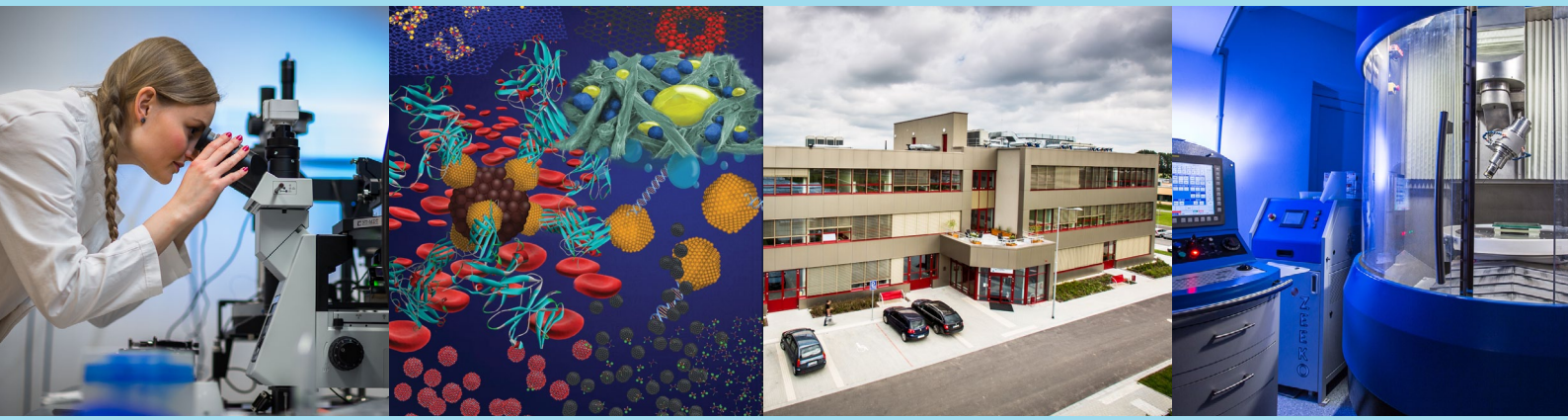
REGIONAL CENTRE OF ADVANCED TECHNOLOGIES AND MATERIALS

2014



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REGIONAL CENTRE
OF ADVANCED TECHNOLOGIES
AND MATERIALS
Regionální centrum pokročilých technologií a materiálů

Palacký University
Olomouc

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MINISTRY OF EDUCATION, YOUTH AND SPORTS

EUROPEAN UNION
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2007–13
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1 RCPTM

Introductory Message from the Director

The year 2014 was crucial for the Regional Centre of Advanced Technologies and Materials in many respects. First of all, the four year realization phase, connected with the ESF support, was successfully closed in September. I am really glad that we were able not only to construct the new building and prepare all the technologies for use, but also to stabilize the scientific team, which keeps probably the highest level of internationalization amongst all of the 48 centres built within the Operational Programme RDI.

Concerning the long term sustainability of the scientific team, as well as the unique technical park, it is very important that we succeeded in an application for the support from the National Sustainability Programme, which is now covering approximately 35 per cent of the Centre's budget until the year 2019.

I am also delighted with the significant rise in the number of scientific publications. If we do not take into account the publications related to our participation in collaborations CERN – ATLAS or Pierre Auger, I have registered more than 220 works in impacted journals in 2014, which means a rise of 25 percent compared to 2013. In my opinion, we have been able to keep the high standard of publications we set which is confirmed by a number of publications in journals with impact factors over 10, including the Accounts of Chemical Research, ACS Nano, Nano Today and Angewandte Chemie.

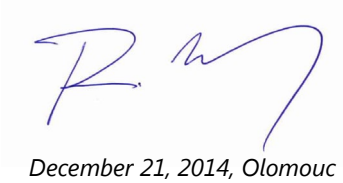
The quality of the scientific papers is starting to be reflected in the high number of citations. In this category our Centre reached, with more than 10 000 citations since 2011, the first place among the all RDI Centres in the Czech Republic, as it was mentioned in the newspaper Lidové noviny at the end of last year. The long-term first-class scientific work brought also a series of awards to our scientists, for example the Neuron grant for prof. Otyepka or prof. Hobza´s enlistment amongst the most cited researchers of the world (Highly Cited Researchers 2014) according to Thomson Reuters Company.

Worth mentioning is as well the Rudolf Zahradník Lecture Series which is evolving promisingly and which last year presented indeed great names of the chemistry world: Mario Ruben from Karlsruhe, Patrik Schmuki from Erlangen and Wolfgang Lindner from Vienna. The series was opened by prof. Rudolf Zahradník himself with the lecture "Word about chemistry in our country and abroad". Also, a few scientific personalities have confirmed their participation in the 2015 Series and this will make it only one more reason why I believe that this Series will likely be an exceptional display of the world of chemistry and physics in the future global context.

Also many technologies which were patented by RCPTM in the last years, shifted in 2014 to the advanced phase of commercialisation. Among the most promising belongs the lactoferin separation from cow's milk or the modifications of functional packages for the food industry. It is also satisfactory that we managed to install a series of unique instruments. Owing to this fact, our microscopic, optical or magnetic laboratories are one of the most well-equipped in

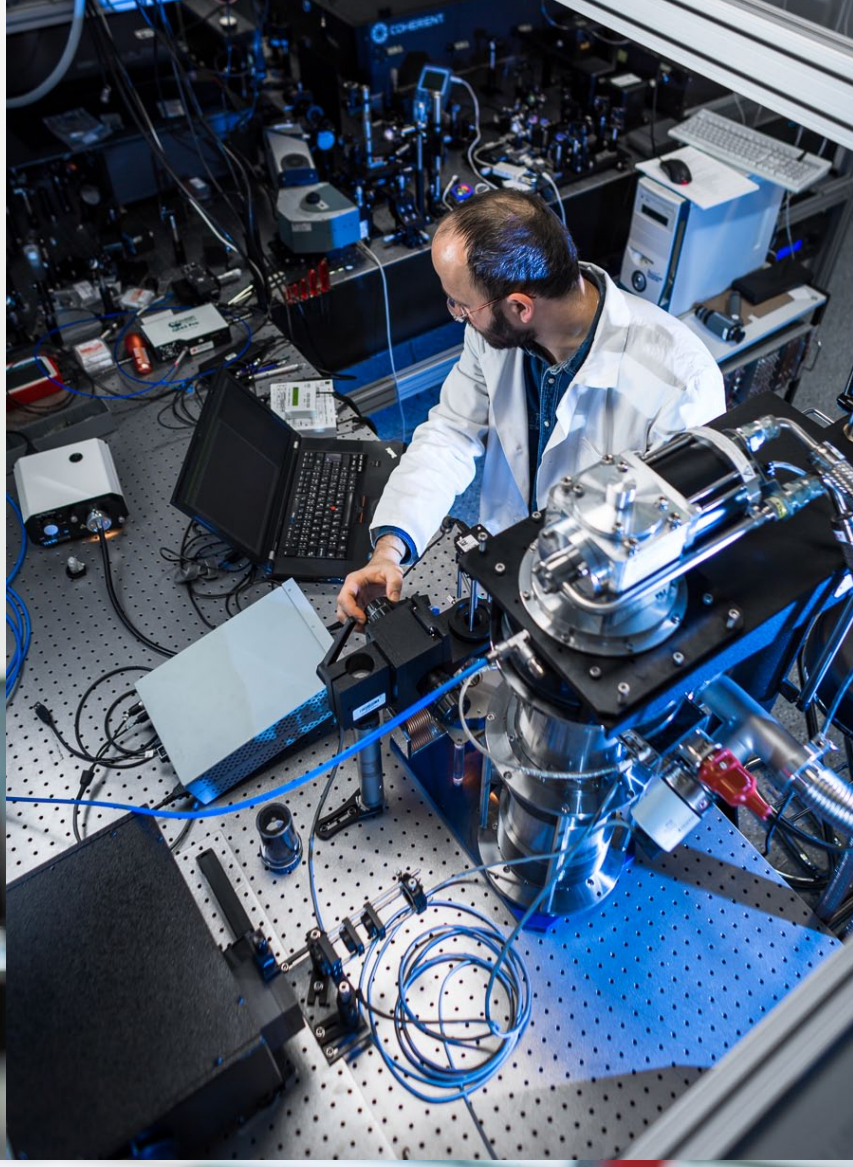
all of Europe.

And what do I wish for the year 2015? Definitely to keep the rising publication and citation trend. I would be also really delighted, if some of our papers were published in some of the most prestigious journals such as *Science* or *Nature Family*. Regarding the promising results of the pilot and operation tests I believe that we will be able to sign the first licence agreements. We will be also waiting eagerly for the results of the competition in European projects H2020 where we submitted a few applications including the ERC grant. And naturally, I wish us all good health, plenty of great ideas, and lots of energy to tackle the next exciting research.



December 21, 2014, Olomouc

Prof. RNDr. Radek Zbořil, Ph.D.

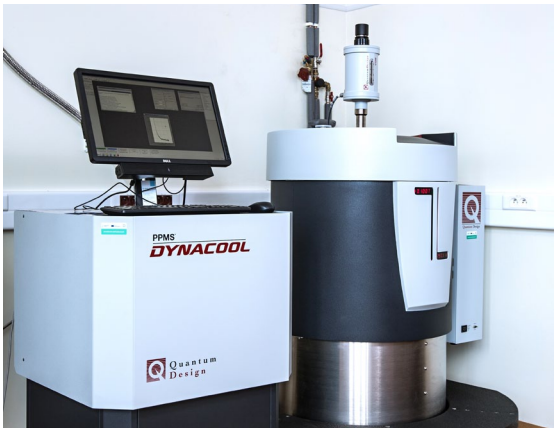


2 NEW INSTRUMENTS FOR THE STUDY OF SURFACE, STRUCTURE AND MAGNETIC PROPERTIES

These days The Regional Centre of Advanced Technologies and Materials in Olomouc represents one of the best equipped workplaces for material, nanotechnological, chemical and optical research in both the European and world scale. The building up of top laboratories has already started in 2005. The wide range of synthetic as well as analytical techniques, which RCPTM disposes of, is given by not only large-scale research orientation of the Centre (Chemistry, Physics, Optics, Materials Research), but also by the large degree of multidisciplinarity of the research in the field of nanotechnologies owing to their application potential overlap in medicine, ecology, biotechnology, energetics and a number of other fields. The instrument park was significantly enlarged by plenty of unique techniques in 2014, which overall rounded off the laboratories of the Centre.

Physical Property Measurement System (PPMS) Dynacool

The laboratory for the measurement in the magnetic field was empowered by a modular instrument named Physical Property Measurement System (PPMS) Dynacool (manufactured by the US company Quantum Design), which allows the characterization of chosen physical properties of the materials and molecular systems in temperature ranges from 1.9 to 400 K, also in the magnetic field up to 9 T. The available measurement modules are intended for getting information about heat capacity, magnetization, magnetic torque and electro-transport properties (electrical resistivity, the Hall effect, I-V curves). The PPMS Dynacool instrument belongs among the most modern instruments capable of studying magnetic and transport properties of the materials, magnetic anisotropy, magnetocaloric effect or supraconductive materials. The system enables fully automatic measurements using programmable sequences.



Grinding of Optical Surfaces

The optical laboratory was significantly replenished in 2014. New technological equipment for the RCPTM optical group was delivered by the ZEEKO company. The CNC machine is designed in a way to be able to generate various shapes of the optical surfaces, from flat surfaces to the surfaces of general shapes. Surface grinding takes place in several steps – from rough surface shaping to final polishing operations, through which the surface gets the final shape with the roughness of the surface in nanometres. The essential part of these technological centres is also a diagnostical instrument for analysing shapes of the element surfaces which are being processed.

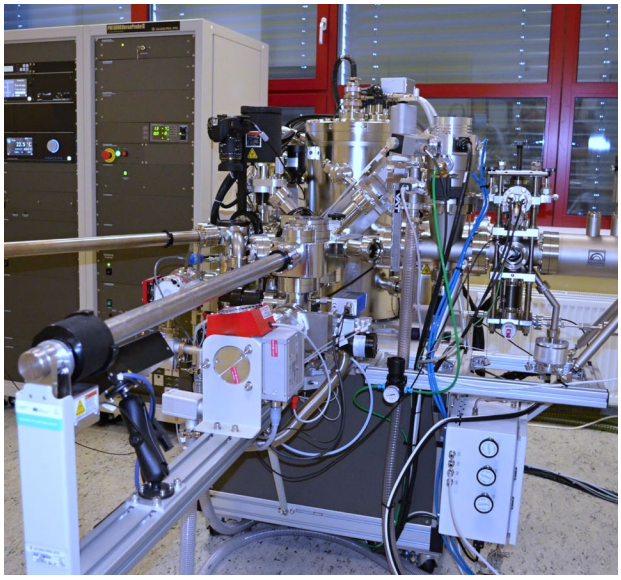
These instruments are used in the Centre for the research, development and the production of the extensive optical elements up to one meter in diameter, which find their usage eg. in big international collaborations in the sphere of astroparticle physics such as The Pierre Auger Observatory or the Cherenkov Telescope Array.

Uniqsis-FlowSyn

The nanocatalysis research group was equipped with the set of instruments including the flow reactor for the study of catalytic organic reactions including amidation, nitration of the electron deficit aromates, esterification, hydrogenation, bromation etc. The flow reactor allows the optimalization of the reactions before their transition from the laboratory conditions to higher yields. Reactants are being mixed up in the T-shape mixer, which enables diffussion via short distances and helps to quick and controlled reactions which take place in microchannels with excellent heat and substance transition.

X-ray Photoelectron Spectroscopy (XPS)

In order to strenghten the X-ray techniques, the laboratories new XPS system was acquired in 2014. X-ray photoelectron spectroscopy (XPS) is an advanced technique used for the chemical analysis of solid surfaces matters (known also as ESCA – Electron Spectroscopy for Chemical Analysis), eventually frozen samples. Device VersaProbe II (manufactured by Physical Electronics) enables the measurement of angle differentiated X-ray photoelectron spectrocsopy, the identification of the elements' content depending on depth (depth profiling) and areal surface mapping. The device is intended for materials research, especially for complex chemical analyses (quantitative and qualitative) and analyses of chemical states of the surfaces of various conductive and nonconductive magnetic samples. Further, the device enables processing of the samples in integrated high-temperature/high-pressure chambre (up to 700 °C/20 bar) with no need of taking the sample out of the spectrometer (i.e. the sample does not leave the environment of ultrahigh vacuum). Navigation on the sample surface is done using the camera snapshot or using the "live"picture of the sample displayed by secondary electrons.



Combined System of AFM and Raman Spectroscopy

The possibility of the Centre to study not only the physical but also chemical properties of surfaces was enlarged highly by obtaining the atomic force microscopy (AFM) and Raman spectroscopy. The device, manufactured by NT-MDT company, enables the investigation of material surfaces in both liquid and air environments in atomic resolutions. Among its equipment belong modules intended for surface topography description and modules for the examination of the magnetic properties of the surfaces or their electric conductivity. An integral part of the instrument is also the spectroscopic part composed by Raman spectroscopy. Its integration enables chemical surface characterization of the examined sample from the standpoint of the present chemical bonds. The Raman spectrometer is equipped with optics reaching the spectral resolution of 0.5 cm^{-1}. The tuned combination of the AFM and Raman part enables to carry out also the so-called TERS analysis (Tip Enhanced Raman Spectroscopy) and obtain the spectral map of the sample with a space resolution less than 20 nm. In this way the system provides the topographic and chemical surface mapping in parallel.

NMR

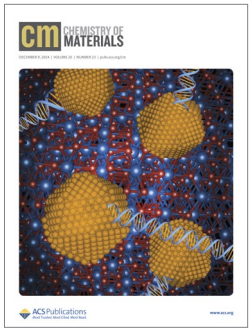
The laboratory of spectroscopy techniques was enriched by the 600 MHz NMR spectrometer by the JEOL company which enables obtaining high-resolution spectra of samples in solution and solid states using 1D and 2D NMR experiments. The spectrometer is equipped with measuring probes with automatic tuning system AutotuneTM 600 MHz 5 mm FG/RO and FG/TH for measuring samples in a solution enabling wide-range 1H a 19F experiments with one or two resonances including the direct measurements 1H, 19F, 23Na, 13C, 31P, 15N, 29Si, 11B, 119Sn and other nuclei. Further, the measuring probe is available for solid samples of 600 MHz 3.2 mm HXMAS in 3.2 zirconium cuvettes suitable for experiments on chemical and biochemical samples in the temperature range from room temperature to 130°C. The spectrometer also allows the studies of the composition and identification of organic and inorganic compounds, including the observation of reaction kinetics of studied substances in various environments.

3 RESEARCH HIGHLIGHTS

MAGNETIC NANOPARTICLES IN MEDICINE AND SENSING APPLICATIONS

Magnetic nanoparticles play an important role in various technical and medical applications. Among them, iron-oxide-based nanoparticles hold a paramount position particularly due to their application promising magnetic and biochemical properties. Nanoparticles of spinel iron oxides show superparamagnetism, have a strong magnetic response even under small applied magnetic fields, are non-toxic, biocompatible and biodegradable. Suitably surface-modified (functionalized) magnetic nanoparticles can be then used in medical diagnostics (contrast agents in magnetic resonance imaging), therapeutic applications (targeted drug delivery, magnetic fluid hyperthermia) or in combined theranostic applications. Moreover, iron oxide nanoparticles have been found effective in sensing applications where they are applied in the form of hybrid systems (e.g., with nanoparticles of noble metals or carbon nanostructures) to detect a series of biologically important molecules and to monitor important biological processes.

The increasing interest of the scientific community to exploit iron oxides in the field of biosensorics inspired the RCPTM researchers to compile and write a review paper. This work, which was showcased on the cover of the prestigious journal, *Chemistry of Materials*, represents the first attempt to summarize possibilities of usage of iron oxide nanoparticles for inducing and monitoring catalytic and enzymatic processes *(Chem. Mater. 26, 2014)*. The attention is devoted to non-enzymatic sensors, enzymatic sensors, advanced immunosensors (nanocomposites made up of iron oxide nanoparticles and noble metal nanoparticles) and hybrid sensors (nanocomposites composed of iron oxide nanoparticles and carbon nanostructures). The work also discusses the applications of hybrid systems involving iron oxide nanoparticles and biological molecules in the field of immunosensors and DNA sensors. In addition, the review paper covers the properties and usage of magnetic, fluorescent and magnetofluorescent sensors exploiting surface plasmon resonance. The main advantages of using iron oxide nanoparticles in sensing applications rests, in particular, in an enhanced area of available surface of an electrode and improved electron transfer associated with the catalytic ability of iron oxide nanoparticles. The work also stimulates further directions in the research of iron-oxide based sensors including development of systems exhibiting multimodal sensing character (magnetic, fluorescent mode, etc.), miniaturization of sensing systems and their expansion in *in vivo* medical applications.



