostructures

HEAD:

Prof. Renata Bilewicz*, PhD DSc

GROUP MEMBERS:

Agnieszka Więckowska, PhD DSc; Krzysztof Stolarczyk, PhD DSc; Ewa Nazaruk, PhD DSc; Dorota Matyszewska, PhD; Olga Święch, PhD; Dominika Majdecka, PhD
PhD students: Michał Kizling, Maciej Dzwonek, Agata Krzak, Monika Szlęzak, Valentina Grippo, Sylwia Dramińska, Aleksandra Buta, Adrianna Cytryniak

RESEARCH PROFILE:

Bioelectrochemistry, Bioinorganic Chemistry, Supramolecular Chemistry, Nanoparticles, Langmuir-Blodgett and self-assembled molecular films at solid-liquid and air-water interfaces.

CURRENT RESEARCH ACTIVITIES:

Lipidic cubic phase nanoparticles, gold and carbonaceous nanoparticles and macrocyclic compounds (e.g. cyclodextrins) as drug delivery systems, Interactions of drugs and drug carriers with model biomimetic membranes and cell membranes. Electron transfer mechanisms of redox enzymes and ion transport through integral proteins – ion pumps and channels immobilized in biomimetic molecular films.
We are searching for new drug carriers decreasing the toxic side effects of drugs by eliminating formation of reactive oxygen species responsible for cardiotoxicity of anthracycline drugs and by providing selective release of the drug in the pathological cells. We found that appropriately designed drug delivery systems e.g. modified lipid cubic mesophase nanoparticles and β-cyclodextrins (see figure above) containing an addressing unit and a pH-sensitive moiety allow to address the carrier to the cancer cell and release the drug through receptor endocytosis. We use liquid crystalline lipid cubic mesophase films also as the biomimetic matrices for the reconstitution of membrane proteins e.g. Na-K-ATPase or chloride channels and studies of their functions.

*e-mail: bilewicz@chem.uw.edu.pl

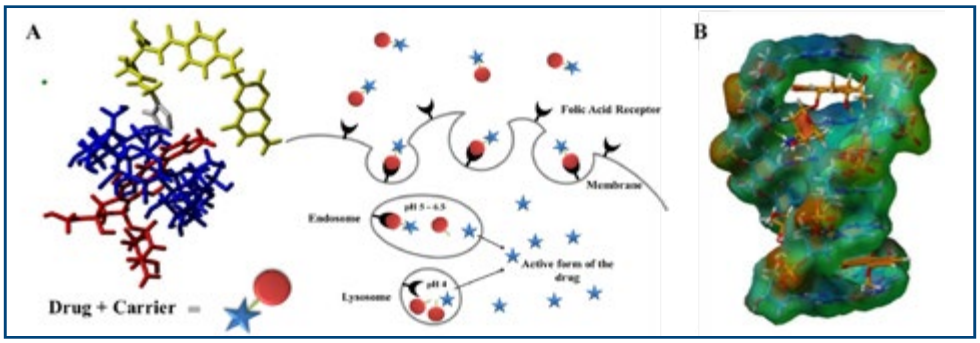

Fig. 1. Scheme showing the function of drug carrier.

We develop new methods of synthesis of metal nanoparticles, especially gold nanoparticles with sizes ranging from one to several hundred nanometers, stabilized physically or chemically by adsorbed compounds. These surface groups determine the properties of the nanoparticles leading to their various applications: in catalysis, sensors, electrode materials, and carriers.

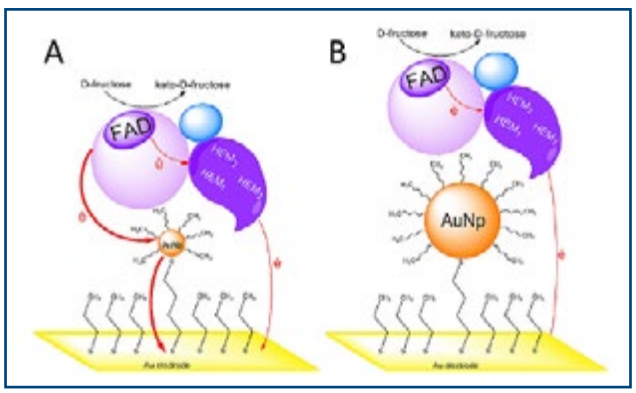

Fig.2. Scheme showing different electron transfer pathways between the electrode and the enzyme active sites in the presence of gold clusters (A) and gold nanoparticles (B).

Enzymes immobilized on the surface of metallic clusters retain their catalytic bioactivity in contrast to similar systems prepared on the metallic electrodes. In these systems, gold nanoparticles act not only as a matrix for immobilization of enzymes, but also provide electron transfer between the enzyme and the electrode, which means, that they may function as mediators, and the systems often do not require any external mediator.
Another topic explored in our group is supramolecular electrochemistry – e.g. electrochemical behaviour of intertwined structures as rotaxanes (see Figure 3) or catenanes. Electrochemical methods allow to trigger movement of one part of molecule versus the second one.

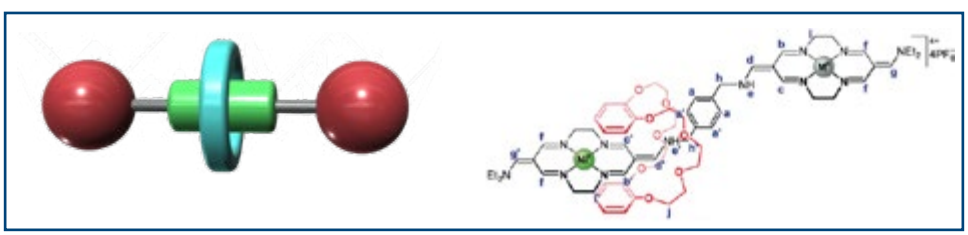

Fig.3. Scheme of rotaxane and chemical structure of exemplary rotaxane

SELECTED PUBLICATIONS:

1. M. Kizling, M. Dzwonek, A. Więckowska, R. Bilewicz, Size Does Matter? Mediation of Electron Transfer by Gold Clusters in Bioelectrocatalysis, ChemCatChem. 10(9) (2018) 1988-1992.
2. K.M. Tomczyk, M. Woźny, S. Domagała, A. Więckowska, J. Pawłowska, K. Woźniak, B. Korybut-Daszkiewicz, Rotaxanes composed of dibenzo-24-crown-8 and macrocyclic transition metal complexing tetraimine units, New J.Chem. 41 (2017) 6004-6013.
3. M. Kizling, M. Dzwonek, B. Olszewski, P. Bącal, Ł. Tymecki, A. Więckowska, K. Stolarczyk, R. Bilewicz, Reticulated vitreous carbon as a scaffold for enzymatic fuel cel designing, Biosensors and Bioelectronics. 95 (2017) 1-7.
4. A. Więckowska, M. Dzwonek, Ultrasmall Au nanoparticles coated with hexanethiol and anthraquinone/hexanethiol for enzyme-catalyzed oxygen reduction, Sensors and Actuators B. 224 (2016) 514-520.
5. D. Matyszewska, R. Bilewicz, F.S. Zhang, F. Abbasi, J.J. Leitch, J. Lipkowski, PM-IRRAS Studies of DMPC Bilayers Supported on Au(111) Electrodes Modified with Hydrophilic Monolayers of Thioglucose, Langmuir. 32 (2016) 1791–1798.
6. O. Święch, M. Majdecki, A. Dębiński, A. Krzak, R. Bilewicz, Competition between self-inclusion and drug binding explains the pH dependence of the cyclodextrin drug carrier – molecular modelling and electrochemistry studies, Nanoscale. 8 (2016) 16733–16742.
7. E. Jabłonowska, E. Nazaruk, D. Matyszewska, Ch. Speziale, R. Mezzenga , E.M. Landau, R. Bilewicz, Interactions of lipidic cubic phase nanoparticles with lipid membranes, Langmuir. 32 (2016) 9640–9648.
8. E. Nazaruk, M. Szlęzak, E. Górecka, R. Bilewicz, Y. Osornio, P. Uebelhart, E.M. Landau, Design and Assembly of pH-Sensitive Lipidic Cubic Phase Matrices for Drug Release, Langmuir. 30 (2014) 1383-1390.
9. K. Stolarczyk, D. Lyp, K. Żelechowska, J.F. Biernat, J. Rogalski, R. Bilewicz, Arylated Carbon Nanotubes for Biobatteries and Biofuel Cells, Electrochim Acta. 79 (2012) 74-81.
10. B. Korybut-Daszkiewicz, R. Bilewicz, K. Woźniak, Tetraimine macrocyclic transition metal complexes as building blocks for molecular devices, Coord. Chem. Rev. 254 (2010) 1637-1658.