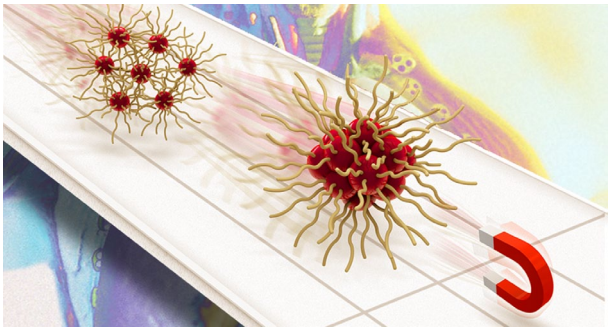
The review work of the RCPTM authors was showcased on the cover of the journal of the American Chemical Society – Chemistry of Materials – in 2014.

RCPTM workers also achieved several interesting results in the field of experimental research regarding the sensing applications of iron oxides in 2014. In particular, the attention was devoted to applications of hybrid systems composed of magnetic nanoparticles with covalently anchored nanosilver. These composite nanostructures can be used, for example, in the methods of magnetically-assisted surface enhanced Raman spectroscopy. In these applications, if suitable antibody is attached to silver nanoparticles, the hybrid can selectively unbind the targeted molecule from the solution. The magnetic properties of this nanocomposite provide easy separation of targeted molecules from a complex matrix while silver nanoparticles act as active components for their determination by surface enhanced Raman scattering. The method was successfully used by the RCPTM researchers to determine the level of dopamine in celebro-spinal fluid and G-immunoglobulin in blood. Both studies were published in the Analytical Chemistry journal *(Anal. Chem. 86, 2014)*.

Cover of the Analytical Chemistry journal showing the work of RCPTM authors. The work describes determination of G-immunoglobulin in blood employing magnetically-assisted surface enhanced Raman spectroscopy with usage of Fe_3O_4/Ag nanoparticles.

It is known that dopamine plays the role of a very important neurotransmitter which mediates a transfer of impulses in certain parts of the brain. Damages of dopamine paths in the brain or decreased concentration of dopamine are closely connected with the evolution of the Parkinson and Alzheimer diseases; other disorders of the dopamine system can result in schizophrenia. Knowledge of dopamine concentration in the human body provides not only to choose proper treatment approach for these brain disorders but also to understand the basic functions of the human brain. The concentration of dopamine can be determined by various methods; electrochemical methods or methods using mass spectrometry are most frequently used. Most of these approaches are complicated and face the problem of relatively high detection concentration limits of the techniques employed, which lie in the range of nmol L^{-1}.

The work of RCPTM researchers introduced a new concept of detecting dopamine by a nanocomposite system composed of Fe_3O_4 and silver nanoparticles *(Anal. Chem. 86, 2014)*. The surface of nanoparticles was secondarily modified with the FTA-based compound, which acts selectively towards dopamine. The synthesized nanocomposite showed a remarkable stability and reproducibility. Comparative data obtained from clinical samples of grey matter of mouse brain confirms that the developed method employing technique of magnetic surface enhanced Raman scattering represents an alternative to the conventional liquid chromatography combined with mass spectrometry. The developed methodology of assessment of dopamine concentration allowing to achieve record detection limits (fmol L^{-1}) is selective, faster and cheaper without the necessity of preconcentration or the derivatization of samples. A similar approach has been used for detection of human G-immunoglobulin in blood *(Anal. Chem. 86, 2014)*. In the work of RCPTM researchers, nanocomposites, made up of Fe_3O_4 and silver nanoparticles coupled with each other through chitosan of carboxylmethyl type, were modified by streptavidin protein and anti-G immunoglobulin, which enabled a high determination selectivity. The nanocomposite could be then used in the method of determination of G-immunoglobulin from blood samples from fingers on hand. By employing these nanocomposites, which are active in the technique of magnetically-assisted surface enhanced Raman scattering, it is feasible to detect concentrations of G-immunoglobulin down to 600 fg mL^{-1}. The exploitation of Fe_3O_4/silver nanocomposites for the determination of targeted molecules by magnetically-assisted surface enhance Raman spectroscopy represents a new direction in analytical chemistry with possibility to determine a broad series of biologically important phases providing record selectivity and sensitivity.



Iron-oxide-based condensed magnetic cluster for usage in theranostic applications.

Among medical applications of magnetic nanoparticles of iron oxides, it is worthwhile to highlight the work of RCPTM researchers published in the *Chemistry of Materials* journal *(Chem. Mater. 26, 2014)*. By using the method of biomineralization and epitaxial aggregation, it was feasible to prepare special magnetic clusters containing iron oxide nanoparticles with prominent characteristics, having the potential to be used not only in magnetic resonance imaging, but also in *in vivo* SPECT imaging. These magnetic clusters also show impressive characteristics for targeted drug delivery with an extraordinary capacity to bind anticancer drugs (doxorubicin) and with possibility to release the drug, in a controllable manner, by changes in temperatures and applied magnetic fields. The developed hybrid system can be thus viewed as a complex theranostic tool applicable in medical diagnostics and therapy.

Apart from sensing and medical applications, iron oxides have been found effective in other fields of human activity. In these areas, composite materials made up of iron oxides and various carbon (nano) structures such as fullerenes, carbon quantum dots, carbon nanotubes, graphene, diamond, and graphite have been identified to play a dominant role. Based on the nature of the interaction between magnetic components and carbon nanoallotropes, it is possible to tune resulting physical properties of such nanocomposites through cooperative and synergetic phenomena. Apart from application acceptable magnetic properties, iron oxide nanoparticles show photocatalytic properties usable in solar cells for the direct splitting of water or easily undergo conversion reactions of principal importance for the storage of electric energy (e.g., lithium-ion batteries). The review work of the RCPTM authors, published in the *ACS Nano* journal, firstly summarizes all the already working and potential applications of nanocomposites containing carbon nanoallotropes and iron oxide nanoobjects (*ACS Nano 8, 2014*). In addition to the physical properties of hybrid systems, the authors describe their applications in the field of storage of electric energy, medicine, remediation of environment or catalysis. The review article also suggests future challenges in applications of iron oxide/carbon hybrids, especially the usage of covalent interactions to tune resulting properties of composite systems.

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A. Balzerova, A. Fargasova, Z. Markova, V. Ranc, R. Zboril: "Magnetically-assisted surface enhanced raman spectroscopy (MA-SERS) for label-free determination of human immunoglobulin G (IgG) in blood using Fe_3O_4@Ag nanocomposite", Anal. Chem. 86, 11107–11114, 2014.

G. Zoppellaro, A. Kolokithas-Ntoukas, K. Polakova, J. Tucek, R. Zboril, G. Loudos, E. Fragogeorgi, C. Diwoky, K. Tomankova, K. Avgoustakis, D. Kouzoudis and A. Bakandritsos: "Theranostics of epitaxially condensed colloidal nanocrystal clusters, through a soft biomineralization route", Chem. Mater., 26, 6, 2062–2074, 2014.

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Grant support:

OPVK 2.3, CZ.1.07/2. 3. 00/20.0155, 2012-2015

Research team of the Regional Centre of Advanced Technologies and Materials with a focus on non-conventional experimental techniques in materials and optical research

Main investigator: Prof. RNDr. Radek Zbořil, Ph.D.

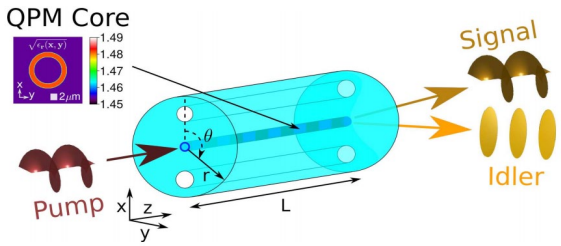
PHOTONS – MESSENGERS OF THE PAST AND FUTURE

At first glance, photons seem to be rather boring when looking into the zoo of particle micro-world recently supplemented with its last anxiously expected capture – theorised Higgs boson. Like ants, photons are everywhere, quietly and discreetly doing their duty. Their job is highly valuable since they bring fragments of information about processes hidden deeply in the hardly accessible vastness of time and space. Watching photons more closely we can see how they manage a lot of business even in our everyday life exhibiting a number of various faces hardly stamped as boring.

Playing with Photons

Photons meet ideal tool requirements for the transmission and processing of information in the way not available using methods of classical physics – we can speak about so-called quantum information processing. Recent research at RCPTM was focused on quantum communication networks using single photons as the carrier of signal. We designed and built-up experimentally a special amplifier of quantum signal (*Phys. Rev. A 89, 2014*), that allows sending quantum information even via lossy communication lines. Furthermore, we proposed and published an approach for digital signature of messages distributed via quantum communication network. We dealt with issues of the quantum computing during research concentrated on the assembly of the quantum simulator for handling natural processes. Using this device we were capable to simulate successfully the behaviour of single atoms.

Even stranger than single photons are photon twins. In cooperation with professor Juan P. Torres from ICFO, Barcelona, we dealt with new sources of photon pairs based on structured optical fibres (*Opt. Express 22, 2014*). We showed that by employing such non-traditional instruments we can produce photon pairs with a very broad spectrum or strongly correlated photon pairs. These processes cannot be realised by means and ideas of classical physics. The properties of each photon twin are highly random, whereas they behave to each other as if they were related by some invisible bond. This bond is very strong and it is preserved even after the twins are subject to undergo random interactions. It also affects properties of optical fields when propagating through the space, or through environment combining layers from metal and dielectric materials.



Design of photon twins generation in a structured optical fibre.

Quantum correlations under our interest, so far examined preferably on the level of single photons, can be observed also in high-power optical fields and they were already observed for instance in the device called optical parametric amplifier. With the help of carefully prepared experiment and together with colleagues from Como, Italy, we have demonstrated, that the nature of these phenomena is very similar, but their manifestations can be dramatically different (*Opt. Express 22, 2014*).

These are not just theoretical mind games distant from reality, because photon pairs can serve, for example, as a very effective metrological tool. With their help we can perform precise absolute measurements of detector efficiency without the need to compare the results with another more precise detector. We have succeeded to show that photon pairs can be exploited also for the arrangement of absolute spectral sensitivity curve of the detector.

Experiments with twin photons.

Earth Being Hit by Space Artillery Barrage

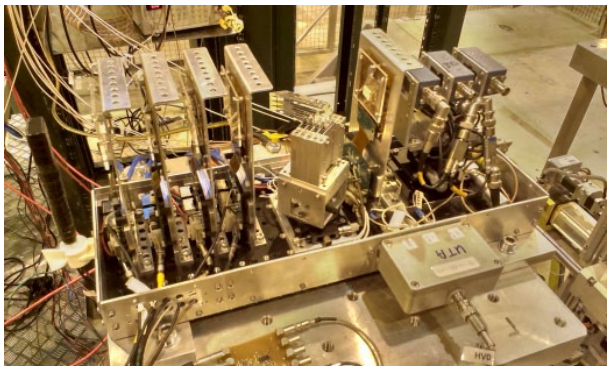
...is the title of the scientific popular lecture that our colleague Dr. Jiří Grygar presented on the Centre ground last year, however the topic is not obsolete even now. Something unknown in the universe is emitting high-energy particles to the surrounding space. Where do these particles come from? Are they from a gigantic cosmic explosion? From the vicinity of a giant black hole swallowing stars? From the place where galaxies collide? From the decay of matter remnants lasting from the short period after Big Bang era? Answers to these questions aiming to understand more thoroughly the basic laws of the universe are being sought by the Pierre Auger Observatory in Argentina in co-operation with RCPTM.

Its main purpose is a study of the properties of cosmic radiation exhibiting the highest observed energies (> 10^{18} eV), only slightly affected by cosmic magnetic fields. Another important research field is the examination of anisotropy of the incident radiation (space distribution of the event directions) with the aim to discover its source. The research is also focused on a study of the structure of incident cosmic rays to decide whether primary particles entering atmosphere are photons, protons, neutrons or nuclei of various chemical elements and to identify the precise chemical composition of cosmic radiation.

Scientists and PhD students of The Academy of Science of the Czech Republic, Faculty of Mathematics and Physics (Charles University in Prague) and RCPTM are all taking part in this project. The Olomouc group designs and operates above all optical parts of fluorescent detectors (they have already delivered 15 telescopes). The group also designed full-sky cameras for monitoring the level of cloudiness and so called optical background of the night sky. Furthermore, the optical telescope was delivered for a novel type of lidar proposed for the purpose of atmosphere monitoring above the observatory ground and the group also takes part in operating the observatory, its maintenance and upgrade. Besides this, the group members also develop specialised optical technologies for various optical elements employed in the observatory, conduct series of unique measurements and data evaluations of distinct parameters supplied by observatory's detection system.

Visualisation of the prospective CTA observatory.

Thanks to successful international collaboration on Pierre Auger Observatory in Argentina, the RCPTM group was also invited to take part in the preparatory stage of another similar project – CTA (Cherenkov Telescope Array). Its purpose is an observation of high-energy gamma radiation. The CTA will serve as an open laboratory to the broad community of astrophysicists and will provide deep insight into high-energy processes in the universe. The community anticipates that it will contribute, for example, to understand a variety of physical mechanisms accelerating particles in the vicinity of black holes. The Olomouc group is dealing with the know-how for spotting suitable locations to build such observatories in the northern and southern hemisphere. Also, the group members concentrate on the development of ultra-thin mirrors and corresponding technologies for their manufacturing.



Configuration of the tested detector with high temporal resolution in the CERN-ATLAS project.

From the Deepness of the Universe to the Heart of the Matter

In the pursuit for understanding of the matter's nature we can redirect our instruments either to deep space, or to the heart of the elementary particles. The latter one we are doing with the use of the largest terrestrial particle accelerator – Large Hydron Collider (LHC) at CERN. ATLAS experiment, that is conducted in cooperation with the group of RCPTM scientists, continued on the preparatory efforts to bring LHC to reopening on higher energies for early 2015. These efforts aim, on one hand, towards detector enhancements (for example applying additional layer of silicon path detectors) and, on the other hand, to software development and collision simulations that are required for the detector calibration and for the comparison with future experimentally acquired data. Simultaneously, analysis of the recently stored data has been accomplished to obtain precise particle characteristics and their spectra (for example of the heaviest top quark that is being currently studied by the Olomouc group members). In greater detail the group studied properties of the Higgs boson (discovered in 2012) in different decay channels and it has been verified that its spin and interactions with other particles are (so far) in good accordance with the standard model of the micro-world.

The Olomouc group took part in the analysis of data obtained by the so-called forward detectors, used for the detection of elastically scattered protons, which physics has not well explored yet. We are taking part in advance workings to develop an innovative forward detector with high temporal resolution (10 ps) which is necessary for distinguishing background events from the real elastically scattered protons. These studies served as a starting point for the design of a new detector's prototype, that was tested at Fermilab in August 2014 and also in CERN laboratories in November 2014. The experimental results helped to optimise glass parts of the detector that is being developed in co-operation with the Olomouc group (*Opt. Express 22, 2014*).

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Grant support:

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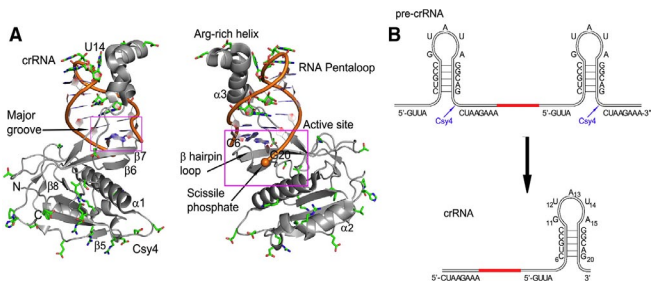
COMPUTATIONAL CHEMISTRY ANALYSING BIOMOLECULES AND ENZYMES

Computer simulations provide a valuable view of fine structural properties with the highest possible resolution which influence mechanical behaviour of DNA, catalytic activity of RNA and enzymes or organization of molecules in crystal structures. Powerful computers give us the answers to many questions from the world of "living" and "non-living" molecules.

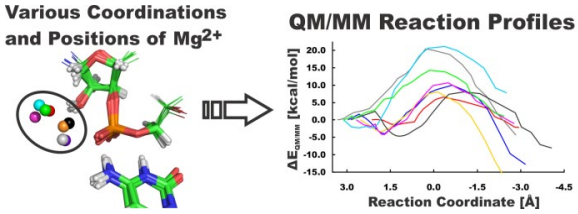
Nucleic Acids

A-tracts are functionally important DNA sequences which induce helix bending and have peculiar structural properties. While A-tract structure has been qualitatively well characterized, their mechanical properties remain controversial. A-tracts appear structurally rigid and resist nucleosome formation, but seem flexible in DNA looping. We investigated the mechanical properties of symmetric and asymmetric A-tracts using two types of coarse-grained models. We found that asymmetric A-tracts are more rigid than the control G/C-rich sequence in localized distortions relevant for nucleosome formation, but are more flexible in global bending and twisting relevant for looping. The symmetric tracts, in contrast, are more rigid than asymmetric tracts and their control, both locally and globally. Our results can reconcile the contradictory stiffness data on A-tracts and suggest symmetric A-tracts to be more efficient in nucleosome exclusion than the asymmetric ones (*Nucleic Acid Res., 42, 2014*). In addition, we studied the importance of allosteric effects in DNA, which is becoming increasingly appreciated. The predicted DNA bending is in quantitative agreement with experiment and suggests that diamidine binding to the alternating TA sequence brings the DNA closer to the A-tract conformation, with potentially important functional consequences (*J. Phys. Chem. Lett., 5, 2014*). Another interesting property of DNA and RNA sequences is the transient opening of their terminal base pairs, called fraying. We show that our new RNA glycosidic torsion potential provides an improved description and substantially more stable MD simulations of RNA molecules. The accurate modeling of fraying is important because of its involvement in nucleic acid end recognition and enzymatic catalysis.



A) Crystal structure of Csy4 CRISPR endonuclease and B) the suggested mechanism of its action yielding to crRNA. Adopted from (Bioch. Biophys. Acta (Gen. Subjects), 10, 2014).

We continued our research focused on a reaction mechanism of small RNA enzymes also called ribozymes. We carefully analyzed the advantages and disadvantages of advanced QM/MM methods for description of the self-cleavage reaction catalyzed by the hairpin ribozyme. (*J. Chem. Theory Comput., 10, 2014*). In the case of hepatitis delta virus (HDV) ribozyme, we carried out extensive QM/MM calculations of the reaction mechanism to understand the role of active site Mg^{2+} ion in catalysis. We showed that a structure of the ribozyme, and particularly the positioning of the active site Mg^{2+} ion, facilitate deprotonation and activation of the 2′-OH nucleophile (*Phys. Chem. Chem. Phys., 17, 2015*).



Specific position and coordination of the Mg^{2+} ion in the active site strongly affects the kinetics of the HDV ribozyme self-cleavage. Adopted from RSC (Phys. Chem. Chem. Phys., 17, 2015).

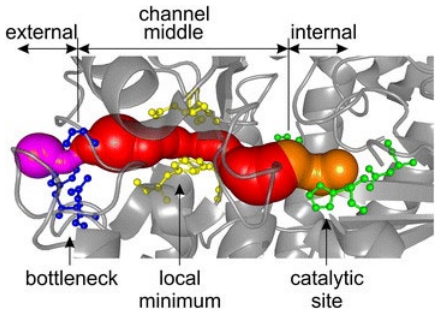
Our molecular dynamics simulations and experimental FRET measurements indicated that the HDV ribozyme structure is conformationaly heterogeneous in solution. We also proposed that the available crystal structures of the HDV ribozyme represent intermediates on an overall rugged RNA folding free-energy landscape (*RNA, 20, 2014*).

During analysis of the molecular mechanism of CRISPR Csy4 endonuclease self-cleavage, which is a backbone of autoimmune system of bacteria, we modeled product and precursor states of the endonuclease. We identified protonation states of the key catalytic amino acid residues mostly compatible with the available structural and mechanistic data. We also highlighted current limitations of molecular dynamics simulations to study protein-RNA complexes (*Bioch. Biophys. Acta (Gen. Subjects), ASAP, 2014*). Recently, we reviewed a current status of molecular dynamics simulations and we clearly explained theunderlying approximations and application potential of MD simulations. On several examples, we showed that MD is a powerful technique, which complements data acquired from experiments, helps to interpret experimental data, and provides testable hypotheses (*J. Phys. Chem. Lett., 5, 2014*).

Anatomy of Enzyme Channels

Enzymes are natural catalysts which help our bodies to sustain life functions. They were also tamed to serve as our tools in various biotechnological processes. The enzymatic reaction occurs in the special spot in the enzyme's structure called the catalytic site. It was already known, that some enzymes like cytochrome P450 and acetylcholine esterase have their catalytic site buried deeply in their structure, though the reason for such complication was not entirely understood. In those enzymes, channels are needed to connect the catalytic site with surrounding environment for their function, but the number of such enzymes was thought to be minor and exceptional.

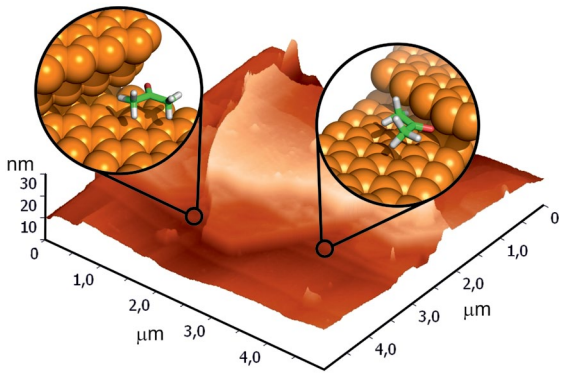
We analyzed channels in all known enzymatic structures and we found that majority of the enzymes have a network of channels leading to their active sites. This indicates that enzymes tend to have buried active sites with channels controlling access to and egress from them. We concluded that the active site access channels play an important role in determining enzyme substrate specificity (*BMC Bioinformatics, 15, 2014*).



An example of an enzyme channel identified by MOLE 2.0. Internal, middle and external parts of the channel in pyridoxal-5'-phosphate-dependent acyl-CoA transferase (PDBID: 3KKI) are colored orange, red and magenta, respectively. Active site amino acids (present in the internal part of the channel) are shown in green, amino acids in the middle part making the wall of a local minimum (channel narrowing) are in yellow, and amino acids in the external part lining the bottleneck are in blue.

Graphene

We continued our studies of the adsorption of organic molecules on graphene by a combination of inverse gas chromatography and theoretical calculations. We mapped in detail the adsorption behavior of acetone on graphene and graphite, revealing the nature of high-energy adsorption sites on these materials (*Carbon, 73, 2014*). The chemisorption of hydrogen on graphene or graphite was studied within an exact quantum formalism involving phonons. Trapping probabilities were obtained as a function of the hydrogen atom kinetic energy and compared to the recent experimental studies (*J. Chem. Phys., 140, 2014*). Our further topic was functionalization of graphene, where we showed that the results of popular n- and p-doping of graphene by nitrogen and boron atoms substituting carbon atoms strongly depend on the method of synthesis (*Phys. Chem. Chem. Phys. 16, 2014*). We also inspected the case of graphene covered by iridium adatoms. This system has been recently proposed as a potential wide gap topological insulator, but our calculation demonstrated that strong correlations inhibit topological properties (*Phys. Chem. Chem. Phys., 16, 2014*). Finally, we used accurate many-body theories to show the importance of electron-hole interactions for predicting low energy excitonic absorption peaks in optical spectra from single- and double-layer fluorographene to graphite fluoride (*Ann. Phys., 526, 2014*).



The AFM image of graphite flake. Insets show the high energy sites for acetone adsorption localized on steps.

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Grant support:

Excellence Centre GAČR P208/12/G016, 2012-2018

Controlling structure and function of biomolecules at the molecular scale: theory meets experiment

Main investigator: Prof. Ing. Pavel Hobza, DrSc., FRSC;

Project participant: Prof. RNDr. Michal Otyepka, Ph.D.

NANOCATALYSTS IN ORGANIC CHEMISTRY AND TECHNOLOGIES OF DIRECT SOLAR SPLITTING OF WATER

The laboratory of nanocatalysis and organic synthesis is the youngest laboratory at the Regional Centre of Advanced Technologies and Materials; it was established in 2014. Nanocatalysis is a dramatically developing branch of physical chemistry with an overlap to materials, environmental, organic, analytical and inorganic chemistry. Nanocatalysts constitute a unique group of materials on the border between homogeneous and heterogeneous catalysis, which allow rapid and selective chemical transformations with excellent product yields. At RCPTM laboratories, the nanocatalysts are prepared by a broad spectrum of synthetic procedures including microwave chemistry of solid-state reaction or traditional colloid chemistry. These complex approaches allow for control of the chemical composition, size and morphology including possibility to synthesize composite (integrated) nanocatalysts, thin films with solid substrate, nanomaterials with core-shell architecture, multidimensional systems and/or magnetically recyclable nanocatalysts. In 2014, the nanocatalysis group contributed significantly to the development of new types of magnetic catalysts with high selectivity and yield, advanced hematite-based photocatalysts for direct solar splitting of water, and also to the description of effect of size of noble metal nanoparticles on the their efficiency in the processes of heterogeneous catalysis.

Boom of Magnetically Recyclable Nanocatalysts

Magnetic nanocarriers are currently in the forefront of the interest of biomedical research for their exploitation in the field of targeted drug delivery, medical diagnostics, separation of cells and/or isolation and detection of biologically important molecules. Owing to the large surface area and easy functionalization, it is readily possible to modify these nanosystems by catalytically active species including nanoparticles. In comparison to traditional catalysts, these integrated catalysts show a number of advantages such as easy separation under external magnetic fields, simple recycling, lower level of contamination of reaction products and significant financial savings due to the possibility of multiple use.

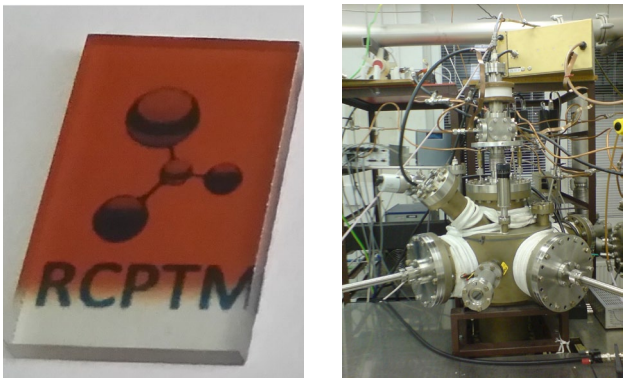
The work of the RCPTM researchers describing the properties and application potential of magnetically separable γ-Fe_2O_3/Au-based catalysts as featured on the cover of the Green Chemistry journal.

In 2014, RCPTM researchers developed new types of magnetic nanocatalysts comprised of magnetite (Fe_3O_4) nanoparticles immobilized with nanoparticles of palladium or gold (*Green Chem. 16, 2014*). The composite Fe_3O_4/Pd system turned out to be highly efficient in the Buchwald-Hartwig reaction of arylation of amines and amides with excellent yields, with a possibility of recycling without the loss of catalytic activity and without any signs of release of palladium to the environment (*Green Chem. 16, 2014*). Composite γ-Fe_2O_3/Au-based catalysts were identified to show similar high catalytic efficiency; these composite catalysts were successfully tested in the reactions of oxidative esterification of aldehydes and reduction of aromatic nitro-compounds. In the work, which has been showcased on the cover of the *Green Chemistry* journal, published by the Royal Society of Chemistry, the RCPTM researchers confirmed maintenance of catalytic efficiency after five separation and catalytic cycles (*Green Chem. 16, 2014*).

New Plasmatic Approaches Toward Development of Photocatalysts for Direct Solar Splitting of Water

Besides nanocatalysts with a broad spectrum of applications in organic and environmental chemistry, the RCPTM researchers also focus on the development of thin films of iron(III) oxide for exploitation in the technologies of direct solar splitting of water. For this purpose, they use a unique device based on high power impulse magnetron sputtering (HiPIMS), allowing control of the thickness of the thin film, size of particles, density of grains, crystalline anisotropy, cation doping and/or film porosity, i.e., the key parameters affecting the efficiency of the transfer of solar energy to chemical energy in the so-called Gratzel cells. If suitable deposition conditions are secured, this technology provides a direct deposition of thin crystalline layers even on thermally sensitive carriers when the temperature of the substrate does not exceed 150 °C during deposition process. As a result, possibilities to use a series of attractive substrates (in particular, flexible polymers) are significantly encouraged. In cooperation with colleagues from the universities in Erlangen and Nebraska, the RCPTM

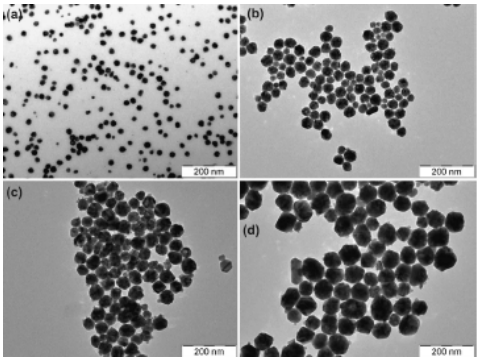
researchers published a study in which they described the advantages of the HiPIMS method for preparation of very thin (to 50 nm), but highly active layers of iron(III) oxide in the hematite crystal phase. Owing to the low thickness and nanocrystalline structure of the layers, backward recombination of photogenerated carriers was suppressed as a result of short diffusion length of holes; thus, high photoelectrochemical activity was achieved (*Appl. Catal. B: Environ. 165, 2015*). The photocatalytic activity of layers was further enhanced by effective passivation of undesired surface states, deposition of isocrystalline ultra-thin (2 nm) films of aluminum(III) oxide nature using the atomic layer deposition (ALD) method.



A thin hematite film for direct solar splitting of water prepared by the HiPMS method.

Nanosilver with Controllable Size and Catalytic Activity

For more than 10 years, RCPTM researchers have focused on the research of silver nanoparticles particularly due to their high antimicrobial activity. In 2006, the authors from RCPTM published a breakthrough work quantifying the effect of size of silver nanoparticles on their antibacterial activity (*J. Phys. Chem. B 2006*, more than 700 citations). In 2014, apart from other topics, the group devoted its attention to describing the effect of size of silver nanoparticles on their catalytic properties in model systems of reduction of organic dyes. For this purpose, an elegant method to control the nanoparticle size was developed; this method is based on the reduction of $[Ag(NH_3)_2]^+$ cation complex by D-maltose in the medium of polyacrylic acid. The specific concentration of polyacrylic acid allowed for the control of the size of nanoparticles and, consequently, to analyze its influence on the reduction of selected organic dyes with clearly confirmed principal effect of surface area of nanoparticles. The work was published in the prestigious journal of the American Chemical Society – *Chemistry of Materials* (*Chem. Mater. 26, 2014*).



Silver nanoparticles with controllable size, prepared in the presence of polyacrylic acid in various concentrations.

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Grant support:
The "Competence Centre" - TAČR TE01020218, 2012-2019.
Environmentally-friendly nanotechnologies and biotechnologies for treatment of water and soils.
Main investigator: Prof. RNDr. Radek Zbořil, Ph.D.

FP7-NMP 2011108, 2013-2017
Taking Nanotechnological Remediation Processes from Lab Scale to End User Applications for the Restoration of a Clean Environment.
Co-investigator: Prof. RNDr. Radek Zbořil, Ph.D.

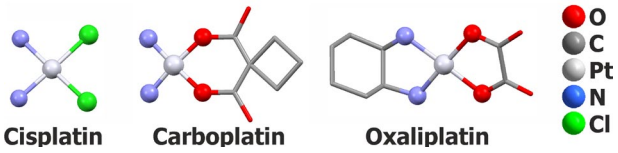
AUSPICIOUS STEPS TOWARDS MORE EFFICIENT THERAPEUTIES FOR THE TREATMENT OF SEVERE AND HARD-TO-TREAT DISEASES

Many sociologists and economists claim that contemporary society is currently experiencing the golden age of its existence. Considering multiple social changes and economic or technical advances, this statement is undoubtedly relevant. However, taking into account the health of the population in advanced economies, the mentioned changes have been clearly connected to the increased incidence of severe and hard-to-treat diseases which are, in essence, related to a combination of multiple factors such as diet quality, stress or environmental pressure. Various types of cancers, diabetes mellitus or inflammatory disorders can be named as the most common and most severe diseases.

The efforts of scientists working in the field of medicinal chemistry, i.e. the chemistry of biologically active compounds, are focused on reversing the unfavourable trend of lowered efficiency of treatment of severe illnesses and on increasing the quality of life of patients suffering from these diseases. The team of the research division "Biologically active complexes and molecular magnets" led by prof. Zdeněk Trávníček has contributed to the field dealing with investigation of more effective therapeutic agents for the treatment of severe human diseases by the development of several new platinum and gold complexes which showed to be up to 50-times more active than currently used anti-cancer/anti-inflammatory drugs.

Platinum and Gold Complexes – Strong Artillery against Cancer Cells

Chemotherapeutics of a varied chemical character are used for the treatment of cancer in oncological practice, while platinum-based drugs, such as cisplatin, oxaliplatin and carboplatin, are still in the frontline position.



Cisplatin **Carboplatin** **Oxaliplatin**

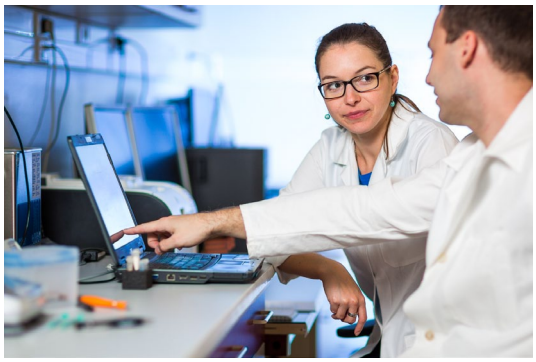
These drugs, however, possess a number of undesired properties, particularly, low selectivity (they affect not only tumour tissues but also healthy ones), which results in many negative side-effects (e.g. damage of kidneys, nervous system, haematogenesis, nausea). What is also a critical complication of this type of treatment is the genetically determined resistance of some tumour types and resistance acquired after repeated application of the platinum-based drugs. Simply, it can be said that efforts to overcome these drawbacks represent the driving force for the development of new chemotherapeutics (not only based on platinum) with a pharmacologically advantageous biological profile.

This field of study is also actively and productively explored by the scientists from the bioinorganic chemistry group of RCPTM. Their research this year was primarily focused on new compounds inspired by the structural properties of cisplatin (*cis*-dichlorido platinum(II) complexes with the derivatives of 7-azaindole – published in *PLoS ONE 9, 2014*) and new gold complexes inspired by the structure of anti-inflammatory drug auranofin (gold(I) complexes involving N-donor ligands based on hypoxanthine or its isosters - PLoS ONE 9, 2014). These compounds represent not only a significant contribution to the general chemical knowledge concerning substances of similar composition, but also exhibit significant biological activity, particularly in the area of cancer and inflammatory diseases.

The first stage of anti-cancer activity testing is performed on the cell models. The investigated compounds from the group of platinum and gold complexes, which were tested on a wide range of human cancer cell lines (e.g. ovarian carcinoma, prostate carcinoma, malignant melanoma, osteosarcoma), several-times exceeded the anti-cancer activity (in vitro) of cisplatin, used as a reference standard due to its therapeutic application in oncological practice.

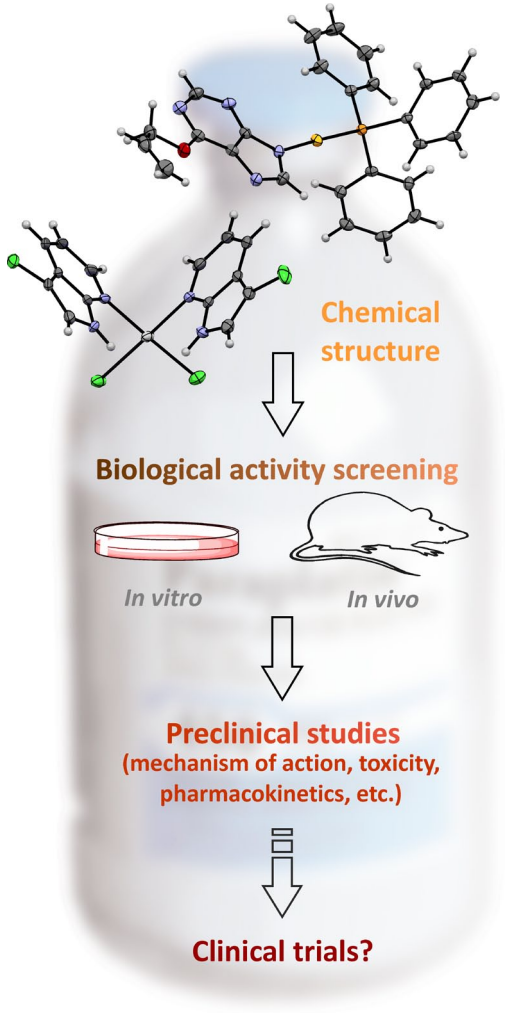
Moreover, it was also found out that the newly developed compounds were able to circumvent effectively the resistance of cancer cells to treatment by cisplatin, which would be very beneficial in their potential practical application, as they could be used as drugs in the case of cancer recurrence after treatment by cisplatin.

Additionally, as resulted from the studies on primary cultures of human hepatocytes, the mentioned compounds had significantly lower undesirable toxicity towards healthy human cells than was their cytotoxicity against cancer cells.