Environmentally Sensitive Polymer Materials and Composites

HEAD:

Marcin Karbarz*, PhD DSc

GROUP MEMBERS:

prof. Zbigniew Stojek, PhD DSc;
Klaudia Kaniewska, PhD; Marcin Maćkiewicz, PhD
PhD students: Kamil Marcisz, Ewelina Wałęka
MSc students: Kinga Drabczyńska,
Jakub Nowakowski, Aneta Rzepniewska

RESEARCH PROFILE:

The main trend of research carried out in the group is to obtain new, structurally advanced and multi-functional polymeric materials.

CURRENT RESEARCH ACTIVITIES:

The research aims at modifying the polymer gels to give them the desired properties. We want them to undergo the phenomenon of volume phase transition under given conditions *(Fig. 1)*, to degrade as external conditions change appropriately and in the presence of specific substances, to become sensitive to new environmental factors, to self- assemble and be capable of self-healing *(Fig. 2)*. We use them also as drug carriers enabling controlled release of active substances *(Fig. 3)*. It is important to obtain these gels in micro- and nano-size in order to reduce phase transition times as much as possible and to achieve a rapid balance with the environment, and to use them in biology and medicine. Thin gel membranes will also be produced on conductive surfaces as the starting substrates for the construction of advanced bioanalytical sensors.

***e-mail:** karbarz@chem.uw.edu.pl

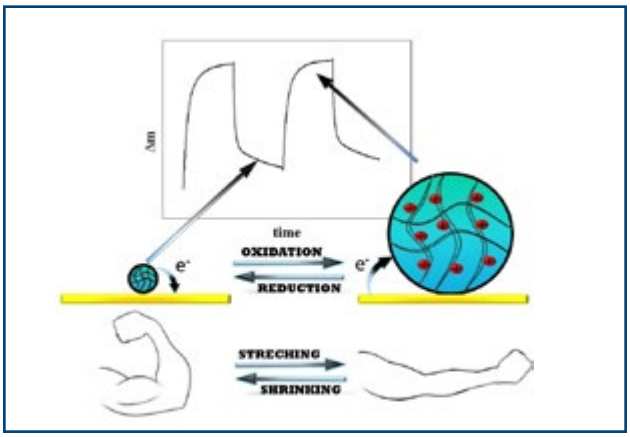

Fig. 1. Potential-triggered microgel volume phase transition, that can mimic muscle activity (monitored with quartz crystal microbalance QCM).

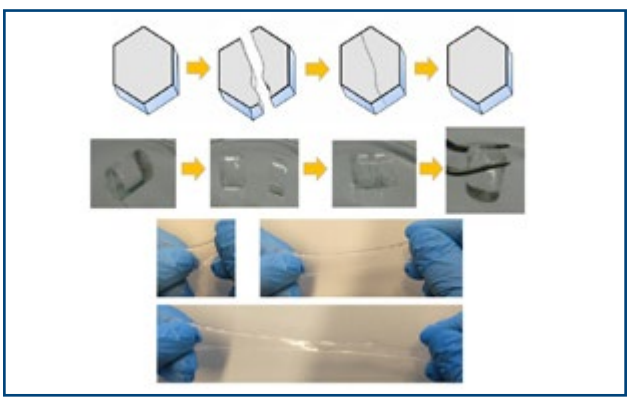

Fig. 2. Scheme and photos of self-healing process of hydrogel material and photos of hydrogels during elongation tests.

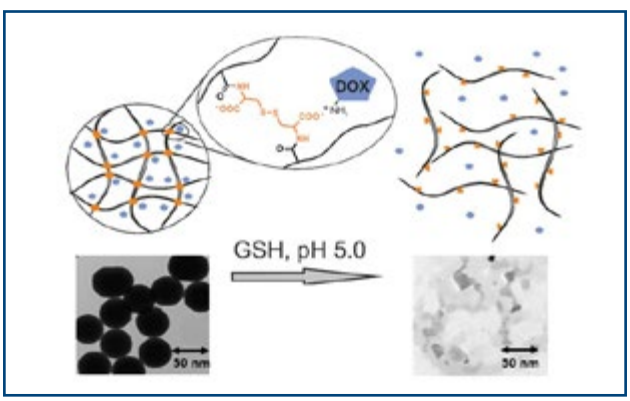

Fig. 3. Degradable micro and nano-gels crosslinked with cystin-derivative as systems for delivery and controlled release of active substances in cancer cells.

SELECTED PUBLICATIONS:

1. K. Marcisz, A. Gawrońska, Z. Stojek, M. Karbarz, Triggering the Shrinking/Swelling Process in Thin Gel Layers on Conducting Surfaces by Applying an Appropriate Potential, ACS Applied Materials and Interfaces. 11 (2019) 12120.
2. K. Marcisz, M. Maćkiewicz, J. Romański, Z. Stojek, M. Karbarz, Significant, reversible change in microgel size using electrochemically induced volume phase transition, Applied Materials Today. 13 (2018) 182.
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4. M. Maćkiewicz, K. Marcisz, M. Strawski, J. Romański, Z. Stojek, M. Karbarz, Modification of gold electrode with a monolayer of self-assembled microgels, Electrochimica Acta. 268 (2018) 531.
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7. M. Karbarz, J. Romański, Dual Sensing by Simple Heteroditopic Salt Receptors Containing an Anthraquinone Unit, Inorganic Chemistry. 55 (2016) 3616.
8. M. Maćkiewicz, K. Kaniewska, J. Romański, E. Augustin, Z. Stojek, M. Karbarz, Stable and degradable microgels linked with cystine for storing and environmentally triggered release of drugs, Journal of Materials Chemistry B. 3 (2015) 7262.
9. K. Kaniewska, M. Karbarz, Z. Stojek, Electrochemical attachment of thermo- and pH sensitive interpenetrating-polymers-network hydrogel to conducting surface, Electrochimica Acta. 179 (2015) 372.
10. M. Maćkiewicz, T. Rapecki, Z. Stojek, M. Karbarz, Environmentally sensitive, quickly responding microgels with lattice channels filled with polyaniline, Journal of Materials Chemistry B. 2 (2014) 1483.

Greenmet Lab

HEAD:

Wojciech Hyk*, PhD DSc

GROUP MEMBERS:

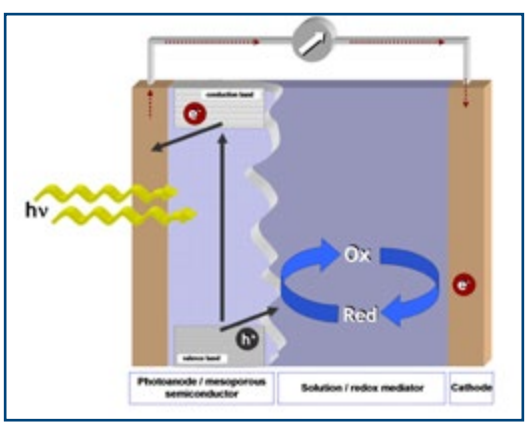
PhD student: Konrad Kitka
MSc students: Magdalena Dziarmaga, Łukasz Kot, Magdalena Radziewicz

RESEARCH PROFILE:

Modelling of mass transport to ultrasmall electrodes: theoretical, environmental and metrological aspects

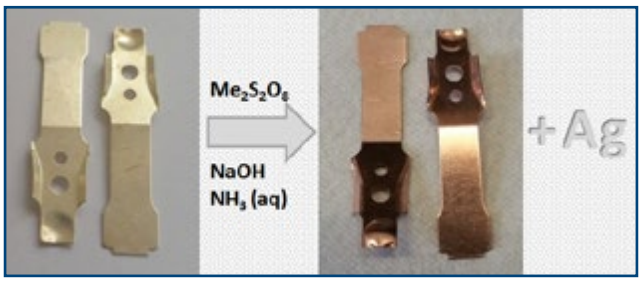
CURRENT RESEARCH ACTIVITIES:

The research activities of our group can be divided into three research areas:



I. Electroanalytical modelling of newly designed redox systems using macroelectrodes, microelectrodes and nanoelectrodes (for extremely small volume samples including intracellular measurements). We develop the procedures for reproducible fabrication of nanoelectrodes and theoretical models of the mass transport to bare and modified electrodes under the diffusion, migration and convection conditions.

*e-mail: wojhyk@chem.uw.edu.pl



II. Green chemistry for environmental protection. This research area has a strictly application character and the proposed solutions are focused on recovery of metals from electronic and technological waste materials. The innovativeness of the proposed methods is expressed by their selective action on a selected metal (targeted recycling), simplicity of operation and environmental friendliness (lack of toxic by-products, ease of regeneration of key reagents). To achieve the assumed indicators, we design and synthesize new inorganic compounds and composite materials, e.g. new persulfate systems and ferro-gel materials, i.e. gel materials sensitive to changes in the external magnetic field.

III. Metrological aspects of analytical methodologies. The employment of fast and reliable methods for multi-element chemical analyses requires the development of detailed quality control systems. We develop new statistical strategies (tools) for data treatment in chemical analysis. These include: quantifying standard uncertainty of the measurands expressed by implicit functions, analyte quantification using the method of serial dilutions and construction of an expert system for quality control assurance in research laboratories. The newly developed tools are incorporated in the e-stat service for on-line statistical analysis in research laboratories (www.e-stat.pl).

SELECTED PUBLICATIONS:

1. W. Hyk, K. Kitka, Water purification using sponge like behaviour of poly (N-isopropylacrylamide) ferrogels. Studies on silver removal from water samples, Journal of Environmental Chemical Engineering. 6 (2018) 6108-6117.
2. W. Hyk, K. Kitka, Highly efficient and selective leaching of silver from electronic scrap in the base-activated persulfate – ammonia system, Waste Management. 60 (2017) 601-608.
3. K. Kaniewska, M. Karbarz, Z. Stojek, W. Hyk, Mass transport affected by electrostatic barrier in ionized gel layers attached to microelectrode surface, Electrochemistry Communications. 81 (2017) 24-28.
4. K. Kaniewska, M. Karbarz, K. Ziach, A. Siennicka, Z. Stojek, W. Hyk, Electrochemical examination of the structure of thin hydrogel layers anchored to regular and microelectrode surfaces, J. Phys. Chem. B. 120 (2016) 9540–9547.
5. W. Hyk, Z. Stojek, Quantifying Uncertainty of Determination by Standard Additions and Serial Dilutions Methods Taking into Account Standard Uncertainties in Both Axes, Anal. Chem. 85 (2013) 5933–5939.
6. W. Hyk, D. Święcicka, S. Garboś, Application of Mixed (Bimodal) Distribution to Human Health Risk Assessment of Cu and Ni in Drinking Water Collected by RDT Sampling Method from a Large Water Supply Zone, Microchemical Journal. 110 (2013) 465-472.
7. W. Hyk, Z. Stojek, Thin and Ultra-Thin Layer Dual Electrode Electrochemistry: Theory of Steady-State Voltammetry without Supporting Electrolyte, Electrochemistry Communications. 34 (2013) 192-195.
8. W. Hyk, Z. Stojek, "Microelectrodes for Electroanalytical Chemistry" in Encyclopedia of Analytical Chemistry, R.A. Meyers (Ed.), John Wiley & Sons Ltd., Chichester, S1-S3 (2010) 1115-1134.

Laboratory of Surface Science

HEAD:

Prof. Sławomir Sęk*, PhD DSc

GROUP MEMBERS:

Joanna Juhaniewicz-Dębińska, PhD;
Jan Pawłowski, PhD
PhD students: Damian Dziubak,
Dorota Konarzewska

RESEARCH PROFILE:

adsorption at solid-liquid interfaces; biomimetic membranes; long-range electron transport.

CURRENT RESEARCH ACTIVITIES:

Scientific interests of our research group are related to adsorption phenomena and self-assembly of organic molecules at solid-liquid interfaces. Currently, our research team is involved in the design of advanced biomimetic lipid bilayers based on the concepts of „polymer cushioned membrane", „tethered membrane" and „floating membrane". The key feature of these systems is an aqueous reservoir between a lipid bilayer and solid surface. It is meant to provide sufficient hydration of lipid polar heads and it enables insertion of transmembrane proteins/ion channels. Apart from quite obvious implications for medicine, the importance of artificial membranes with embedded functional channels also stems from their potential applications in biosensors and bioelectronics devices.

Other research activities of our group are related to peptide-mediated electron transport phenomena. In particular, we strive to reveal how the efficiency of electron transport is affected by the conductance of individual amino acids and the higher-order structures adopted by peptide molecules. Another important issue is to evaluate whether it is possible to modulate peptide conductance through conformational structural changes triggered either by physical or chemical stimuli including external electric field, nanomechanical modulation or variation of pH value. This would enable construction of a molecular switch with two conductance values depending on the instantaneous secondary structure of the system.

*e-mail: slasek@chem.uw.edu.pl

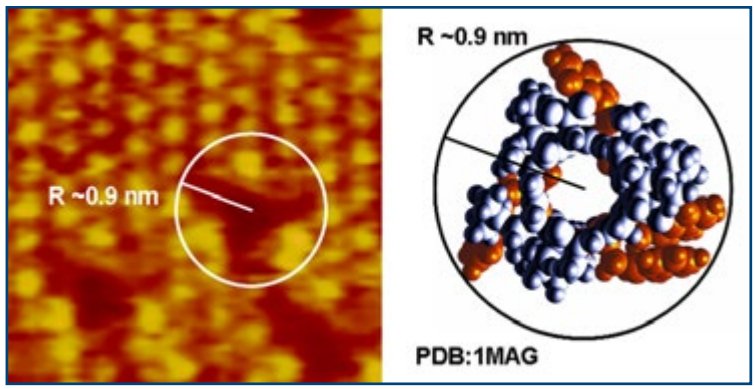


Fig. 1 High resolution image of the ion channel of gramicidin D embedded into the lipid membrane supported on gold surface. Adapted with permission from Sek et al. Journal of the American Chemical Society, 131 (2009) 6439–6444. Copyright (2009) American Chemical Society.