This information, which is crucial from the pharmacological point of view, was further complemented by studies of mechanism of action of the compounds in direct comparison with cisplatin (*J. Biol. Inorg. Chem. 18, 2013*). It was proven that the basic mechanism of action of the developed platinum complexes involves, analogously to cisplatin, covalent bonding to nuclear DNA. Significant mechanistic differences for the complexes were found in connection to the accumulation in tumour cells (up to ca. 50 times higher as compared to cisplatin), to the influence on tumour cell division, and last but not least, to a higher deficiency in cellular DNA repair mechanisms. These overall positive results of the experiments on the molecular level

were extended by in vivo studies of anti-cancer activity on a mouse model for lymphocytic leukaemia L1210. This investigation also used cisplatin as a comparative standard. The newly developed complexes reduced the tumour tissue volume to a similar extent as cisplatin, however, their impact on overall health status of the treated laboratory animals was less negative, i.e. the loss of appetite or weight was not observed during the experiments, which suggests less adverse negative side effects and organ toxicity of the prepared complexes as compared to cisplatin.



The positive biological profile and high potential for the medicinal application of the newly developed complexes have resulted in legal protection of the compounds and their use in cancer therapy in the form of utility models and national and international patent applications. In 2014, three utility model certificates were granted.

The "Gold" Path towards the Treatment of Inflammatory Diseases

Inflammatory illnesses belong among the most painful disease states affecting patients of all age groups and rank among the most common disabling diseases with difficult full recovery. The treatment of complicated inflammatory disorders, especially of the autoimmune origin, is realized, mostly at specialized clinics, by the administration of a gold-based drug auranofin.

The optimization of the structure of this drug by our team has led to the successful preparation of a series of highly effective gold complexes with significant in vitro and in vivo anticancer and anti-inflammatory activity, which in some cases exceeded the activity of the reference standard auranofin and other (e.g. non-steroidal) anti-inflammatory drugs. For this reason, these complexes have been legally protected in the form of two utility models (*CZ 27030 U1, CZ 27032 U1*).

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Grant support:

Centre of Excellence P303/12/G163, 2012-2018:

Centre of Interactions of Dietary Supplements with Drugs and Nutrigenetics,

Co-investigator: Prof. RNDr. Zdeněk Dvořák, DrSc. et Ph.D

GAČR P207/11/0841, 2011-2014:

Functionalized iron oxide nanoparticle-based magnetic carriers with bound biologically active and/or magnetically interesting compounds,

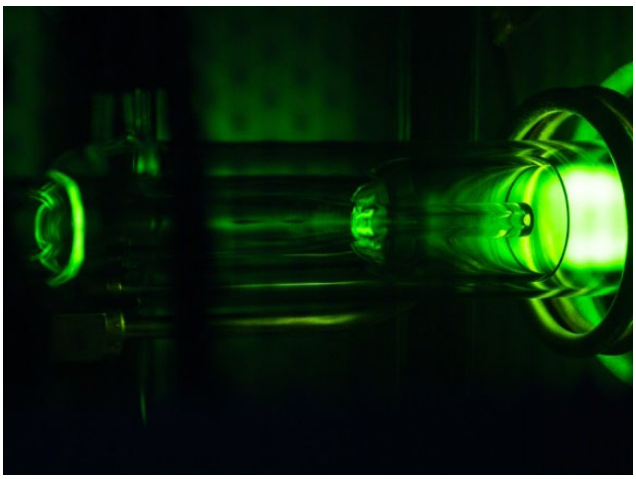
Main investigator: Prof. RNDr. Zdeněk Trávníček, Ph.D.

NANOTECHNOLOGIES IN ANALYTICAL CHEMISTRY

Nanotechnologies are involved today in many fields of human lives. One can meet nanotechnologies, for instance, in the form of nanoparticles in the textile industry (antibacterial silver nanoparticles), in medicine (nanoparticles and liposomes as drug carriers), as miniaturized technologies e.g. in chemistry (analysis of nanoliter-scale samples, nanoreactors) or electronics (nanosensors). An indispensable role in nanotechnology research is played by analytical chemistry which, as a multidisciplinary science, is a rich source of knowledge vital for the development of all of these fields.

Hiding silver

Silver nanoparticles, thanks to their antibacterial properties, have penetrated into many fields of human activity. They can be encountered in textile materials, cosmetics, healthcare products and, last but not least, in clinical research. With a constantly growing number of applications, however, the danger of polluting the environment with silver nanoparticles is also on the rise. For this reason, the team of scientists from RCPTM was established, aimed for the development and validation of a method suitable for determination of trace level of this metal in tissues of laboratory animals. In preliminary experiments using an ICP-MS spectrometer – one of the most suitable analytical instruments for determination of very low (trace) levels of metals – only about a half of expected concentrations were found. Further experiments have shown that the desired result is strongly influenced by the sample mineralization procedure. Consequently, a specific mixture of acids suitable for mineralization and stabilization of samples was proposed, allowing determination of silver using ICP-MS with great accuracy and in unprecedently low concentrations.

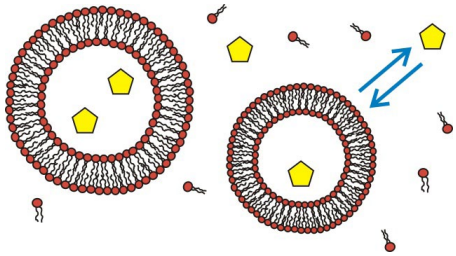


Inductively coupled plasma in the ICP-MS instrument.

The developed method featuring high-performance microwave digestion followed by mass spectrometry with argon plasma ionization was successfully validated using a number of certified reference materials of animal origin *(Spectrochim. Acta B 102, 2014)*.

Liposomes: "Nanoassistants"

Phospholipids, as a natural and inseparable constituent of cell membranes of all plant and animal cells, are substances inherently connected to the life on Earth. A remarkable feature of phospholipids is the formation of bilayers characterized by thickness in the nanometer range. These, according to the surrounding environment, can assume various shapes from spherical vesicles (liposomes) to planar membranes. This feature stems from the structure of phospholipids molecules.



A scheme of liposome interaction.

Phospholipids are species of an elongated shape, having a polar group bound on one end of the molecule and nonpolar fatty acid chains on the other end. While the polar group provides water wettability, the nonpolar chains impart adhesiveness to the lipids and lipid-soluble substances in general. Currently, liposomes are routinely used e.g. in cosmetic preparations or in drug formulations to facilitate transport of active ingredients across the cell membrane into the intracellular space. In our laboratory, we pursue the preparation and utilization of liposomes and phospholipid layers for the purposes of chemical analysis. The surface of a carbon electrode is coated with a thin phospholipid layer (thickness of a few nanometers). This sensor is immersed into a solution containing an investigated oxidizable or reducible compound. If the compound permeates through the layer, a current change is detected on the electrode. Such an approach can be used to study newly synthesized substances, e.g. drug candidates, that need to be assessed in terms of the ability to permeate through cell membranes and get into the intracellular space of target cells. Another possible application is the analysis of small amounts of lipophilic compounds, e.g. pesticides or drugs, in aqueous matrices containing a significant excess of polar substances, especially salts. Under such conditions, the phospholipid layer on the electrode serves as a barrier for the polar compounds that are prevented from getting to the electrode surface and interfering with the analysis. At the same time, the layer can act as a "trap" and accumulate the lipophilic compounds. An increased amount of a compound in the layer causes a greater current signal and, consequently, affords a more sensitive analytical method *(Eur. J. Lipid. Sci. Tech. 116, 2014)*.

Characterization of nanoparticles

When designing novel nanoparticles, we face the issue of monitoring the behaviour of these "very small objects". Basic characteristics can be obtained using electron microscopy, infrared and Raman spectroscopy or light scattering measurements. The group of electromigration techniques is involved in application of capillary electrophoresis in nanoparticles characterization. The technique of capillary electrophoresis reflects the behaviour of nanoparticles in solution. Specifically, it allows studying their dissociation, interactions with other molecules or monitoring reactions occurring at the surface. Capillary electrophoresis is particularly unique in studying interactions since it affords information about nanoparticle behaviour in environments containing e.g. proteins, phospholipids or nucleic acids. In this manner, knowledge about how nanoparticles interact with cells is obtained which facilitates better structural design vital for applications focused on drug delivery into cells.

The investigation of interactions has shown that it is essential to describe the behaviour of nanoparticles in media of various pH values. The influence of pH on the electrophoretic properties of selected nanoparticles was studied. Scientists observed that the extent of aggregation of nanoparticles may change when crossing a boundary between regions of different pH. This conclusion is significant in terms of possible pH deviations in different parts of cells and tissues. It proves that nanoparticles may change structure depending on pH which may alter their interaction with cells and, in turn, their biological activity.

Phytopharmaceuticals

The design of novel drugs is a paramount research direction of contemporary science. Besides purely synthetic approaches, another option is to exploit substances contained e.g. in plants (so-called phytopharmaceuticals). In the liquid chromatography / mass spectrometry research group, we focus on separation techniques enabling the development of phytopharmaceuticals. Specifically, analyses of extracts prepared from white cedar (*Thuja occidentalis*) and greater celandine (*Chelidonium majus*) were performed. Alkaloid profiles related to region and year of harvest were determined for the latter species while phenolic and polyphenolic compounds were monitored in the white cedar extracts. Both plants were historically used for treatment of skin diseases, warts, clavuses and for other medical purposes. The results of the aforementioned analyses will become a basis for preparation of respective medicinal formulations and methods for determination of active ingredients therein. Another important research direction involves metabolic studies investigating the transformation pathways of alkaloids in human organism and monitoring the products of such transformations (*J. Pharm. Biomed. Anal. 102, 2015*). The purpose of metabolic studies is to evaluate the ability of medical preparations to exert a curative effect and detect potential formation of toxic metabolites.

L. Veverkova, S. Hradilova, D. Milde, A. Panacek, J. Skopalova, L. Kvitek, K. Petrzelova, R. Zboril: "Accurate determination of silver nanoparticles in animal tissues by inductively coupled plasma mass spectrometry", Spectrochim. Acta B 102, 7-11, 2014.

H. Svecova, J. Souckova, M. Pyszkova, J. Svitkova, J. Labuda, J. Skopalova, P. Bartak: "Phospholipids improve selectivity and sensitivity of carbon electrodes: Determination of pesticide Paraquat", Eur. J. Lipid. Sci. Tech. 116, 1247–1255, 2014.

C. Cacho, Z. Markova, J. Sevcik, R. Zboril, J. Petr: "Study of behavior of carboxylic magnetite core shell nanoparticles on a pH boundary", J. Chromatogr. A 1364, 59–63, 2014.

J. Vrba, B. Papouskova, M. Pyszkova, M. Zatloukalova, K. Lemr, J. Ulrichova, J. Vacek: "Metabolism of palmatine by human hepatocytes and recombinant cytochromes P450", J. Pharm. Biomed. Anal. 102, 193–198, 2015.

Grant support:

GA ČR, P206/12/1150, 2012-2016

Sampling and efficiency of atmospheric pressure desorption/ionization in mass spectrometric experiment

Main investigator: Prof. RNDr. Karel Lemr, Ph.D.

TA ČR, TA03010458, 2013-2015

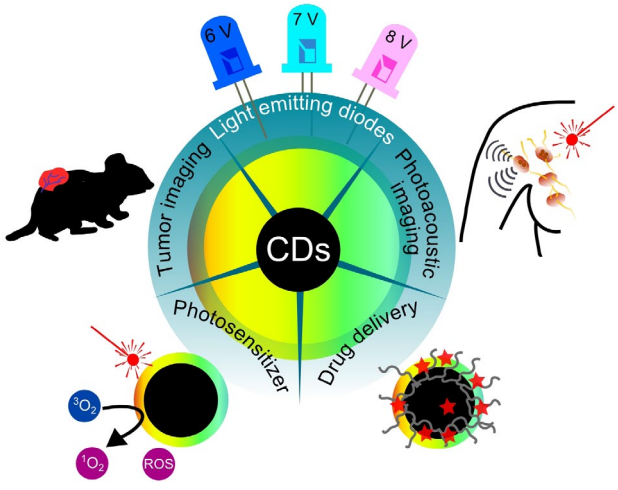
New separation procedures for analytical sample treatment and their application in development of phytopharmaceuticals

Main investigator: Prof. RNDr. Karel Lemr, Ph.D.

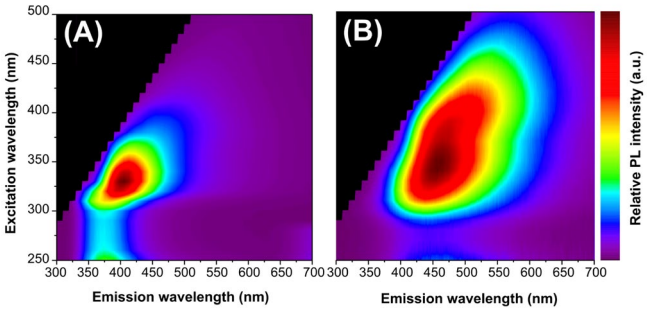
CARBON DOTS – A NEW GENERATION OF NANOMATERIALS FOR DIAGNOSTIC, THERAPEUTIC AND OPTOELECTRONIC APPLICATIONS

Carbon dots (CDs) represent a new emerging class of carbon nanomaterial with unique fluorescent properties. Huge scientific effort has been paid to this material thanks to its high biocompatibility, specific optic properties and size of up to 10 nanometers. The application potential of CDs can be found mainly in cell labelling proved by many *in vitro* studies. Moreover, the recent *in vivo* studies showing the biodistribution of CDs open the doors to other possible applications in diagnoses and therapy. The other fast growing application field of this material except the biomedical one is in optoelectronics, mainly in the field of Light Emitting Diodes (LED). The scientists of RCPTM have revealed some interesting news in the field of CDs in 2014.

Carbon dots (CDs) were accidently discovered in 2004 during the preparation of carbon nanotubes. Carbon nanotubes do not typically exhibit fluorescence in visible range of the spectrum. However, the prepared material exhibited blue, green, yellow and red photoluminescence depending on the mobility in agarose gel. In other words, the prepared sample of CDs emitted different colours under UV light depending on size of the particles. Over the course of time, it has been discovered that this newly discovered material is composed of small carbon particles in the nanometer range (up to 10 nm) with a graphitic structure of the core and high amount of oxygen. These nanoparticles have gained wide popularity in science thanks to their excellent biocompatibility (harmlessness for organism). In comparison with traditional quantum dots based on metal chalocogenides (CdSe, CdTe), CDs do not exhibit any cytotoxicity thanks to their ideal chemical composition (C, N, H, O) without any heavy metals. Therefore, they have found an application in optical imaging of tumours, in cell labelling, LED diodes, photocatalysis or as a component of biosensors. Very perspective is also a utilization of CDs as nanocarrier for drug delivery, in photodynamic and photothermal anticancer therapy or for photoacoustic imaging. The broad spectrum of CDs applications, different methods of their preparation and approaches for controlling their fluorescent properties can be found in recent invited review written by the RCPTM scientists published in 2014 (*Nano Today 9, 2014*).

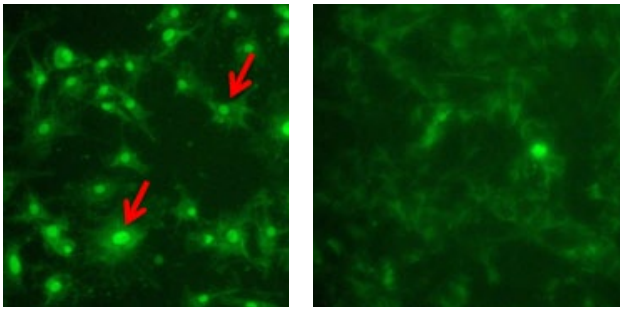


The main applications of carbon quantum dots.



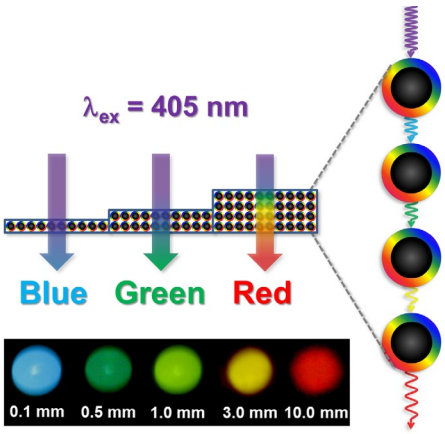
The fluorescent maps of carbon quantum dots showing the effect of surface functional groups on their optical properties.
A) Fluorescent map of CDs with alkyl chains on the surface,
(B) CDs with carboxylic groups on the surface.

The frequently discussed phenomenon of CDs is the origin of their photoluminescence. The most discussed issue is the dependence of the emission maximum (the colour of the fluorescence) on the size of CDs graphitic core and the amount of surface functional groups. The optical properties of CDs are between the semiconductor particles and organic fluorescent dyes (carotenoids, fluorescein etc.) thanks to their aromatic character and nanometer range. The RCPTM scientists brought up new knowledge in the field of controlling the photoluminescence properties of CDs and published it in the journal *Carbon* (*Carbon 70, 2014*). They have been able to determine the size, hydrophilicity and photoluminescence properties of CDs by simple syntheses from organic precursors (derivatives of galic acid with variable length of alkyl chains). The size of the graphitic core determined the colour of the emission of CDs. A bigger carbon dot can reach more intense emission in red region of the spectrum. However, this property can be also observed for surface functional groups. A significant red-shift was observed after simple transformation of prepared CDs with alkyl chains on the surface into the carboxylic groups. This red-shift caused by carboxylic groups can have significant influence on the application of CDs in biomedicine. The prepared particles also exhibited record values of biocompatibility.

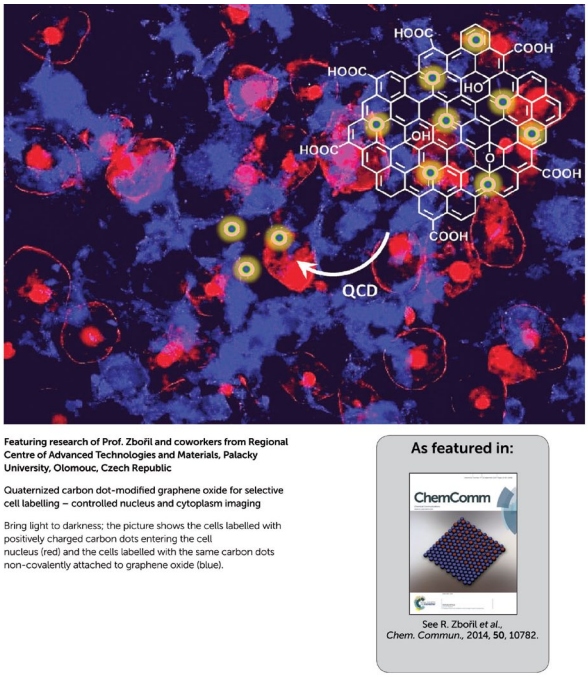


Images of mouse fibroblasts obtained by fluorescent microscope showing selective labelling of the cell nucleus by positively charged CDs (left, the red arrow points the particles in the nucleus) and labelling of the cell cytoplasm by hybrid nanosystem CDs/graphene oxide (right).