SELECTED PUBLICATIONS:

1. J. Juhaniewicz-Dębińska, D. Tymecka, S. Sęk, Diverse effect of cationic lipopeptide on negatively charged and neutral lipid bilayers supported on gold electrodes, Electrochimica Acta. 298 (2019) 735-744.
2. K. Pułka-Ziach, A.K. Puszko, J. Juhaniewicz-Dębińska, S. Sęk, Electron Transport and a Rectifying Effect of Oligourea Foldamer Films Entrapped within Nanoscale Junctions, Journal of Physical Chemistry C. 123 (2019) 1136–1141.
3. J. Pawłowski, J. Juhaniewicz, A. Guzeloglu, S. Sęk, Mechanism of Lipid Vesicles Spreading and Bilayer Formation on a Au(111) Surface, Langmuir. 31 (2015) 11012–11019.
4. J. Juhaniewicz, S. Sęk, Atomic Force Microscopy and Electrochemical Studies of Melittin Action on Lipid Bilayers Supported on Gold Electrodes, Electrochimica Acta. 162 (2015) 53-61.
5. J. Pawłowski, J. Juhaniewicz, D. Tymecka, S. Sęk, Electron Transfer Across α-Helical Peptide Monolayers: Importance of Interchain Coupling, Langmuir. 28 (2012) 17287–17294.

Modern Nano- and Bioelectroanalysis

HEAD:

Anna M. Nowicka*, PhD DSc

GROUP MEMBERS:

Agata Kowalczyk, PhD; Edyta Matysiak-Brynda, PhD
PhD students: Patrycja Kowalik, Monika Nisiewicz, Jakub P. Sęk

RESEARCH PROFILE:

Nanomaterials, biomaterials, bioelectrochemistry, biosensors, medical diagnostic, drug carrier systems, targeted therapy

CURRENT RESEARCH ACTIVITIES:

Our scientific activity is focused on the preparation and characterisation of nanomaterial-based assemblies on electrodes that would effectively bind biological materials with the electrode surface, in appropriate orientation and conformation (see Figure 1), and allow the rapid transformation of chemical signals into electrical signal, which are directed to eventual application in catalysis, biofuel cells or as a biomolecular electrochemical devices.

We also focus on modern nano-electrochemistry of DNA and immuno-electrosensors used in POC diagnostics and modern nanomedicine. The developed by us modern electrochemical bioassays are mainly based on the antigen-antibody specific interactions, aptamer-protein interactions or hybridization processes between two complementary DNA fragments. To enhance the sensitivity of such novel devices, different nanomaterials including quantum dots, metal nanoparticles, dendrimers, polymer-metal nanoparticle composites, carbon-based nanomaterials are applied as a new

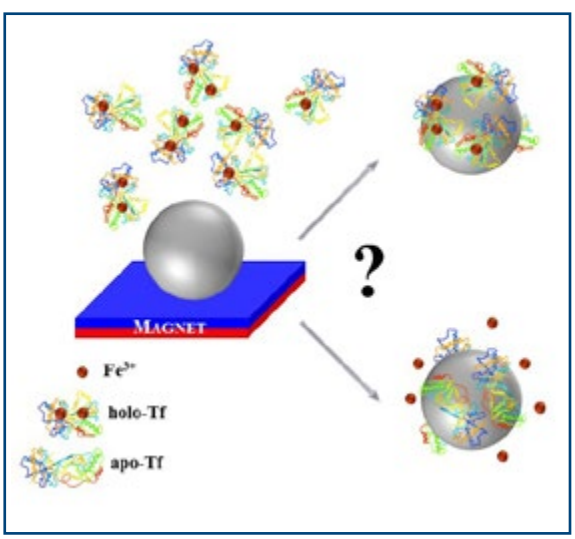


Fig. 1. Consequences of protein interaction with magnetic nanoparticles.

*e-mail: anowicka@chem.uw.edu.pl

carriers for immobilization of biomolecules or targeted signal molecules (see Figure 2).
One of the major challenges of medicine is effectively combating diseases of civilization. Despite the enormous technological and scientific progress, effective methods to combat cancer are still scarce and limited to particular forms of this disease. The difficulty issue of cancer treatment consists of a number of factors, however the biggest problem is the cytotoxic activity of the drug against both tumor and healthy cells. This fact is the main driving force of research aimed at reducing / elimination the cytotoxic activity of the anticancer drugs toward the healthy cells. One way to limit the negative effects of anti-tumor drugs on healthy cells is targeted therapy employing functionalized drug carriers. We also carry out research in the field of searching for and designing new drugs / drug carriers that will allow the active substance to be transported in a suitable concentration and time to the desired place (e.g. tumor tissue). Among our interests are multitarget drugs (MTD), which act simultaneously on more than one molecular target.

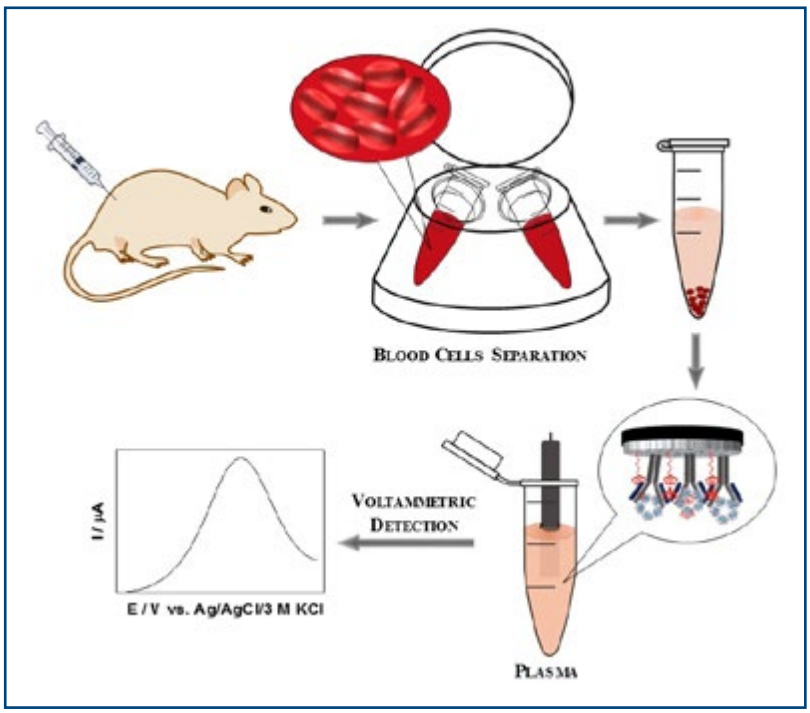


Fig. 2. Immunosensor for C-reactive protein detection

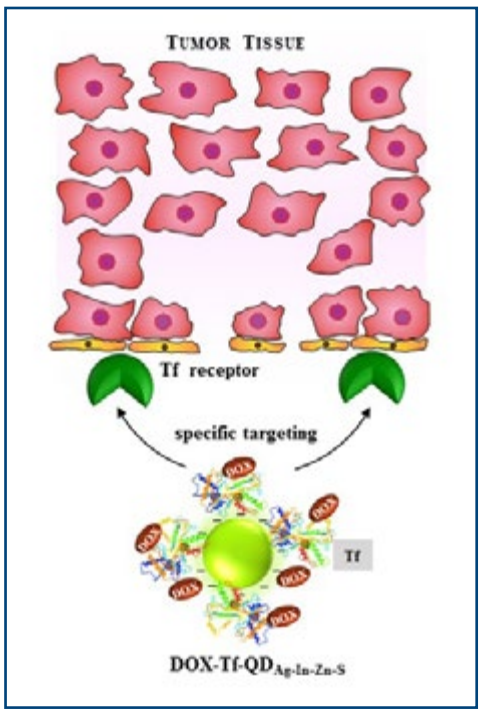


Fig. 3. Drug delivery system.