The biggest application potential of CDs is in cell labelling for *in vitro* imaging of cell organelles. In the year 2014, the RCPTM scientists developed a unique and selective method for cell labelling. This method was published in the journal *Chemical Communications* and is based on the application of CDs with highly positive charge (*Chem. Commun. 50, 2014*). These particles have an ability to enter the cell nucleus (tested on mouse fibroblasts NIH/3T). However, after coupling of these particles with graphene oxide, the material can be used for labelling of cell cytoplasm. This non-covalent interaction between graphene oxide and carbon quantum dots offers a preparation of well-defined hybrid nanosystem without bleaching of the fluorescence of CDs.



One of the properties of carbon quantum dots is also an ability to emit different colour after excitation by appropriate wavelength. This property can cause an effect known as reabsorption, that can occur in the case that the CDs are captured in gels with different thicknesses. The thinnest gel will emit, in this case, a blue colour after exposition to the violet light. If the gel is wider, the particles will still emit the blue colour after irradiation by violet light. However, this colour will be absorbed by surrounding particles and these particles will emit green light (the gel will be green). In wider and wider gel the re-absorption will be more dominant and the gel will be yellow or even red.



The backside cover art in the journal Chemical Communication showing the work of the RCPTM scientists on selective cell labelling (nucleus versus cytoplasm).

K. Hola, Y. Zhang, Y. Wang, E. P. Giannelis, R. Zboril, A. L. Rogach: "Carbon dots - Emerging light emitters for bioimaging, cancer therapy and optoelectronics", Nano Today 9, 590–603, 2014.

K. Hola, A. B. Bourlinos, O. Kozak, K. Berka, K. M. Siskova, M. Havrdova, J. Tucek, K. Safarova, M. Otyepka, E. Giannelis, R. Zboril: "Photoluminescence effects of graphitic core size and surface functional groups in carbon dots: COO– induced red-shift emission", Carbon 70, 279–286, 2014.

K. K. R. Datta, O. Kozak, V. Ranc, M. Havrdova, A. B. Bourlinos, K. Safarova, K. Hola, K. Tomankova, G. Zoppellaro, M. Otyepka, R. Zboril: "Quaternized carbon dots modified graphene oxide for selective cell labelling – controlled nucleus and cytoplasm imaging", Chem. Commun. 50, 10782-10785, 2014.

Y. Wang, S.Kalytchuk, L. Wang, O. Zhovtiuk, K. Cepe, R. Zboril and A. Rogach: "Carbon dot hybrids with oligomeric silsesquioxane: Solid-state luminophores with high photoluminescence quantum yield and applicability in white light emitting devices", Chem. Commun. 51, 2950-2953, 2015.

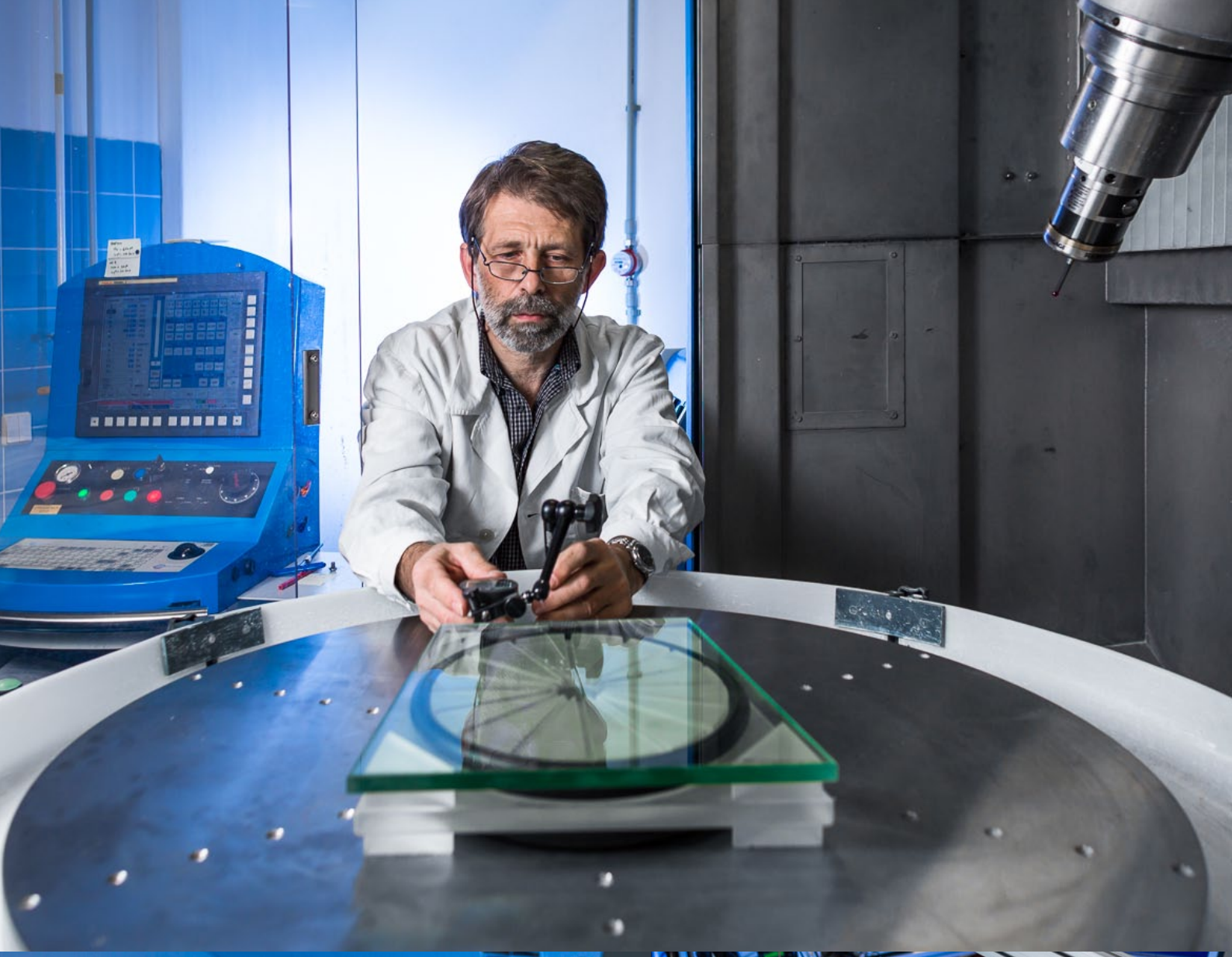
Grant support:

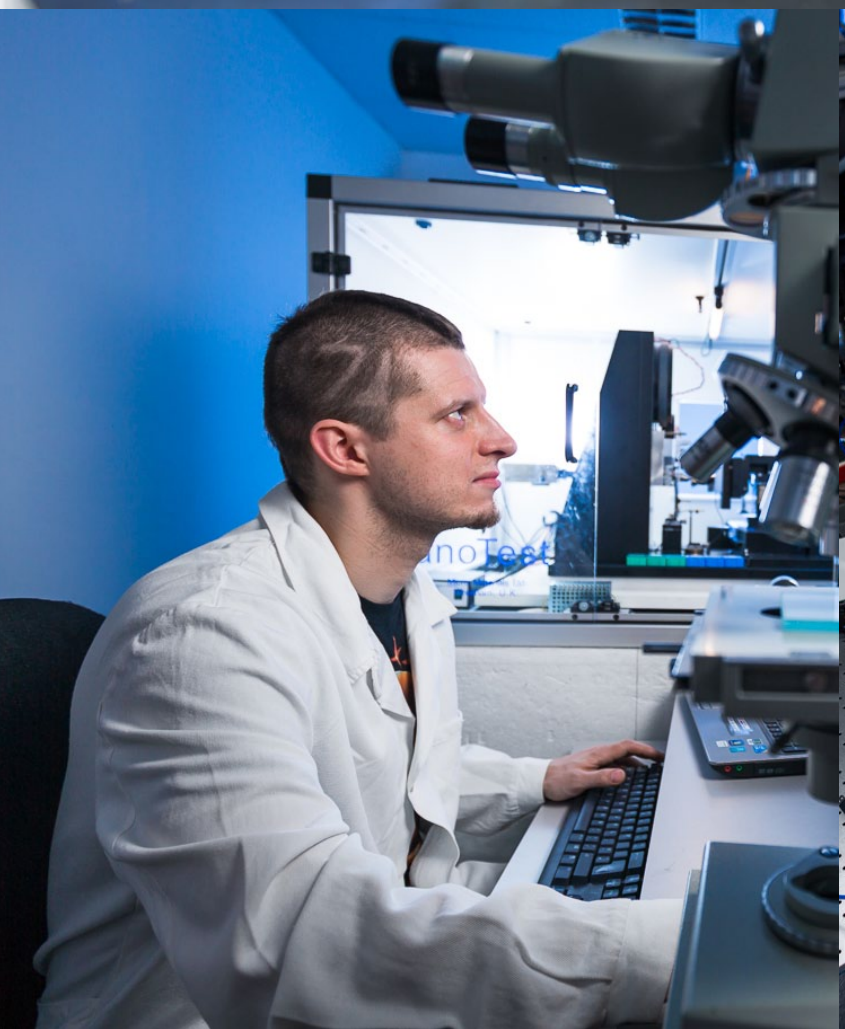
Excellence Centre GAČR P208/12/G016, 2012-2018

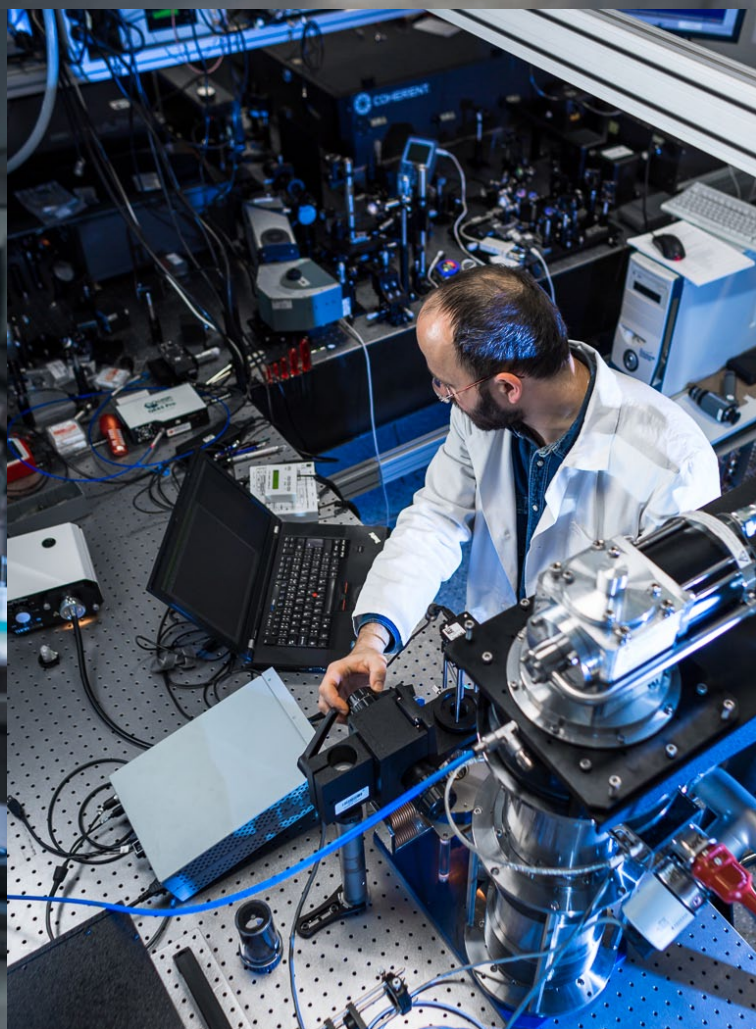
Controlling structure and function of biomolecules at the molecular scale: theory meets experiment

Main investigator: Prof. Ing. Pavel Hobza, DrSc., FRSC;

Project participant: Prof. RNDr. Michal Otyepka, Ph.D.







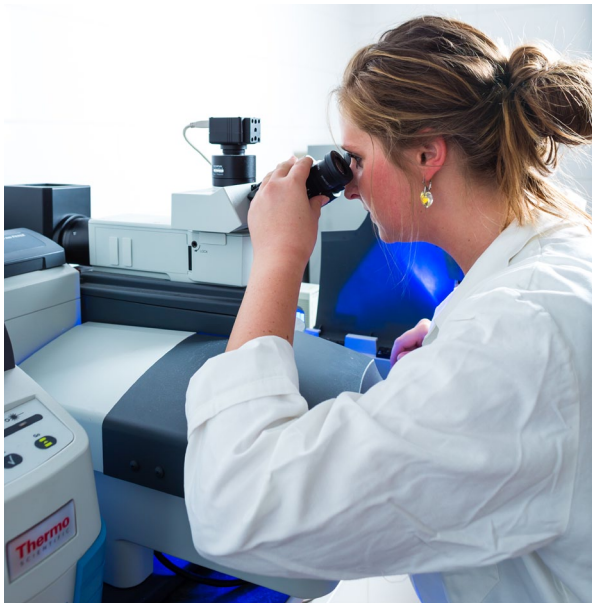
4 APPLICATIONS HIGHLIGHTS

Excellent basic research is a very important building block for quality and commercially attractive applied results. RCPTM is successful, owing to the interconnection with basic research, also as a centre of applied research and it cooperates within a number of projects of The Technological Agency of the Czech Republic, FP7 projects and has contracted research with more than 80 commercial partners, both national and foreign. The RCPTM researchers stand out within the frame of these activities for the technology transfer to the spheres of environment protection, medicine, industrial applications, chemical industry, optics and photonics.

RESEARCH OF SURFACE PROPERTIES OF PIGMENTS

The cooperation of RCPTM and Precheza has proceeded in the last three years in the field of research focused on surface particle properties of titanium white, fundamental product of the above mentioned industrial company. The Precheza emulates with the growing competition in the production and retail of the inorganic pigments by intensive development in the field of quality improvement of its key products, where titaoium white (titanium dioxide) belongs. Research and development cooperation with RCPTM focuses on optimalization of the surface modification of this significant inorganic pigment, with the aim of improving not only the dispersibility of the pigment particles in currently used disperse systems, but predominantly in enhancing the quality of the final coating by polishes containing this pigment, where the important part is played by the covering power and gloss. These physical parametres are influenced by the size of titaoium white particles, as well as by the quality of coating of single particles. RCPTM takes part in the development of quality characterization methods of commonly used coating, and in the first place in the development of new methods of titaoium white pigment particles coating, which will lead to higher quality of final polish films containing this inorganic pigment for the final customer.

Precheza

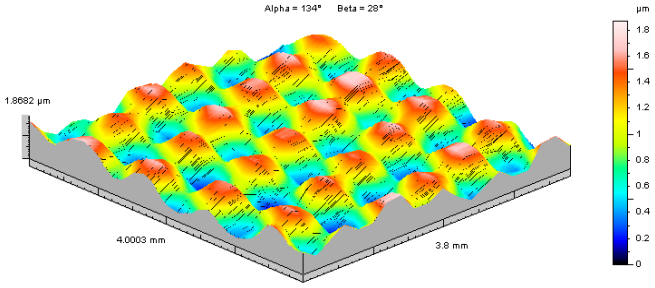


The principal aim of the joint research lies in the development of the technologically usable method of the compact oxide layer preparation, which is being commonly used for the titanium dioxide pigment coating, such as silicon dioxide and aluminum oxide. Such coating improves not only dispersibility of the pigment particles in polish disperses, but at the same time improves the optical properties of the final polish film. Currently, the research cooperation focuses particularly on the understanding of the influence of physically chemical parametres of the coating silicon dioxide and aluminum oxide layers preparation on width and structure of the emerging pigment layers. Another topic of cooperation focuses on the development of new methods of coating characterisation using modern mathematical methods (fractal dimension) of electron microscopy and using the classical methods of coating quality evaluation based on the principle of stating the surface energy of the powder material.

OPTICAL TECHNOLOGIES FOR ENGINEERING

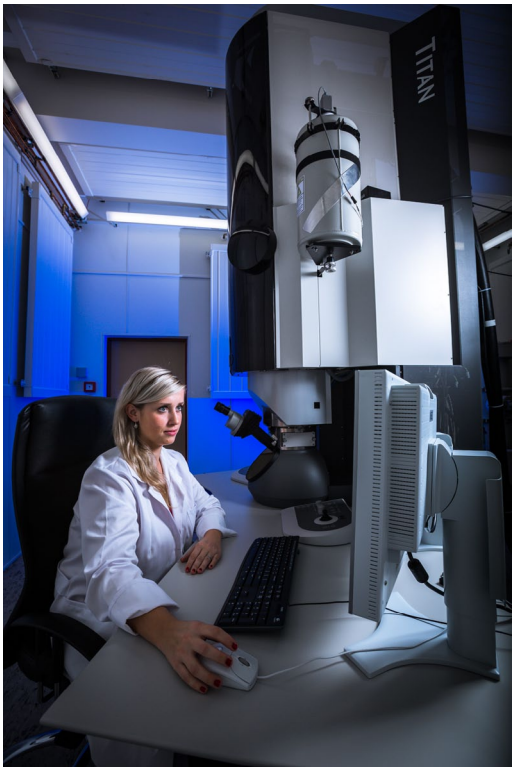
Optics, optoelectronics and photonics bring a wide range of technologies and measuring methods with applications in engineering. RCPTM develops application activities in many engineering branches, especially by applying its research results in nonstandard optical elements, appliances and instruments. In the field of optic and laser technologies, the applications are focused on calculations and realizations of nonstandard optical elements, related technologies, and control and analytical measuring methods. One of the examples is the axonometrical view of the small space (see the picture) app. 4 x 4 mm of plastic car headlamp surface. From such obtained data it is possible to find out, with high accuracy, the dimensions of very fine details on the surface of solids and correct reversibly the manufacturing technology of the headlamp optical parts.

The surface materials and thin micro/nano layer structure properties are being analyzed for the customers also using the nanoindentation methods (measuring of local mechanical properties). RCPTM also produces complex optoelectronic appliances. One of the applications in the branch of monitoring and managing the flow line production is the unique device for controlling the colour marking of coiled car springs or control software for the optimalization of this production. The example of the nonstandard techniques might be the new generation of the appliance for visualisation, monitoring and analysis of burning process in the real time in heating boilers, steel and cement furnaces etc., or optical sensors and guidance system for power plant reactors service.



Topography of the plastic car headlamp.