SELECTED PUBLICATIONS:

1. J. Pilch, E. Matysiak-Brynda A. Kowalczyk, P. Bujak, Z. Mazerska, A.M. Nowicka, E. Augustin, New unsymmetrical bisacridine derivatives noncovalently attached to quaternary quantum dots improve cancer therapy by enhancing cytotoxicity towards cancer cells and protecting normal cells, ACS Appl. Mater. Inter. 12 (2020) 17276-17289.
2. W. Kiciński, J.P. Sęk , E. Matysiak-Brynda, K. Miecznikowski, M. Donten, B. Budner, A.M. Nowicka, Enhancement of PGM-free oxygen reduction electrocatalyst performance for conventional and enzymatic fuel cells: the influence of an external magnetic field, Appl. Catal. B-Environ. 258 (2019) 117955.
3. J.P. Sęk, A. Kasprzak, M. Bystrzejewski, M. Popławska, W. Kaszuwara, Z. Stojek, A.M. Nowicka, Nanoconjugates of ferrocene and carbon-encapsulated iron nanoparticles as sensing platforms for voltammetric determination of ceruloplasmin in blood, Biosens. Bioelectron. 102 (2018) 490-496.
4. E. Matysiak-Brynda, P. Bujak, E. Augustin, A. Kowalczyk, Z. Mazerska, A. Proń, A.M. Nowicka, Stable nanoconjugate of transferrin with alloyed quaternary nanocrystals Ag-In-Zn-S as biological entity for tumor recognition, Nanoscale. 10 (2018) 1286-1296.
5. A. Kowalczyk, J.P. Sęk, A. Kasprzak, M. Popławska, I.P. Grudziński, A.M. Nowicka, Occlusion phenomenon of redox probe by protein as a way of voltammetric detection of non-electroactive C-reactive protein, Biosens. Bioelectron. 117 (2018) 232-239.
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8. A.M. Nowicka, A. Kowalczyk, A. Jarzębińska, M. Donten, P. Krysiński, Z. Stojek, E. Augustin, Z. Mazerska, Progress in targeting tumor cell by using drug-magnetic nanoparticles conjugate, Biomacromolecules. 14 (2013) 828-833.
9. A. Kowalczyk, A.M. Nowicka, R. Jurczakowski, M. Fau, A. Królikowska, Z. Stojek, Construction of DNA biosensor at glassy carbon surface modified with 4-aminoethyl-benzenediazonium salt, Biosens. Bioelectron. 26 (2011) 2506-2512.
10. A.M. Nowicka, U. Hasse, M. Hermes, F. Scholz, Hydroxyl radicals attack metallic gold, Angew. Chem. Int. Edit. 49 (2010) 1061-1063.

Laboratory of Theory of Biopolymers

UNIVERSITY OF WARSAW

WCh Faculty of Chemistry University of Warsaw

Andrzej Koliński's Research Group

HEAD:

Prof. Andrzej Koliński*, PhD DSc

GROUP MEMBERS:

Dominik Gront, PhD DSc; Sebastian Kmiecik, PhD DSc; Maciej Błaszczyk, PhD; Maksim Kouza, PhD; Mateusz Kurciński, PhD

RESEARCH PROFILE:

Theoretical Chemistry. Theory of polymers and biopolymers. Theoretical structural biology. Theory of protein folding. Theory of protein structure and function. Computer simulations of complex biopolymer systems. Structural bioinformatics. Computational biology. Molecular docking in drug design.

CURRENT RESEARCH ACTIVITIES:

Our research areas include:

- coarse-grained modeling and multiscale modeling of proteins and their complexes
- prediction of protein structure: from comparative modeling to de novo folding
- simulations of protein dynamics
- prediction of protein interactions/ molecular docking
- bioinformatics and biological statistics
- computer aided drug design/ structure-based drug design
- modeling and predicting of biomacromolecular interactions: prediction of protein function
- development of software for molecular modeling and computational analysis of experimental data on biomacromolecules

*e-mail: kolinski@chem.uw.edu.pl

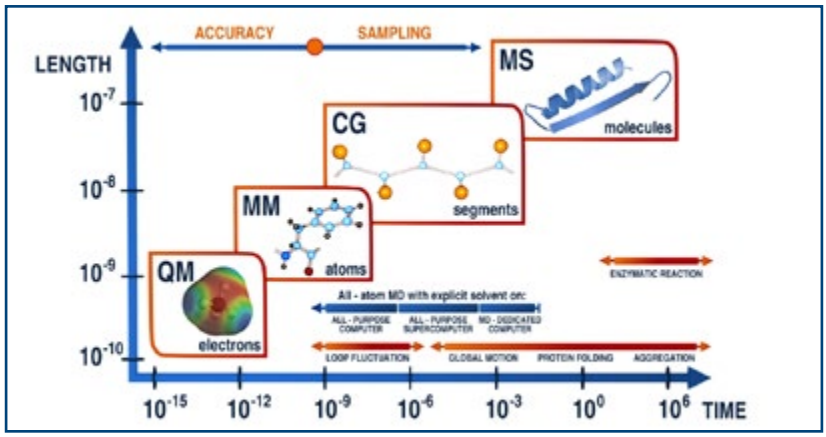

Fig. 1. Application ranges for molecular modeling at different resolutions: quantum, all-atom, coarse-grained, and mesoscale. The plot shows approximate ranges of time scales and system sizes (lengths). The presented application ranges can be expanded by merging tools of different resolution into multiscale schemes.

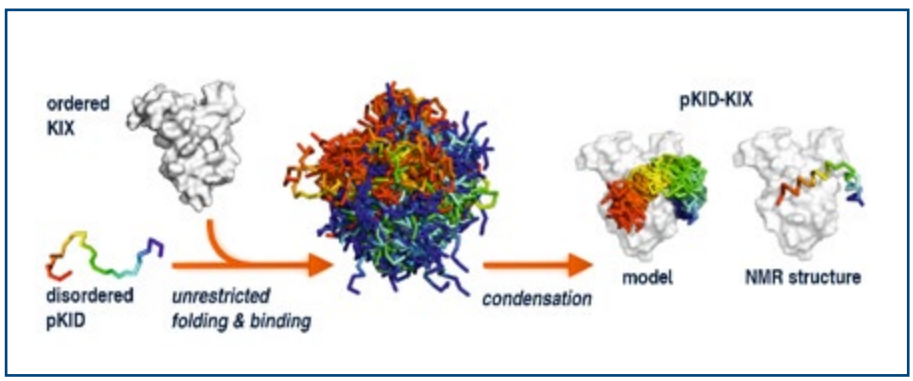

Fig. 2. Mechanism of coupled folding and binding of the pKID/KIX complex as revealed by coarse-grained modeling. Docking simulations allowed full flexibility of the disordered pKID during a blind search for the binding site onto the KIX surface. During docking, the movement of the KIX backbone was limited to near-native fluctuations.

SELECTED PUBLICATIONS:

1. M.P. Ciemny, M. Kurciński, K. Kamel, A. Koliński, N. Alam, O. Schueler-Furman, S. Kmiecik, Protein-peptide docking: opportunities and challenges, Drug Discovery Today. 23(3) (2018) 1530-37.
2. A.E. Dawid, D. Gront, A. Koliński, Coarse-grained modeling of the interplay between secondary structure propensities and protein fold assembly, J. Chem. Theory Comp. 14(4) (2018) 2277-2278.
3. A.E. Dawid, D. Gront, A. Koliński, SURPASS low–resolution coarse–grained protein modeling, J. Chem. Theory Comp. 13(11) (2017) 5766–5779.
4. S. Kmiecik, D. Gront, M. Koliński, L. Wieteska, A. Dawid, A. Koliński, Coarse-grained protein models and their applications, Chemical Reviews. 116(14) (2016) 7898–7936.
5. M.P. Ciemny, A. Dębiński, M. Paczkowska, A. Koliński, M. Kurciński, S. Kmiecik, Protein-peptide molecular docking with large-scale conformational changes: the p53-MDM2 interaction, Scientific Reports – Nature. 6 (2016) 37532.
6. M. Błaszczyk, M. Kurciński, M. Kouza, L. Wieteska, A. Dębiński, A. Koliński, S. Kmiecik, Modeling of protein-peptide interactions using the CABS-dock web server for binding site search and flexible docking, Methods. 93 (2016) 72-83.
7. M. Kurciński, M. Jamróz, M. Błaszczyk, A. Koliński, S. Kmiecik, CABS-dock: web server for flexible docking of peptides to proteins without prior knowledge of the binding site, Nucleic Acids Research. 43(W1) (2015) W419-W424.

Modeling of Cellular Processes

HEAD:

Dorota Latek*, PhD DSc

GROUP MEMBERS:

PhD student: Mikołaj Mizera (Assistant promoter, UMP)
MSc student: Szymon Wiśniewski
Former group members: Krystiana Krzyśko (FUW), Szymon Niewieczerzał (CeNT), Paweł Pasznik, Ewelina Rutkowska (Selvita), Maria Turant

RESEARCH PROFILE:

G protein-coupled receptors (structure prediction, drug design, signal transduction), Solute Carrier Transporters, web applications for computational biology & drug discovery, molecular dynamics simulations of cellular processes

CURRENT RESEARCH ACTIVITIES:

We are focused on transmembrane proteins involved in cell signaling and transportation. Our aim is to characterize them in two major aspects: structure and mechanism of action and as a consequence, we strive for drug discovery.
Main research areas include:

- drug design based on off-target interactions /virtual screening/
- mechanisms of GPCR activation /molecular switches/
- SLC transport cycle /toxins & drug metabolites efflux/
- structure modeling of GPCRs using multiple templates approach and sequence profiles comparison / GPCRM/
- drug design targeting GPCRs from class A and B using flexible-receptor Boost-implementing software /GUT-DOCK/
- NMR methods for biological systems /CABS-NMR, INPHARMA/

*e-mail: dlatek@chem.uw.edu.pl

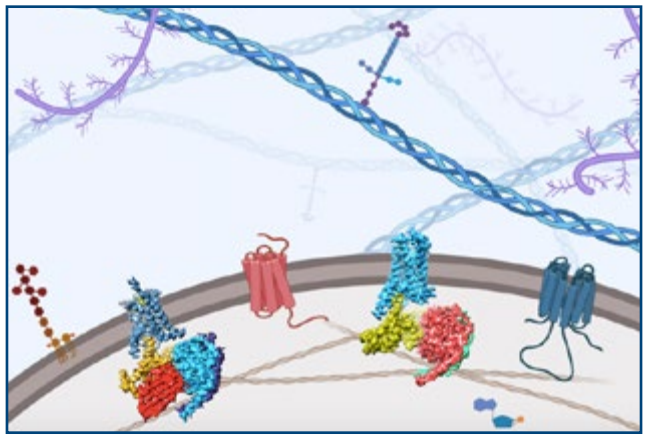

Fig. 1. Extracellular matrix with G protein-coupled receptors located in the cellular membrane. For more information, please visit: http://dlatek.chem.uw.edu.pl/. This figure has been prepared with BioRender (https://biorender.com/).

SELECTED PUBLICATIONS:

1. P. Pasznik, E. Rutkowska, S. Niewieczerzał, J. Cielecka-Piontek, D. Latek, Potential off-target effects of beta-blockers on gut hormone receptors: In silico study including GUT-DOCK—A web service for small-molecule docking, PLOS ONE. 14(1) (2019).
2. D. Latek, E. Rutkowska, S. Niewieczerzal, J. Cielecka-Piontek, Drug-induced diabetes type 2: In silico study involving class B GPCRs, PLOS ONE. 14(1) (2019).
3. D. Latek, I. Langer, K.A. Krzyśko, L. Charzewski, A Molecular Dynamics Study of Vasoactive Intestinal Peptide Receptor 1 and the Basis of Its Therapeutic Antagonism, Int J Mol Sci. 20(18) (2019) 4348.
4. D. Latek, P. Pasznik, T. Carlomagno, S. Filipek, Towards improved quality of GPCR models by usage of multiple templates and profile-profile comparison, PLOS ONE. 8(2) (2013).
5. D. Latek, M. Bajda, S. Filipek, A hybrid approach to structure and function modeling of G protein-coupled receptors, J Chem Inf Model. 56(4) (2016) 630-641.
6. P. Miszta, P. Pasznik, J. Jakowiecki, A. Sztyler, D. Latek, S. Filipek, GPCRM: a homology modeling web service with triple membrane-fitted quality assessment of GPCR models, NAR. 46(W1) (2018) W387–W395.
7. D. Latek, Rosetta Broker for membrane protein structure prediction: concentrative nucleoside transporter 3 and corticotropin-releasing factor receptor 1 test cases, BMC Struct Biol. 17(1) (2017) 8.
8. B. Trzaskowski, D. Latek, S. Yuan, U. Ghoshdastider, A. Dębiński, S. Filipek, Action of molecular switches in GPCRs-theoretical and experimental studies, Curr Med Chem. 19(8) (2012) 1090-1109.
9. S. Yuan, R. Wu, D. Latek, B. Trzaskowski, S. Filipek, Lipid receptor S1P1 activation scheme concluded from microsecond all-atom molecular dynamics simulations, PLOS Comp Biol. 9(10) (2013).
10. L. Skjærven, L. Codutti, A. Angelini, M. Grimaldi, D. Latek, P. Monecke, M.K. Dreyer, T. Carlomagno, Accounting for conformational variability in protein–ligand docking with NMR-guided rescoring, JACS. 135(15) (2013) 5819-5827.