THE USE OF MICROSCOPIES FOR THE PHARMACEUTICAL AND CAR INDUSTRIES



Microscopic measurements belong among the methods which are most widely used by the external subjects, both industrial and academical. The scanning electron microscopy and the atomic force microscopy characterise the aggregate sizes and crystal surfaces of API substances for TEVA company. Another industrial company, for which the regular microscopic analyses are carried out, is Mubea. It uses the scanning electrone microscopy including analytical methods for defectoscopy of the surface layers of components for the car industry. The NanoComposix company makes use of the complex RCPTM microscopy park for the description of size morphological and structural nanomaterial properties.

NANOPARTICLES IN THE DEVELOPMENT OF NEW FUNCTIONAL PACKAGES

The development of new types of active package foils intended for use in both food-processing and non-food fields is the long-term subject of cooperation with the Invos company. The active function (antibacterial activity, oxygen removal, diffusion barrier) of the developing foils is given by the incorporation of the technologically progressive materials, such as nanomaterials or natural substances, into the package foil structure. Recyclable foils constructed in this way decrease material and energy losses connected with their production and durability of the packaged products.

invos®
výroba obalových materiálů, flexotisk

hopi popi®

The content of the cooperation with the Hopi Popi company was the technology verification of the preparation of papers highly filled by inorganic filling agents based on kaolin with the aim of increasing their resistance against the exfiltration of food fats and moisture. Also the verification of the surface modification technology of package materials based on ferromagnetic pigments suitable for effective microwave energy absorption and its transfer to food-stuff (e.g. pizza, popcorn etc.) took place. The aim of the cooperation is the technology transfer from the laboratory to pilot scale and the attestation of the production effectivity and resulting utility of these packages in the final application (e.g. popcorn).

COMPUTATIONAL PREDICTIONS OF THE SKIN PERMEABILITY AS AN ALTERNATIVE TO TESTING ON ANIMALS

P&G

The skin represents the biggest and so far the most neglected human body organ, which is the first protective shield against adverse effects of the environment. For the application of cosmetics it is necessary to be acquainted with mechanisms of permeability of chemical substances through the skin layers. The cooperation with Procter and Gamble company is based especially on the investigation of physico-chemical properties of chemical substance permeability through skin. Such research is always connected with testing on animal and human tissues, which, however, brings along a number of ethical questions.

The RCPTM workplace evolved methods which can be used for these purposes and for which the tests on animals and humans are not necessary. The advantage of computer simulations is their limitless reproducibility, possibility of immediate modification and quick reaction. The only and the biggest public EDETOX test database contains 2,500 measurements, which together with a number of substances included in REACH database (12,276) offer place for big added value. It can be said, that according to the ChEMBL statistics, there are app. 1.4 million of such compounds.

BREAKTHROUGH NANOTECHNOLOGIES FOR THE ENVIRONMENT

RCPTM is involved in key national and international projects for water and soil treatment. The common factor of all of these applications are nanomaterials which are being developed at RCPTM. The biggest help so far are iron nanoparticles. They alternate the physico-chemical parametres of groundwater, react with certain types of pollutants and are capable of removing them in a chemical way absolutely, or transform them from highly toxic soluble substances into less toxic solid phase.

Tens of toxic substances can be removed from the water owing to nanotechnologies and it can be contributed to disposal of the old ecological load connected with former non-ecological production or the stay of the Soviet army troops. The high effectiveness of the new technologies has been proven in pilot treatment as well as in real practice. They helped to clean, for example, the premises of the industrial complex in Hořice, Podkrkonoší, where the groundwater was contaminated with chlorohydrocarbons. In the premises of Kara company (Trutnov) they contributed to the removal of groundwater contamination with hexavalent chromium, which is widely used in the fur industry. Nanotechnologies have played an important role in solving two other serious ecological problems of today – the presence of cyanobacteria in natural waters and the presence of arsenic in drinking water in many Asian countries, as well as in Europe, the USA and South America.

Cooperating companies

AECOM

mega

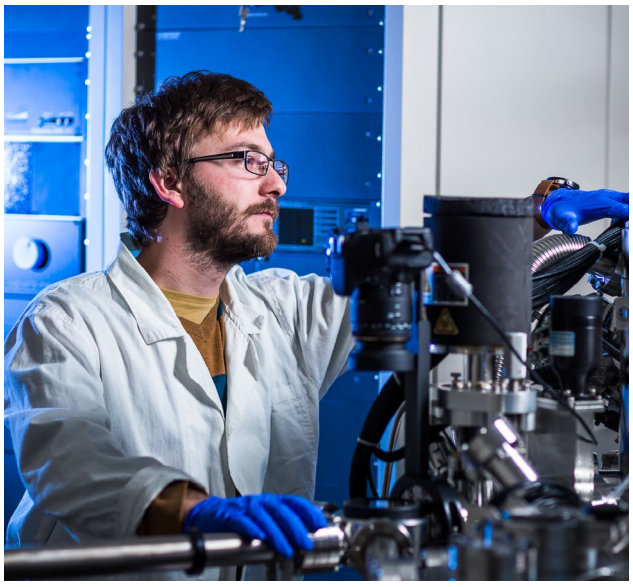
aquatest

Asio čištění a úprava vod

GEOtest

dekonta

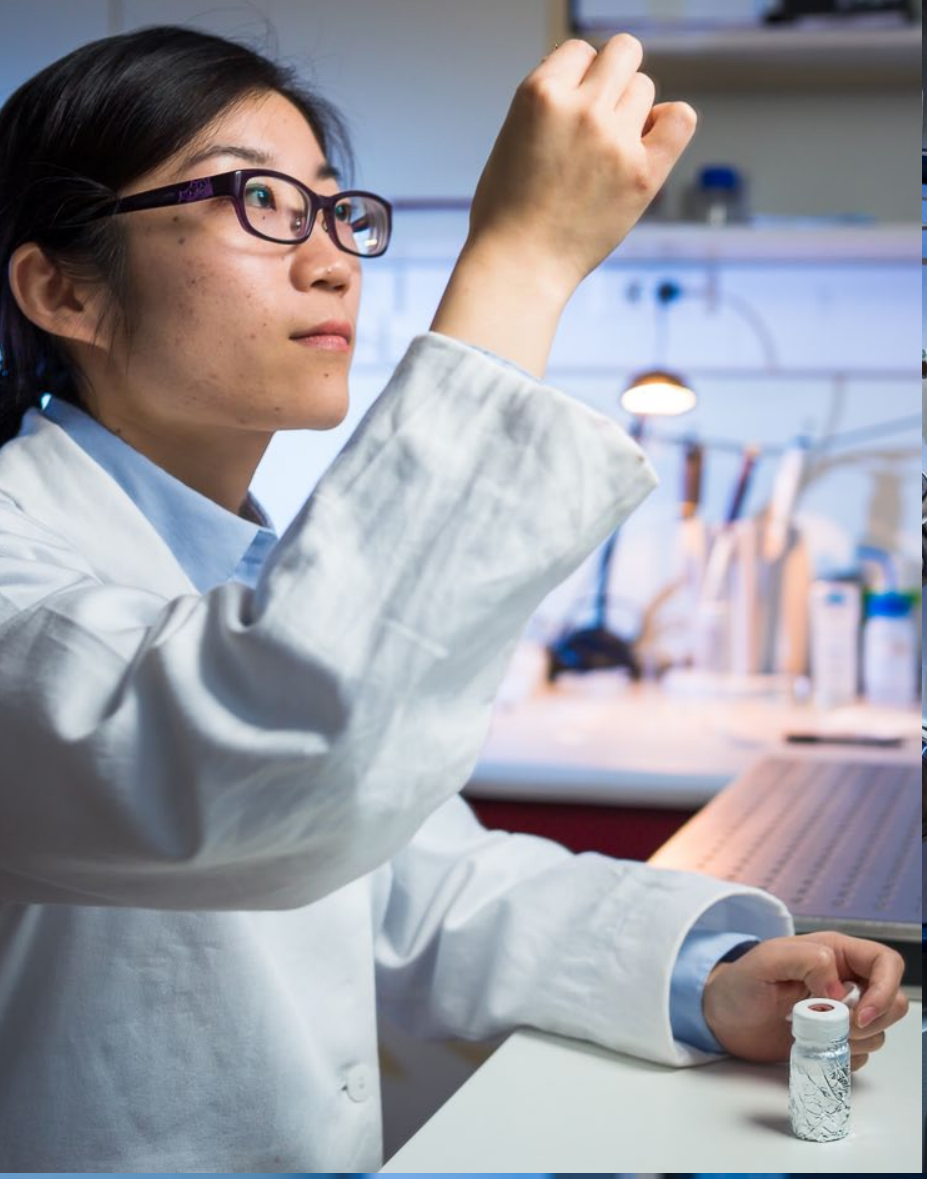
NANOPARTICLES FOR THE ADVANCED BIOTECHNOLOGIES – LACTOFERIN SEPARATION

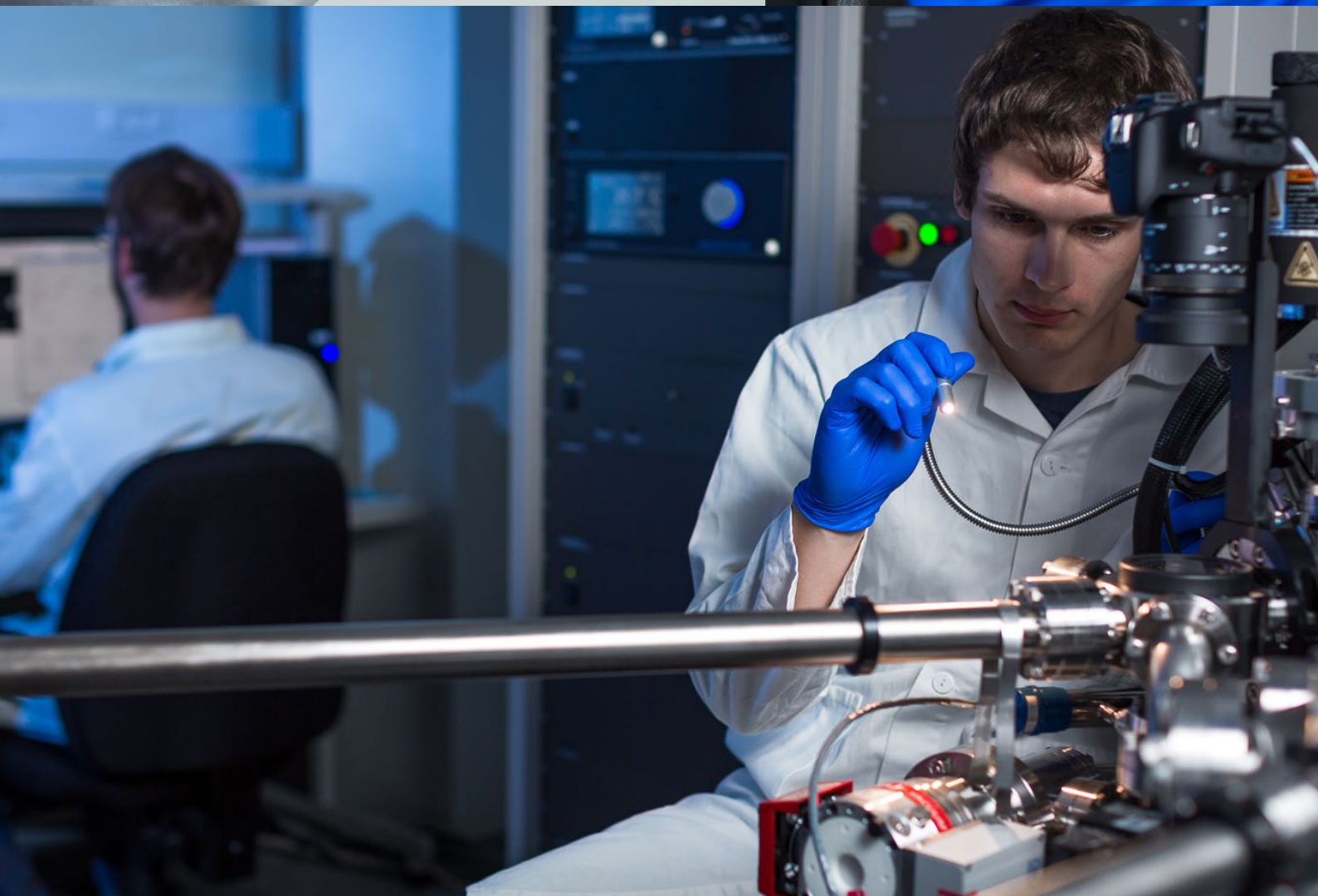


In the frame of cooperation with the Ingredia company, RCPTM develops new technology of the magnetic lactoferin separation from cow's milk. Lactoferin is a basic glycoprotein, which has antimicrobial and anticarcinogenic effects. Unfortunately, even the ordinary pasteurisation depreciates this protein in such a way, that the consumer receives it in an inactive form. The result of the cooperation will be the unique technology which will be able, owing to magnetic nanoparticles, to separate this active protein before the pasteurisation and keep in this way its highly useful properties.

ingredia

GRAN MORAVIA





5 RCPTM – AN INTERNATIONAL CENTRE OF RESEARCH AND EDUCATION

One of the chief objectives since the very beginning of The Regional Centre of Advanced Technologies and Materials has been the achievement of a high level of internationalisation on all levels. Historically, the name RCPTM has been connected with a great deal of prestigious foreign collaborations and many international scientific capacities act in the Centre across all of its groups. Also in 2014, a few significant personalities of the world chemical and materials research field joined the activities of RCPTM. The Centre has become, in this manner, a harbour for a number of researchers who, under the colours of RCPTM, submit projects to the European Research Council (ERC) and in the Maria Curie-Skłodowska programme.

Foreign Scientists about RCPTM

Prof. Dr. Patrik Schmuki

FRIEDRICH-ALEXANDER UNIVERSITÄT ERLANGEN-NÜRNBERG

Head of the Surface Chemistry Group
Friedrich-Alexander University,
Erlangen-Nuremberg, Germany

- **Highly Cited Researcher 2014 (Thomson Reuters Award)**
- **H-index: 72**
- **More than 500 publications with more than 20,000 citations (according to the Web of Science)**

"I had the pleasure to visit the RCPTM for the first time this year in the frame of the Rudolf Zahradník Lecture Series. I was highly impressed by the width and depth of the research activities pursued at the Center, as well as by the very warm welcome from my hosts. The research center certainly offers great opportunities for research from many important fields of science and technology, and the research topics tackled cover many of the most significant future challenges, such as various projects related to energy research and life sciences. During the personal encounters at the Center I could feel the excitement and motivation of the researchers.

This certainly has been the key to the success of the Center, which is demonstrated by the excellent academic output.

I am therefore very happy to have established a collaboration between my group in Erlangen and the RCPTM in the field of functional oxide nanostructures. I believe that this collaboration will be very fruitful and lead to even more novel and exciting findings."

Joint publications in 2014:

S. Kment, Z. Hubicka, J. Krysa, D. Sekora, M. Zlamal, J. Olejnicek, M. Cada, P. Ksirova, Z. Remes, P. Schmuki, E. Schubert and R. Zboril: "On the improvement of PEC activity of hematite thin films deposited by high-power pulsed magnetron sputtering method", APPLIED CATALYSIS B: ENVIRONMENTAL, vol. 165, pp. 344-350, 2015.

Prof. Kwang S. Kim

UNIST
ULSAN NATIONAL INSTITUTE OF SCIENCE AND TECHNOLOGY

Director of the Center of Superfunctional Materials
Ulsan National Institute of Science and Technology (UNIST)
The School of Natural Science, Ulsan, South Korea

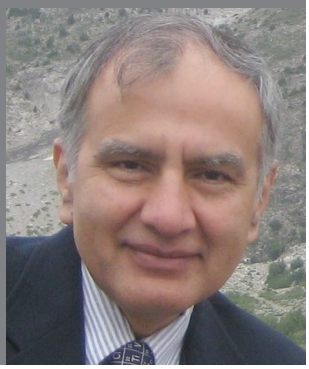
- **One of the TOP 500 chemists in South Korea (2011)**
- **H-index: 70**
- **More than 400 publications with more than 25,000 citations (according to the Web of Science)**

"Creativity, commitment, conviction. These are some words that spring to mind when I consider my collaboration with Prof. Zboril and other colleagues at RCPTM. RCPTM is still a young research center, but a quick glance at their accomplishments would not leave you thinking that. Any new research center requires strong leadership and key members who can drive it forward by making smart decisions which are in the best interest of the center. In this vein, there have clearly been smart choices made at RCPTM, as the output and the quality of the research is growing year by year. The future of RCPTM should be bright when one looks at its past performance, as well as the infrastructure that has been put in place. These factors, combined with the motivated staff and students as well as educational and industrial collaborators, surely can only lead to a bright future. With all of this in mind, it is with eagerness that I look forward to future collaborations with RCPTM."

Joint publications in 2014:

J. Tucek, K. C. Kemp, K. S. Kim and R. Zboril: "Iron-Oxide-Supported Nanocarbon in Lithium-Ion Batteries, Medical, Catalytic, and Environmental Applications", ACS NANO, vol. 8, iss. 8, pp. 7571-7612, 2014.

Dr. Rajender S. Varma



Head of the National Risk Management Laboratory
U. S. Environmental Protection Agency
Cincinnati, Ohio, USA

- **Holder of the "Visionary of the Year 2009" award by VeruTEK company**
- **H-index: 70**
- **More than 600 publications with more than 17,000 citations (according to the Web of Science)**

"I strongly believe the everything is chemistry and it clicked when I had Prof. Zboril in my lecture at the Regional Centre of Advanced Technologies and Materials (RCPTM) couple of years back. In view of our similar and intense love for what we engage in everyday, we formed a bond instantaneously. The vision of Radek to have a world-class interdisciplinary research center and to ensure the diversity of researchers, both in terms of discipline and their origin, is very much aligned with my life-long thinking. Indeed, the facilities have come a long way in a very short span of time and I am sure it will be an exemplary center for everyone to behold in not-so-distant future. Endowed with the proper vision and a cluster of enthusiastic and hardworking researchers, this dream will soon translate into a reality. I am glad and honored to be associated with Radek and the research center we all call home."

Joint publications in 2014:

M. B. Gawande, A. K. Rathi, J. Tucek, K. Safarova, N. Bundaleski, O. M. N. D. Teodoro, L. Kvitek, R. S. Varma and R. Zboril: "Magnetic gold nanocatalyst (nanocat-Fe–Au): catalytic applications for the oxidative esterification and hydrogen transfer reactions", GREEN CHEM., vol. 16, iss. 9, pp. 4137-4143, 2014.

Z. Markova, P. Novak, J. Kaslik, P. Plachtova, M. Brazdova, D. Jancula, K. M. Siskova, L. Machala, B. Marsalek, R. Zboril and R. Varma: "Iron(II,III)–Polyphenol Complex Nanoparticles Derived from Green Tea with Remarkable Ecotoxicological Impact", ACS SUSTAINABLE CHEM. ENG., vol. 2, iss. 7, pp. 1674-1680, 2014.