Polymer Group

HEAD:

Andrzej Sikorski*, PhD DSc

GROUP MEMBERS:

PhD student: Aleksander Kuriata

RESEARCH PROFILE:

physicochemical properties of polymer and biopolymer systems

CURRENT RESEARCH ACTIVITIES:

- Transport in crowded environments: models of motion in biomembranes and in random media
- Structure of branched polymers and highly branched polymers, dendrimers as drug carriers
- Structure and dynamics of polymer systems in confined geometries
- Percolation of polymer systems: the structure of polymer melts and composites, models of plastic electronics
- Simulation tools used: Cooperative Motion Algorithm Dynamic Lattice Liquid, Random Sequential Adsorption

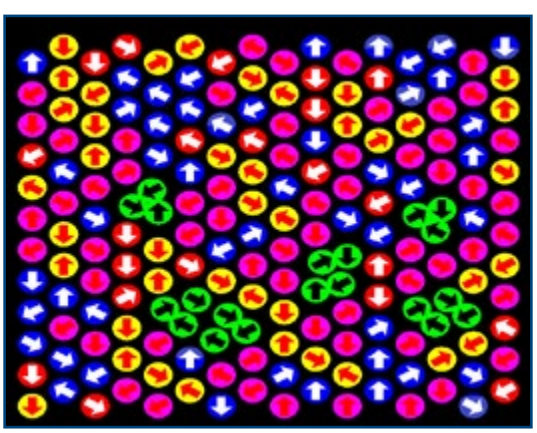

Fig. The idea of the DLL algorithm

*e-mail: sikorski@chem.uw.edu.pl

SELECTED PUBLICATIONS:

1. P. Polanowski, A. Sikorski, Diffusion of Small Particles in Polymer Films, J. Chem Phys. 147 (2017) 014902.
2. P. Polanowski, A. Sikorski, Simulation of Molecular Transport in Systems Containing Mobile Obstacles, J. Phys. Chem. B. 120 (2016) 7529-7537.
3. P. Polanowski, A. Sikorski, Simulation of Diffusion in a Crowded Environment, Soft Matter. 10 (2014) 3597-3607.
4. E. Wawrzyńska, S. Eisenhaber, P. Parzuchowski, A. Sikorski, G. Zifferer, Simulation of Hyperbranched Polymers. 1. Properties of Regular Three Generation Dendrimers, Macromol, Theory Simul. 23 (2014) 288-299.
5. P. Polanowski, J.K. Jeszka, A. Sikorski, Dynamic Properties of Linear and Cyclic Chains in Two Dimensions. Computer Simulation Studies, Macromolecules. 47 (2014) 4830-4839.

Quantum Chemistry Laboratory

UNIVERSITY OF WARSAW

WCh Faculty of Chemistry University of Warsaw

Electronic structure theory for high-precision spectroscopy, collisions, and attosecond processes

HEAD:

Prof. Robert Moszyński*, PhD DSc

GROUP MEMBERS:

Piotr Gniewek, PhD; Małgorzata Jeziorska, PhD; Michał Lesiuk, PhD; Aleksandra Tucholska, PhD
PhD students: Justyna Balcerzak, Tomasz Grining, Iwona Majewska, Aleksander Woźniak
MSc student: Mateusz Szczygieł

RESEARCH PROFILE:

Development of new tools of the electronic structure theory for an accurate description of high-resolution spectroscopic and collisional processes occurring in the ultracold regime, and also for the description of time-resolved electronic dynamics in the attosecond scale.

CURRENT RESEARCH ACTIVITIES:

New tools of the electronic structure theory for molecules in the ultracold regime

Molecules cooled to temperatures below T = 10^{-3} K allow for tackling questions touching upon the very fundamentals of quantum mechanics. They are promising candidates in novel applications, ranging from ultracold chemistry and precision measurements to quantum computing. Cold and ultracold molecules are thus opening up new and exciting areas of research in chemistry and physics due to their manifestly quantum nature. Understandably, to describe the processes occurring in the ultracold regime new tools of the electronic structure theory must be developed. In the course of the this research task we seek to:

- develop explicitly correlated coupled cluster methods for the ground state and the corresponding properties (dipole moments, electronic densities, etc.);
- apply Slater-type orbitals as a one-electron basis set and the explicitly correlated Kołos-Wolniewicz functions in the calculations for diatomic molecules;
- develop explicitly correlated electronic structure methods for excited states;
- generalise the expectation value formalism of the coupled cluster theory for the calculation of the coupled cluster linear and quadratic response functions at the explicitly correlated level;
- calculate coupling matrix elements (e.g., spin-orbit, nonadiabatic) between arbitrary excited states, as well as the transition moments and related quantities, based on the aforementioned newly developed methods;
- apply these newly developed methods to interpret current experiments in the ultracold regime.

*e-mail: rmoszyns@chem.uw.edu.pl

New tools of the electronic structure theory for molecules in the attosecond laser fields

Attoscience is a rapidly developing area of research with unparalleled application possibilities in fields of broadly understood chemistry, biology and physics. It focuses on processes occurring in extremely short timescale (1 as = 10^{-18} s) which allows for a direct study of the dynamics of electrons within atoms or molecules. Most of the attosecond processes involve irradiation of the sample (single atom, molecule, solid sample, gas sample etc.) with short but strong infrared impulses. This produces a variety of sample's responses, such as: (i) generation of high-order harmonics (HHG) by sample molecules, (ii) above-threshold ionization (ATI), accompanied by release of high-energetic free electrons, (iii) generation of multiply charged atomic and molecular ions, detection and analysis of which may be of value
in understanding the processes occurring within the electronic structure of molecules. However, without sufficiently developed theoretical description of attosecond processes these experiments may not fulfill their intended purposes. We are planning to create a range of advanced quantum chemistry methods for analysis and interpretation of gathered experimental data. These methods will be based on:

- numerical solutions of the time-dependent Schrödinger equation (TDSE) and it's non-linear version (TDNS) for one-dimensional atoms with one or two electrons, three-dimensional atoms with one or two electrons and one-dimensional molecules with one electron,
- the strong-field approximation (SFA) for one-dimensional atoms with one or two electrons, three-dimensional atoms with one or two electrons and one-dimensional molecules with one electron,
- classical Wigner methods for atoms, molecules and many-electron clusters,
- real-time time-dependent coupled cluster (TDCC) theory and density functional theory (TDDFT), which allow to obtain explicitly the time-dependent wavefuction and electron density for the many-electron systems;
- application of the electronic structure tools developed in our group for the time-independent case to an accurate description of time-dependent processes in the attosecond time scale.

SELECTED PUBLICATIONS:

1. M. McDonald, I. Majewska, C.-H. Lee, S.S. Kondov, B.H. McGuyer, R. Moszyński, T. Zelevinsky, Control of Ultracold Photodissociation with Magnetic Fields, Phys. Rev. Lett. 120 (2018) 033201.
2. A.M. Tucholska, M. Lesiuk, R. Moszyński, Transition moments between excited electronic states from the Hermitian formulation of the coupled cluster quadratic response function, J. Chem. Phys. 146 (2017) 034108.
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4. M. McDonald, B.H. McGuyer, F. Apfelback, C.-H. Lee, I. Majewska, R. Moszyński, T. Zelevinsky, Photodissociation of ultracold diatomic strontium molecules with quantum state control, Nature. 535 (2016) 122.
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7. M. Lesiuk, R. Moszyński, Reexamination of the calculation of two-center, two-electron integrals over Slater-type orbitals. I. Coulomb and hybrid integrals, Phys. Rev. E. 90 (2014) 063318.
8. M. Lesiuk, R. Moszyński, Reexamination of the calculation of two-center, two-electron integrals over Slater-type orbitals. II. Neumann expansion of the exchange integrals, Phys. Rev. E. 90 (2014) 063319.
9. M. Lesiuk, B. Jeziorski, R. Moszyński, On the large interelectronic distance behavior of the correlation factor for explicitly correlated wave functions, J. Chem. Phys. 139 (2013) 134102.
10. B.H. McGuyer, C.B. Osborn, M. McDonald, G. Reinaudi, W. Skomorowski, R. Moszyński, T. Zelevinsky, Nonadiabatic E_ects in Ultracold Molecules via Anomalous Linear and Quadratic Zeeman Shifts, Phys. Rev. Lett. 111 (2013) 243003.

Chałasiński Group

HEAD:

Prof. Grzegorz Chałasiński*, PhD DSc

GROUP MEMBERS:

Michał Hapka, PhD; Marcin Modrzejewski, PhD

RESEARCH PROFILE:

weak intermolecular interactions, density functional theory

CURRENT RESEARCH ACTIVITIES:

Our group is focused on the development and applications of electronic structure methods for weak intermolecular interactions. Recent works included advances in symmetry-adapted perturbation theory (SAPT) and density functional theory (DFT) methods based on Kohn-Sham formalism.

We introduced a variant of SAPT based on unrestricted Kohn-Sham treatment of the interacting monomers. Open-shell SAPT has been applied in a series of studies of small dimers relevant for ultracold chemistry. Moreover, we have investigated the possibility of merging the DFT-SAPT method with range-separated exchange-correlation density functional approximations. We have shown that the resulting LRC-SAPT method rivals the accuracy of the best-performing DFT-SAPT approaches.

Our work on improving hybrid semilocal DFT approximations has been focused on removing unnecessary empirical parameters and merging DFT with a proper description of long-range correlation effects. We devised a method for converting an arbitrary GGA or a meta-GGA functional into a range-separated hybrid which is free from DFT's shortcomings for, e.g., charge transfer systems. We have also analyzed the performance of different DFT approaches for calculations of many-body interaction energies. Our work established which nonadditive interaction energy components pose a considerable challenge even for best-performing modern DFT functionals. Works to properly account for these effects in the existing DFT approximations are under development in our group. Our current research involves merging DFT with the random-phase approximation model for electron correlation.

*e-mail: chalbie@chem.uw.edu.pl

SELECTED PUBLICATIONS:

1. M. Hapka, Ł. Rajchel, M. Modrzejewski, R. Schäffer, G. Chałasiński, M.M. Szczęśniak, The nature of three-body interactions in DFT: exchange and polarization effects, J. Chem. Phys. 147 (2017) 084106.
2. M. Modrzejewski, M. Hapka, G. Chałasiński, M.M. Szczęśniak, Employing range separation on the meta-GGA rung: New functional suitable for both covalent and noncovalent interactions, J. Chem. Theory Comput. 12(8) (2016) 3662-3673.
3. M. Hapka, Ł. Rajchel, M. Modrzejewski, G. Chałasiński, M.M. Szczęśniak, Tuned range-separated hybrid functionals in the symmetry-adapted perturbation theory, J. Chem. Phys. 141 (2014) 134120.
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5. J.V. Koppen, M. Hapka, M. Modrzejewski, M.M. Szczęśniak, G. Chałasiński, DFT for gold-ligand interactions: Separating true effects from artifacts, J. Chem. Phys. 140 (2014) 244313.
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7. M. Modrzejewski, Ł. Rajchel, G. Chałasiński, M.M. Szczęśniak, Density-dependent onset of the long-range exchange: A key to donor–acceptor properties, J. Phys. Chem. A. 117(45) (2013) 11580-11586.

Intermolecular interactions and electron correlation

HEAD:

Tatiana Korona*, PhD DSc

GROUP MEMBERS:

PhD students: Michał Chojecki,
Michał Śmiałkowski, Emran Masoumifeshani
Former group member: Sirous Yourdkhani, PhD

RESEARCH PROFILE:

intermolecular interactions analysis, electron correlation in molecules, molecular properties

CURRENT RESEARCH ACTIVITIES:

- Modelling of intermolecular interactions of large molecules with state-of-art quantum-chemistry methods (symmetry-adapted perturbation theory, functional-group SAPT, interacting quantum atoms etc.)
- Method development of molecular properties of large molecules, including local electron correlation and molecular fragmentation approaches
- Investigation of electronic excited states of large molecules
- Development of Molpro suite of programs

SELECTED PUBLICATIONS:

1. G. Wälz, D. Usvyat, T. Korona, M. Schütz, A Hierarchy of Local Coupled Cluster Singles and Doubles Response Methods for Ionization Potentials, J. Chem. Phys. 144 (2016) 084117.
2. S. Yourdkhani, M. Chojecki, M. Hapka, T. Korona, Interaction of Boron-Nitrogen Doped Benzene Isomers with Water, J. Phys. Chem. A. 120 (2016) 6287-6302.
3. A. Heßelmann, T. Korona, Intermolecular Symmetry-Adapted Perturbation Theory Study of Large Organic Complexes, J. Chem. Phys. 141 (2014) 094107.
4. H. Dodziuk, T. Korona, E. Lomba, C. Bores, Carbon Nanotube Container: Complexes of $C_{50}H_{10}$ with Small Molecules, J. Chem. Theory Comp. 8 (2012) 4546-4555.
5. T. Korona, First-order exchange energy of intermolecular interactions from coupled cluster density matrices and their cumulants, J. Chem. Phys. 128 (2008) 224104.

*e-mail: tania@chem.uw.edu.pl

Theoretical studies of interatomic forces and atomic properties

HEAD:

Prof. Bogumił Jeziorski*, PhD DSc

GROUP MEMBERS:

Paweł Czachorowski, PhD; Jakub Lang, PhD; Michał Przybytek, PhD

RESEARCH PROFILE:

Development of quantum theory of atomic properties and interatomic interactions and applications of this theory to metrology and high-resolution molecular spectroscopy.

CURRENT RESEARCH ACTIVITIES:

Development of methods to include relativistic and quantum electrodynamics effects in calculations of atomic properties and interatomic interaction energies. Developments of methods to include the effects of the coupling of electronic and nuclear motion in calculations of interatomic potentials. Development of new perturbation theory techniques for accurate determination of interatomic potentials. Development of new accurate methods of the electronic structure theory. Accurate calculations of electric and refractive properties of atomic gases for applications in metrology.

SELECTED PUBLICATIONS:

1. M. Lesiuk, B. Jeziorski, Size consistency and counterpoise correction in explicitly correlated calculations of interaction energies and interaction-induced properties, Phys. Rev. A. 99 (2019) 032712-1 - 032712-10.
2. M. Przybytek, W. Cencek, B. Jeziorski, K. Szalewicz, Pair potential with submillikelvin uncertainties and nonadiabatic treatment of the halo state of helium dimer, Phys. Rev. Lett. 119 (2017) 123401-1 - 123401-6.
3. P. Gniewek, B. Jeziorski, Determination of the exchange interaction energy from the polarization expansion of the wave function, Phys. Rev. A. 94 (2016) 042708-1 – 042708-6.
4. K. Piszczatowski, M. Puchalski, J. Komasa, B. Jeziorski, K. Szalewicz, Frequency-dependent polarizability of helium including relativistic effects with nuclear recoil terms, Phys. Rev. Lett. 114 (2015) 173004-1 – 173004-5.
5. P. Gniewek, B. Jeziorski, Exchange splitting of the interaction energy and the multipole expansion of the wave function, J. Chem. Phys. 143 (2015) 154106-1 – 154106-10.

*e-mail: jeziorsk@chem.uw.edu.pl

Index of Research Group Members

UNIVERSITY OF WARSAW

WCh Faculty of Chemistry University of Warsaw

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University of Warsaw
Krakowskie Przedmieście 26/28
00-927 Warsaw
www.uw.edu.pl

Faculty of Chemistry
University of Warsaw
Pasteura 1
02-093 Warsaw
www.chem.uw.edu.pl

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