S. N. Shelke, S. R. Bankar, G. R. Mhaske, S. S. Kadam, D. K. Murade, S. B. Bhorkade, A. K. Rathi, N. Bundaleski, O. M. N. D. Teodoro, R. Zboril, R. S. Varma and M. B. Gawande: "Iron Oxide-Supported Copper Oxide Nanoparticles (Nanocat-Fe-CuO): Magnetically Recyclable Catalysts for the Synthesis of Pyrazole Derivatives, 4-Methoxyaniline, and Ullmann-type Condensation Reactions", ACS SUSTAINABLE CHEM. ENG., vol. 2, iss. 7, pp. 1699-1706, 2014.

M. B. Gawande, S. N. Shelke, R. Zboril and R. S. Varma: "Microwave-Assisted Chemistry: Synthetic Applications for Rapid Assembly of Nanomaterials and Organics", ACC. CHEM. RES., vol. 47, iss. 4, pp. 1338-1348, 2014.

S. S. Kahandal, S. R. Kale, M. B. Gawande, R. Zboril, R. S. Varma and R. V. Jayaram: "Greener iodination of arenes using sulphated ceria–zirconia catalysts in polyethylene glycol", RSC ADVANCES, vol. 4, iss. 12, pp. 6267, 2014.

Prof. Andrey Rogach

香港城市大學
City University of Hong Kong

Director of the Centre for Functional Photonics
Department of Physics and Materials Science
City University of Hong Kong

- **8th place among "20 TOP AUTHORS publishing on nanocrystals in the past decade"**
- **H-index: 72**
- **More than 300 publications with more than 19,000 citations (according to the Web of Science)**

"I enjoy my collaboration with RCPTM colleagues. The team is dynamic and truly international, which makes this Centre a perfect location for Czech and international students and postdocs to advance their careers. I was very happy to contribute to their team build-up by recommending two of my former PhD students and postdocs (a Chinese and a Ukrainian) to move to Olomouc to join RCPTM. Thanks to the competitive support from the European Union funds, the Centre is perfectly equipped with a wide range of analytical and structural characterisation of (nano) materials, including a very advanced HRTEM, which my Czech colleagues generously offered us for joint use. The team of its director, Prof. Zbořil, has long-term experience in carbon dots and related carbon nano-allotropes, including the bio-applications of these materials, and this is one topic of our ongoing collaboration where my own group in Hong Kong contributes with the material synthesis and optical spectroscopy expertise. Another active topic of our efforts is on composite oxides for lithium ion batteries, where we have already published a half-dozen well-cited papers. We are currently actively exploring possibilities to attract extra funding for our joint research, and I am very much looking forward to the extension of our collaboration and to the bright future of RCPTM."

Joint publications in 2014:

Y. Wang, S. Kalytchuk, L. Wang, O. Zhovtiuk, K. Cepe, R. Zboril, and A. Rogach, "Carbon dot hybrids with oligomeric silsesquioxane: Solid-state luminophores with high photoluminescence quantum yield and applicability in white light emitting devices," CHEM. COMMUN., vol. 51, iss. 14, pp. 2950-2953, 2015.

K. Hola, Y. Zhang, Y. Wang, E. P. Giannelis, R. Zboril and A. L. Rogach: "Carbon dots—Emerging light emitters for bioimaging, cancer therapy and optoelectronics", NANO TODAY vol. 9, iss. 5, pp. 590-603, 2014.

H. Wang, M. Wang, B. Li, X. Yang, K. Safarova, R. Zboril, A. L. Rogach, and M. K. H. Leung, "Hydrothermal synthesis and electrochemical properties of tin titanate nanowires coupled with SnO2 nanoparticles for Li-ion batteries," CRYSTENGCOMM, vol. 16, iss. 32, pp. 7529-7535, 2014.

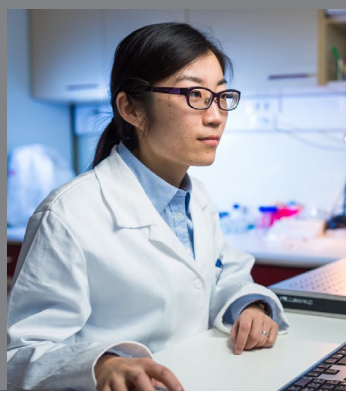
The Rising Generation of RCPTM

Every scientific centre grows due to the way it treats its future in its human resource policy. As, the immortality pill has not yet been invented it is inevitable the best researchers will be one day forced to hand over the reigns to the next generation. The average age of the Centre's employees in 2014 did not exceed 35 years old. This was part in thanks to the involvement of many young scientists from both the Czech Republic and abroad, in Ph.D. positions as well as Junior researcher positions.

Mgr. Sandra Štěpánková

"I began my academic studies at the Faculty of Science, Charles University in Prague, where I received my bachelor's degree in chemistry in 2012. During the bachelor study I was working at the Jaroslav Heyrovský Institute of Physical Chemistry where I gained valuable experience and it was there where I first came across the topic of nanomaterials. It was my colleague from the J. Heyrovský Institute who told me about his studies in Olomouc, where he studied Material Chemistry – a field of study that interests me. I started to become more interested in the possibilities in my hometown, Olomouc. New research centres were arising and there was an indubitable growing potential that Olomouc has had to offer. After the first weeks of my study of Material Chemistry in Olomouc I knew that my choice was good. In my diploma thesis I was dealing with nanomaterials - quantum carbon dots. The possibility to study and to get to know two different universities was (and still is) for me very valuable. Still I wanted to and I was quite persuaded to study the PhD program in Prague. But after some time of studying in Olomouc, the city, our University and mainly the RCPTM enthused me so much that I decided to stay here. In June 2014 I received my master's degree and since September I have been studying in the PhD program at the Palacký University and RCPTM. The possibility to work at RCPTM means I can do work that I enjoy, among a team of capable people in a modern, fully-equipped centre. It is a job that motivates me and pushes me to improve myself. It also allows me to travel, gain new experience, new contacts and improve my English. RCPTM is an exquisite centre and I am grateful to be a part of it."

MEng. Lingyun Wang



"After four years of working in the photovoltaic industry, I went to City University of Hong Kong as a research assistant for continuing my scientific research. In late 2013, my husband got a good opportunity to work as a Junior Researcher at RCPTM, and at the same time Prof. Zbořil kindly offered me a PhD position. Thus, we made a decision to come to the Czech Republic together. We were very impressed by the warm-hearted and helpful colleagues in RCPTM as well as the state-of-the-art instruments. In RCPTM, scientific researchers with different expertise and background not only can share ideas and discuss questions within the Center, but also have a great opportunity to visit and cooperate with other advanced labs around the world. I am happy here that I can work with these outstanding researchers and learn from the brilliant professors to broaden my scientific horizons and improve my research capabilities. Building a photoelectrochemical testing system here is a good challenge and opportunity for me, where I could have the chance to use what I have learnt in HK, also to continue the research I am fond of. The training and skills I learned in this big family will benefit me for a lifetime."

Dr. Manoj B. Gawande

"When, I joined RCPTM, last year in July 2013, there were less facilities for catalysis and nanocatalysis research. When I shared my ideas with Prof. Radek Zboril (Director, RCPTM), he was very supportive to provide all necessary funding for the establishment of "Nanocatalysis Research Group". He has a great vision of multidisciplinary research, and is always ready to support new ideas including all necessary facilities required for research. My research interests are supported nanocatalysis, core-shell nanomaterials, magnetically recyclable nanomaterials, and their applications for organic transformations by using various advanced tools including continuous flow reactor etc. In general, the catalysis research in our group unites together heterogeneous, photo- and bio-catalysts for the industrial and academic sectors. We focus mainly on the design, growth and expenditure of nanocatalysts/catalysts for the organic transformations, catalytic applications, and environmental applications. I strongly believe that every year publications and patents output are increasing tremendously."

6 RCPTM IN 2014

THE RUDOLF ZAHRADNÍK LECTURE SERIES

RCPTM organizes a unique and internationally significant lecture series connected with the worldwide known name of this Czech scientist. The Rudolf Zahradník Lecture Series is an honorary lecture series organized under the patronage of the director of the Regional Centre of Advanced Technologies and Materials, Radek Zbořil. The ambition is to introduce the most famous and the most successful world scientists, particularly from the field of chemical, materials and physical research, to the Czech world.

Prof. Ing. Rudolf Zahradník, DrSc. was born in 1928 in Bratislava. In 1952 he graduated from the Institute of Chemical Technology in Prague. Rudolf Zahradník´s first place of work was the Institute of Work Hygiene and Occupational Diseases where he studied the relationships between structure and biological effectiveness. He was one of the first people in the Czech Republic who started to deal with quantum chemistry. In 1961 he joined the Institute of Physical Chemistry of the Czechoslovak Academy of Sciences where he was the Head of the Applied Quantum Chemistry Department for many years. Later on, he was the leader of Chemistry Reactivity Theory Group in the same institute. He habilitated at the Faculty of Sciences of Charles University in 1968 in the field of physical chemistry, and became the professor at the same faculty in 1992. Between the years 1965 – 1990 he was the visiting scientist at eleven European universities. In 1990 he became the Head of the J. Heyrovský Institute of Physical Chemistry of the Czech Academy of Sciences. He was elected the first president of the Czech Academy of Sciences in 1993 and, in 2001, its honorary president. In 1994 he also became the first president of the Learned Society of the Czech Republic. For his contribution to the Czech science and society prof. Zahradník was honoured by many awards; in 1998 he was given the State Award of the Czech Republic by President Václav Havel for the contributions to scientific and social activities.

Prof. Ing. Rudolf Zahradník, DrSc. *source: www.cas.cz*

"Prof. Zahradník is a doyen of Czech chemistry, the pioneer of the quantum and computational chemistry. Many significant scientific works can be found under him, as well as students who grew up under his leadership into the world science personalities. The fact that he lent his name to the lecture series, means honour not only for RCPTM itself, but also for the whole university. I believe, that in future this series will be tightly connected to the name of Palacký University just like, for example, the Academia film Olomouc," said the director of RCPTM prof. Zbořil after the opening of the series.

Rudolf Zahradník joined his name with the series with feelings of joy and gratefulness. "Man would have to be conceited to take the compliment which I was given here, as something ordinary. As God is my witness, I do not consider it in this way," said prof. Zahradník during his introductory lecture of this series.

During the two years that the series has been in progress, Olomouc has welcomed Professor Josef Michl of Colorado University, Andrey Rogach from Hongkong, Mark Ratner from Chicago, Wolfgang Lindner from Vienna, Patrik Schmuki from German Erlangen and Mario Ruben from Karlsruhe - all belonging to the most distinguished representatives of the current chemistry world.

Prof. Josef Michl

October 10, 2013

University of Colorado & IOCB AS CR

"Alkylation of Gold Surfaces"

Prof. Andrey L. Rogach

November 14, 2013

City University of Hong Kong

"Functional Hybrid Structures of Semiconductor and Metal Nanocrystals"

Prof. Rudolf Zahradník

March 26, 2014

J. Heyrovsky Institute of Physical Chemistry, AS CR

"A Word about Chemistry in Our Country and Abroad"

Prof. Mark A. Ratner

November 25, 2013

Northwestern University

"Molecular Mesoscopics: Transport in Molecular Junctions"

Prof. Patrik Schmuki

May 7, 2014

Friedrich-Alexander-Universität Erlangen-Nürnberg

"Self-organized TiO_2 Nanotube Arrays: Formation, Properties, Applications"

Prof. Wolfgang Lindner

February 14, 2014

University of Vienna

"Chromatographic Resolution of Enantiomers on Chiral Ion Exchanger: Conceptional Reflections"

Prof. Mario Ruben

May 20, 2014

Karlsruhe Institute of Technology

"(Supra)Molecular Quantum Spintronics"

NANOCON

The Regional Centre of Advanced Technologies and Materials became, for the fourth time, one of the organizers of the international conference Nanocon, which during its existence has achieved the reputation of one of the best events among European nanotechnological symposiums. Prof. Zbořil is, at the same time, the main scientific guarantor of this international meeting, which took place in Brno, Czech Republic, in 2014. More than 400 participants from over 40 countries presented their research results in the fields of preparation, characterisation and applications of nanomaterials.

Nanocon is the first Czech conference concentrating entirely on nanomaterials, their investigation, applications and potential influence on the environment and human health. In individual sections scientists deal with controlled nanostructures preparation, bionanotechnologies, nanomaterials for medicine or industrial and environmental nanoparticle applications. Also, Olomouc´s scientists presented their results here. The youngest take part in the Dr. Tasil Prnka Award competition for young scientists under the age of 30, which was won by Eleni Petala from RCPTM in 2013.

2014 NANOCON®

This year belonged, without question, among the most successful ones in regard to both the number of participants and the quality of single entries. More than 400 participants from more than 40 countries enrolled working in the various spheres of nanotechnologies – from theoretical and computational chemistry to representatives of academical background and companies presenting the nanomaterial applications in practice. Just like every year, this year the brilliant names of the scientific world accepted the invitation to this outstanding meeting.

Among the speakers was professor Michael Grätzel from Swiss Federal Institute of Technology in Lausanne, who belongs among the ten most highly cited scientists of the world (H-index 176). His name is a regular participant among the names of Nobel Prize candidates, especially thanks to the discovery and revolutionary papers about the use of nanomaterials in direct solar water splitting. No less distinguished was the world renowed polymer chemist Krysztof Matyjaszewski from Carnegie Mellon University in Pittsburgh. He gained in the scientific world vast publicity for the discovery of atomic radical polymerisation – a new method of the polymer synthesis which represents revolution in the creation and macromolecules organisation manner and provides possibilities in the new materials development. Prof. Matyjaszewski is the author of more than 50 US patents and more than 1,000 publications with more than 65,000 citations.

B R N O

Conference venue – hotel Voroněž, Brno, Czech Republic.

Meeting during the Nanocon conference 2014 in front of the Holy Trinity Column, Olomouc. From left side: Prof. Alexander Eychmüller, Prof. Radek Zbořil, Prof. Dionysios D. Dionysiou, Prof. Krysztof Matyjaszewski, Ing. Tasilo Prnka and Dr. Athanasios B. Bourlinos.

Grant Successes

Also in 2014, the employees of Regional Centre of Advanced Technologies and Materials were successful in many grant competitions and they submitted a number of projects now waiting for the evaluation process results. The Centre was successful, predominantly with projects of applied research such as the Competence Centres of the Technology Agency of the Czech Republic, or the Pre-seed Project of the Operational Programme Research and Development for Innovations. When taking into account the long-term point of view, then the obtained support from National Sustainability Programme of Ministry of Education, Youth and Sport is quite significant.

Ministry of Education, Youth and Sport

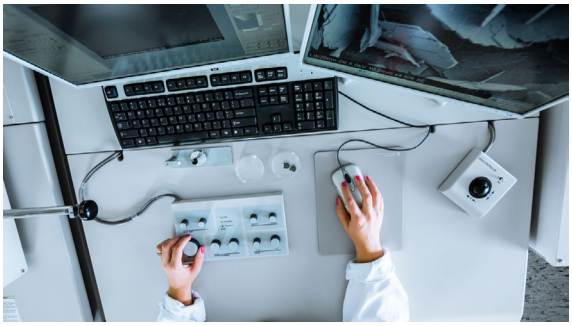
MINISTRY OF EDUCATION, YOUTH AND SPORTS

The Development of the Centre of Advanced Technologies and Materials

MŠMT LO 1305

Principal Investigator: Prof. RNDr. Radek Zbořil, Ph.D.

The main objective of the project is the maintenance and development of the research infrastructure of The Regional Centre of Advanced Technologies and Materials (RCPTM), which was built at Palacký University in Olomouc between the years 2010 – 2014 with the support of OP RDI. The term research infrastructure means not only the outstanding instrument equipment but also quality human resource infrastructure and long-term involvement of the Centre to international research structures.



New Technologies UP in Chemistry and Biology

MŠMT CZ.1.05/3. 1. 00/14.0302

Principal Investigator: Prof. Ing. Lubomír Lapčík, Ph.D.

The aim of the project is to create a quick and flexible system for the support of commercialization and prompt protection of Industrial Property (IP), originating especially in the two OP RDI Centres at UP, based on the connection of the current infrastructure for technology transfer with concrete RD teams.

PRE-SEED

Nové technologie UP v chemii a biologii

http://preseed.upol.cz/

Technology Agency of the Czech Republic

T A
Č R

The Centre for Alternative Environment Friendly High Effective Polymer Antimicrobial Agents for Industrial Applications

TE02000006

Principal investigator at Palacký University:

Prof. RNDr. Radek Zbořil, Ph.D.

The objective of the project is research, development and commercialization proposal for innovative antimicrobiological systems for plastics, coating, cosmetics and textile. Proposed antimicrobial substances will have strong bonds in polymer system, therefore they will protect only the surface of the material without the influence on the environment. This will lead to a long-term protection of treated materials against the effects of antimicrobial attacks excluding the undesirable health and ecological impacts.

alterbio

http://www.alterbio.eu/

Selected Publications and Applied Results

In 2014 RCPTM employees published 220 publications in impacted journals, 40 publications out of these were published in journals with impact factors higher than 5. The Centre also contributed to another 80 collaborative papers within the Pierre-Auger and CERN-Atlas projects.

TOP 40 publications

1. M. B. Gawande, S. N. Shelke, R. Zboril, R. S. Varma: "Microwave-assisted chemistry: synthetic applications for rapid assembly of nanomaterials and organics", Accounts Chem. Res. 47, 1338 – 1348, 2014. IF = 24.35
2. K. Hola, Y. Zhang, Y. Wang, E. P. Giannelis, R. Zboril, A. L. Rogach: "Carbon dots—Emerging light emitters for bioimaging, cancer therapy and optoelectronics", Nano Today 9, 590–603, 2014. IF = 18.43
3. J. Tucek, K. C. Kemp, K. S. Kim, R. Zboril: "Iron-oxide-supported nanocarbon in lithium-ion batteries, medical, catalytic, and environmental applications", ACS Nano 4, 7571 – 7612, 2014. IF = 12.03
4. V. V. T. Doan-Nguyen, S. A. J. Kimber, D. Pontoni, D.R. Hickey, B. T. Diroll, X. H. Yang, M. Miglierini,C. B. Murray, S. L. J. Billinge: "Bulk metallic glass-like scattering signal in small metallic nanoparticles", ACS Nano 9, 6163 – 6170, 2014. IF = 12.03
5. J. Fanfrlik, A. Prada, Z. Padelkova, A. Pecina, J. Machacek, M. Lepsik, J. Holub, A. Ruzicka, D. Hnyk, P. Hobza: "The dominant role of chalcogen bonding in the crystal packing of 2D/3D aromatics", Angew. Chem.-Int. Edit. 10, 10139 – 10142, 2014. IF = 11.34
6. T. Drsata, N. Spackova, P. Jurecka, M. Zgarbova, J. Sponer, F. Lankas: "Mechanical properties of symmetric and asymmetric DNA A-tracts: implications for looping and nucleosome positioning", Nucleic Acids Res. 6, 7383 – 7394, 2014. IF = 8.81
7. T. A. P. de Beer, K. Berka, J. M. Thornton, R. A. Laskowski: "PDBsum additions", Nucleic Acids Res. 42, D292 - D296, 2014. IF = 8.81
8. V. K. Sharma, K. M. Siskova, R. Zboril, J. L. Gardea-Torresdey: "Organic-coated silver nanoparticles in biological and environmental conditions: Fate, stability and toxicity", Adv. Colloid Interface Sci. 204, 15 – 34, 2014. IF = 8.64
9. G. Zoppellaro, A. Kolokithas-Ntoukas, K. Polakova, J. Tucek, R. Zboril, G. Loudos, E. Fragogeorgi, C. Diwoky, K. Tomankova, K. Avgoustakis, D. Kouzoudis, A. Bakandritsos: "Theranostics of epitaxially condensed colloidal nanocrystal clusters, through a soft biomineralization route", Chem. Mat. 12, 2062 – 2074, 2014. IF = 8. 54.
10. A. Panacek, R. Prucek, J. Hrbac, T. Nevecna, J. Steffkova, R. Zboril, L. Kvitek: "Polyacrylate-assisted size control of silver nanoparticles and their catalytic activity", Chem. Mat. 1332 – 1339, 2014. IF = 8.54
11. V. Urbanova, M. Magro, A. Gedanken, D. Baratella, F. Vianello, R. Zboril: "Nanocrystalline iron oxides, composites, and related materials as a platform for electrochemical, magnetic, and chemical biosensors", Chem. Mat. 26, 6653–6673, 2014. IF = 8.54
12. B. Narayanamoorthy, K. K. R. Datta, M. Eswaramoorthy, S. Balaji: "Highly active and stable Pt3Rh nanoclusters as supportless electrocatalyst for methanol oxidation in direct methanol fuel cells", ACS Catal. 4, 3621 – 3629, 2014. IF = 7.57
13. M. B. Gawande, V. D. B. Bonifacio, R. Luque, P. S. Branco, R. S. Varma: "Solvent-free and catalysts-free chemistry: a benign pathway to sustainability", ChemSusChem 5, 24 – 44, 2014. IF = 7.12
14. M. B. Gawande, A. K. Rathi, J. Tucek, K. Safarova, N. Bundaleski, O. M. N. D. Teodoro, L. Kvitek, R. S. Varma, R. Zboril: "Magnetic gold nanocatalyst (nanocat-Fe-Au): catalytic applications for the oxidative esterification and hydrogen transfer reactions", Green Chem. 9, 4137 – 4143, 2014. IF = 6.85
15. S. Sa, M. B. Gawande, A. Velhinho, J. P. Veiga, N. Bundaleski, J. Trigueiro, A. Tolstogouzov, O. M. N. D. Teodoro, R. Zboril, R. S. Varma, P. S. Branco: "Magnetically recyclable magnetite-palladium (Nanocat-Fe-Pd) nanocatalyst for the Buchwald-Hartwig reaction", Green Chem. 11, 3494 – 3500, 2014. IF = 6.85
16. K. K. R. Datta, O. Kozak, V. Ranc, M. Havrdova, A. B. Bourlinos, K. Safarova, K. Hola, K. Tomankova, G. Zoppellaro, M. Otyepka, R. Zboril: "Quaternized carbon dot-modified graphene oxide for selective cell labelling - controlled nucleus and cytoplasm imaging", Chem. Commun. 11, 10782 – 10785, 2014. IF = 6.72
17. W. Liu, X. Bao, L. L. Mao, J. Tucek, R. Zboril, J. L. Liu, F. S. Guo, Z. P. Ni, M. L. Tong: "A chiral spin crossover metal-organic framework", Chem. Commun. 9, 4059 – 4061, 2014. IF = 6.72
18. K. K. R. Datta, O. Kozak, V. Ranc, M. Havrdova, A. B. Bourlinos, K. Safarova, K. Hola, K. Tomankova, G. Zoppellaro, M. Otyepka, R. Zboril: "Quaternized carbon dots modified graphene oxide for selective cell labelling – controlled nucleus and cytoplasm imaging", Chem. Commun. 50, 10782 – 10785, 2014. IF = 6.72
19. K. K. R. Datta, E. Petala, K. J. Datta, J. A. Perman, J. Tucek, P. Bartak, M. Otyepka, G. Zoppellaro, R. Zboril: "NZVI modified magnetic filter paper with high redox and catalytic activities for advanced water treatment technologies", Chem. Commun. 50, 15673 – 15676, 2014. IF = 6.72
20. J. Sponer, P. Banas, P. Jurecka, M. Zgarbova, P. Kuhrova, M. Havrila, M. Krepl, P. Stadlbauer, M. Otyepka: "Molecular Dynamics Simulations of Nucleic Acids. From Tetranucleotides to the Ribosome", J. Phys. Chem. Lett. 5, 1771 – 1782, 2014. IF = 6.69
21. T. Drsata, M. Zgarbova, N. Spackova, P. Jurecka, J. Sponer, F. Lankas: "Mechanical model of DNA allostery", J. Phys. Chem. Lett. 5, 3831 – 3835, 2014. IF = 6.69
22. M. Magro, D. Baratella, G. Salviulo, K. Polakova, G. Zoppellaro, J. Tucek, J. Kaslik, R. Zboril, F. Vianello: "Core-shell hybrid nanomaterial based on prussian blue and surface active maghemite nanoparticles as stable electrocatalyst", Biosens. Bioelectron. 52, 159 – 165, 2014. IF = 6.45

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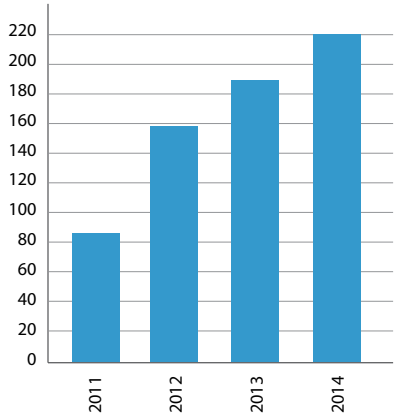
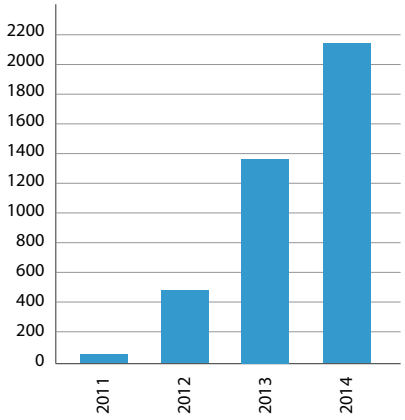
The development of the number and citations of RCPTM publications since 2011



Number of publications without collaborative works



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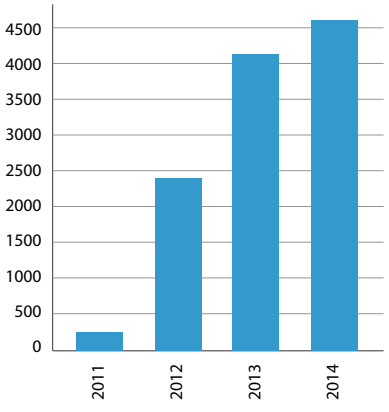
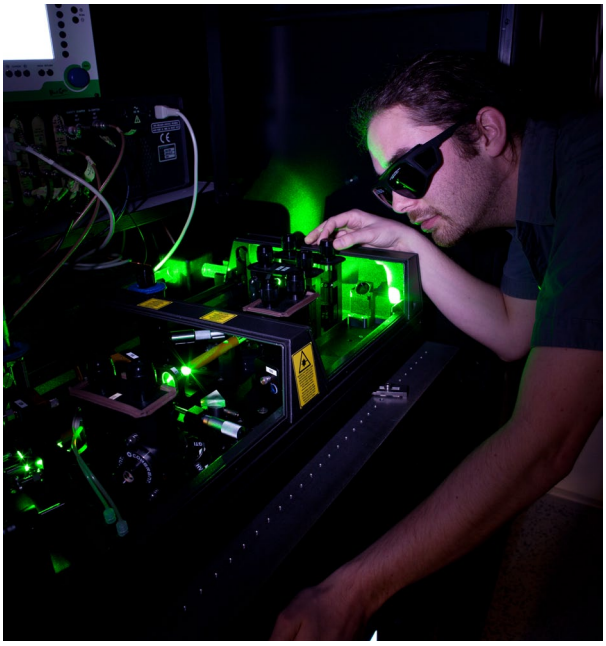


Number of citations with collaborative works

The most significant publications within the Pierre-Auger and CERN-Atlas collaborations

1. ATLAS Collaboration: Search for Scalar Diphoton Resonances in the Mass Range 65-600 GeV with the ATLAS Detector in pp Collision Data at root s=8 TeV. *Phys. Rev. Lett.* (2014) 113171801. DOI = 10.1103/PhysRevLett.113.171801. IF = 7,73.
2. ATLAS Collaboration: Measurements of Four-Lepton Production at the Z Resonance in pp Collisions at root s=7 and 8 TeV with ATLAS. *Phys. Rev. Lett.* (2014) 112231806. DOI = 10.1103/PhysRevLett.112.231806. IF = 7,73.
3. ATLAS Collaboration: Search for Invisible Decays of a Higgs Boson Produced in Association with a Z Boson in ATLAS. *Phys. Rev. Lett.* (2014) 112201802. DOI = 10.1103/PhysRevLett.112.201802. IF = 7,73.
4. ATLAS Collaboration: Search for Quantum Black Hole Production in High-Invariant-Mass Lepton plus Jet Final States Using pp Collisions at root s=8 TeV and the ATLAS Detector. *Phys. Rev. Lett.* (2014) 11291804. DOI = 10.1103/PhysRevLett.112.091804. IF = 7,73.
5. ATLAS Collaboration: Search for Dark Matter in Events with a Hadronically Decaying W or Z Boson and Missing Transverse Momentum in pp Collisions at root s=8 TeV with the ATLAS Detector. *Phys. Rev. Lett.* (2014) 11241802. DOI = 10.1103/PhysRevLett.112.041802. IF = 7,73.
6. Pierre Auger Collaborat: A search for point sources of EeV photons. *Astrophys. J.* (2014) 789160. DOI = 10.1088/0004-637X/789/2/160. IF = 6,28.
7. Pierre Auger Collaboration; Telescope Array Collaboration:Searches for large-scale anisotropy in the arrival directions of cosmic rays detected above energy of 10(19) eV at the Pierre Auger observatory and the telescope array. *Astrophys. J.* (2014) 794172. DOI = 10.1088/0004-637X/794/2/172. IF = 6,28.
8. ATLAS Collaboration: Search for top quark decays t -> q H with H -> gamma gamma using the ATLAS detector. *J. High Energy Phys.* (2014) 68. DOI = 10.1007/JHEP06(2014)008. IF = 6,22.
9. ATLAS Collaboration: Search for squarks and gluinos with the ATLAS detector in final states with jets and missing transverse momentum using root s=8 TeV proton-proton collision data. *J. High Energy Phys.* (2014) 9176. DOI = 10.1007/JHEP09(2014)176. IF = 6,22.
10. ATLAS Collaboration: Measurements of fiducial and differential cross sections for Higgs boson production in the diphoton decay channel at TeV with ATLAS. *J. High Energy Phys.* (2014) 9161. DOI = 10.1007/JHEP09(2014)112. IF = 6,22.



Selected applied results

- Device to carry out separation of whey proteins from milk medium. *CZ 26415 U1;* Katerina Hola; Radek Zboril; Ivo Medrik.
- Complexes of gold with omega-substituted derivatives of 6-alkyloxy-9-deazapurins and phosphane derivatives as well as the use of these complexes for the preparation of medicaments for the treatment of inflammatory and tumor diseases. *CZ 27030 U1;* Zdenek Travnicek; Jana Galikova; Jan Hosek; Jan Vanco.
- Platinum diiodo-complexes and their use for the preparation of medicaments intended for the treatment of tumor diseases. *CZ 27031 U1;* Zdenek Travnicek; Pavel Starha; Zdenek Dvorak.
- Complexes of gold with hypoxanthine derivatives and phosphane derivatives as well as their use for the preparation of medicaments for the treatment of inflammatory and tumor diseases. *CZ 27032 U1;* Zdenek Travnicek; Radka Krikavova; Jan Hosek; Zdenek Dvorak.
- Composite material based on zero-valent iron nanoparticles bound to the matrix surface and use thereof. *CZ 26708 U1*; Zdenka Markova; Jan Filip; Ivo Medrik; Radek Zboril.

Awards

The quality of scientific work is measurable according to standard scientometrical criteria, although the community might award it sometimes after few years or decades. Such acknowledgement may have the form of a simple announcement of the best works within the frame of young scientists presentations (Best Poster Award), which can help bring higher motivation for further scientific work. Next time experienced researchers are honoured for their longtime creative work. RCPTM employees also received several prestigious awards in 2014.

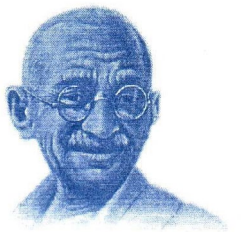
Prof. RNDr. Michal Otyepka, Ph.D. won the 2014 Neuron Impuls competition in chemistry. He succeeded with the project: Graphene Interface – A biomolecule as the way to cyborgs. Grant competition organizes Neuron – Fund for Support of Science.

Prof. Ing. Pavel Hobza, Dr.Sc., FRSC, dr.h.c. in 2014 became part of the list of the world's most highly cited scientists - Highly Cited Researchers 2014 – according to the Web of Science.

THOMSON REUTERS

The selection of approximately 3000 names of the most influential scientists from the fields of physical and social sciences is published by the Thomson Reuters company, the provider of the Web of Science.

Scientists earn enlistment among the upper percentage of the highly cited researchers owing to the high number of publications and their acceptance in the world of science.



MAHATMA GANDHI PRAVASI SAMMAN

Dr. Manoj B. Gawande was honoured with the "Mahatma Gandhi Pravasi Samman – 2014" award in May 2014. This is a prestigious award from the Indian government to Indian citizens who work abroad and achieve significant success there. Every year about 30 researchers from different fields are honoured with this award.

The RCPTM scientific team led by Ing. Štěpán Kment, Ph.D. won first place for the poster at SPEA 8 conference (8th European Meeting on Solar Chemistry and Photocatalysis: Environmental Applications), which took place in Greek Thessaloniki in June 2014. The name of the poster: "On the improvement of pec activity of hematite thin films deposited by high-power pulsed magnetron sputtering method."

Mgr. Martin Kuba won first prize for his poster on the Symposium on Atomic Spectrometry, which took place in Prague, March 2014. The name of the poster: "Determination of metals released from particular replacements in clinical samples by ICP-MS."

CONCLUSION

This year was, for The Regional Centre of Advanced Technologies and Materials of Palacký University in Olomouc, a crucial year – the building phase of the Centre, supported by OP RDI project of the European Regional Development Fund, has been finished. The year 2015 represents a new period in Centre's existence, a time when it must live and support its research intentions from its own sources and activities.

While for most centres this fact is a nightmare, because reaching the point of self sufficiency (even partial) in financial means is impossible for them, The Regional Centre of Advanced Technologies and Materials of Palacký University in Olomouc is prepared for this step. Both the scientific and applied results of the Centre are excellent, and the Centre has joined, taken from the viewpoint of evaluations by ISI statistics of the Web of Science, or Elsevier´s Scopus, the TOP 10 of the best research institutions in the Czech Republic and has also gained a significant position in the international scale. The great results indicate that the Centre stands on solid foundations based on outstanding scientific results, successful grant policy and cooperation with chief regional and international commercial subjects. It is not surprising then that the Centre got the support of 20.4 milion EUR within the National Sustainability Programme for the years 2014 – 2019.

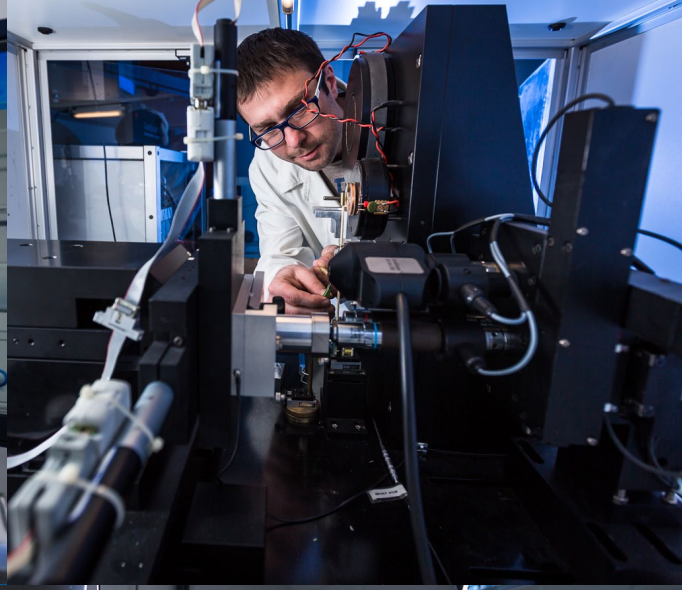
Centre employees published more than 250 publications in first rank European and world scientific journals in 2014. Being published in such journals means a high number of citations, which presents one of the most important indicators of the institution´s success. In this context, I cannot forget to mention one of the best publications of the Centre from 2012. This work has been cited more than 250 times this year. Works compiling the current state of knowledge in the specific sphere of research mean for the Centre´s employees significant appreciation of their work. In 2014, the employees of The Regional Centre of Advanced Technologies and Materials made a few great discoveries of the basic research such as the verification of full graphene dispersibility in water with the help of carbon nanotubes (Adv. Funct. Mater., 2015) and the targeted marking of cell nuclei using the carbon dots (Chem. Comm., 2014).

The Centre keeps its international character and this is good news. Foreign employees identify themselves with the Centre: a good example is the application for the ERC grant, which submitted under RCPTM one of the most significant researchers in nanotechnology – prof. Andrey Rogach.

How to conclude? The Centre is firmly anchored in the small group of the best scientific institutions in our republic and has clearly profiled scientifically. The research team of the Centre is stabilised, its management has got a clear concept about the scientific orientation for the coming years and this means that the Centre has the potential to become one of the chief research institutions not only in the Czech Republic, but also in Europe.

December 11, 2014, Prague

Prof. Ing. Pavel Hobza, Dr.Sc., FRSC, dr.h.c.



REGIONAL CENTRE
OF ADVANCED TECHNOLOGIES
AND MATERIALS

Regionální centrum pokročilých technologií a materiálů