

## REGIONAL CENTRE OF ADVANCED TECHNOLOGIES AND MATERIALS 2010-2013

## research · innovation · education





## REGIONAL CENTRE OF ADVANCED TECHNOLOGIES AND MATERIALS

Šlechtitelů 11, 783 71 Olomouc, Czech Republic +420 585 634 973 http://www.rcptm.com rcptm@upol.cz

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## RCPTM

2

Introductory Message from the Director

## **RCPTM IN BRIEF**

- 6 RCPTM Research Groups
- 8 Technologies and Research Infrastructure

## **RCPTM - RESEARCH HIGHLIGHTS**

- 12 The Kingdom of Graphene Materials with Limited Dimensions and Unlimited Possibilities
- 14 Photons Messengers in Studies of Space and the Nature of Matter
- 16 Environmentally Friendly Nanotechnologies for Water Treatment
- 18 Nanomedicine New Options for Diagnostics and Therapy
- 20 Coordination Compounds in Biomedical and Materials Research
- 22 The World of Biomolecules and their Interactions as Seen by Supercomputers and Nanosensors
- 24 Miniaturization a New Challenge in Analytical Chemistry

## RCPTM AND TECHNOLOGY TRANSFER

- 27 Looking into Heaven and Hell
- 28 Looking inside Materials
- 29 Looking under the Skin
- **30** Groundwater Treatment
- **30** Rapid Quality Control

## **RCPTM – INTERNATIONAL CENTRE FOR SCIENCE AND EDUCATION**

- 31 Leading Foreign Researchers at RCPTM
- **34** The Rising Generation at RCPTM

## **RCPTM IN NUMBERS**

- 36 Grant Successes
- 37 Selected Publications and Patents
- 40 Awards
- 4) Conclusion

## RCPTM Introductory Message from the Director

"RCPTM indeed has the makings of a significant international research centre, founded on three pillars, which in my judgment form the basis of sustainability for any research institution. The first of these is a high quality of applied research growing out of an excellent basic research. The second pillar is the multisource funding consisting of balanced income streams from publication, grants, technology transfer and educational activity. The final pillar is the internationalization at all levels emphasizing the high research quality of foreign and returning researchers."

It has already been three years since the founding of the Centre, which today bears the impressive designation Regional Centre of Advanced Technology and Materials. I am not sure to what extent that name itself has become known, but its abbreviation (RCPTM) is gradually becoming a label associated with quality research at the national, European and global levels. When it came into being in 2010, RCPTM was no new-born child unable to care for itself. Even at that time, the institution was able to benefit from the personnel and technological capacity developed for a number of large national projects, particularly Research Plans and Research Centres. An especially gifted generation of young researchers with the ability to generate leading results in both basic and applied research areas has also gathered in the Chemistry and Physics departments at RCPTM.

Nevertheless, it is the funding from the European Structural Funds under OP RDI which have been responsible without any doubt for the institution growing from its childhood into the healthy, mature individual of today, enjoying its best years (the average age of employees is 33) and with broad international experience.

The main pillars on which RCPTM systematically relies are its extensive international reach, its high quality workforce balanced in terms of age and involving individuals of varied nationalities and, last but not least, the unique technology it possesses. What regards international collaboration, the Centre has a long-term history of working together with more than 30 leading international institutions. Strong ties have thus come into being in several fields of research, creating an international network, which is partially responsible for forming their research development. Examples would be research on carbon quantum dots together with partners at Cornell University and the University of Ioannina, environmental research on new environmentally friendly technologies in collaboration with colleagues at the Florida Institute of Technology and research on the biomedical, catalytic and magnetic applications of nanoparticles in collaboration with colleagues at EPFL Lausanne and universities in Padua



and Tokyo. The interaction and applications of grapheme are being studied together with partners at universities in Pohang and Aarhus. And there are dozens of other examples, which could be given. The Centre is also involved in international projects, including projects being developed under the EU Seventh Framework Program, prestigious projects at the Pierre Auger Observatory, CERN-ATLAS and a number of others.

Key, in my opinion, is the involvement of young researchers at the doctoral student level and postdocs in these research projects involving foreign partners. Just in 2012, our researchers took part in more than 60 internships in almost 20 countries.

The interest of foreign researchers in positions and internships at RCPTM is also very important. In my opinion, this is the greatest shift compared to the previous years. Almost every day, postdocs and PhDs submit applications for positions in individual working groups at the Centre. Another benefit of this is that the Centre today has become significantly internationalized with almost thirty researchers from abroad. These are young researchers primarily from countries like Italy, the USA, Germany, Poland and Greece. Centre employs also outstanding scientific personalities from the USA, Israel or Hong Kong, professors who have been awarded a number of prestigious prizes and participate in the editorial boards of leading global journals, who also make valuable contributions in scientific education of the younger generation. If I should answer the question of what attracts both young and experienced researchers from around the world to RCPTM, I definitely would not say the high salary.

Today we are able to offer salaries at a level comparable with laboratories in Western Europe and the USA but young people, particularly those involved in research, are much more interested in their scientific growth and working on interesting projects with unique facilities at hand. I think, that it is the quality of research, interesting projects with great potential for applications and the first-rank technologies and instrumentation the Centre possesses that bring them here.

In the three years of its existence the Centre published more than five hundred high-impact publications in top journals such as Science, Chemical Reviews, Nature Communications, Accounts of Chemical Research, ACS Nano, Physical Review Letters and the Journal of the American Chemical Society. All these prove the quality of basic research done in the Centre. It is interesting to note that more than 30% of these papers were published in journals with impact factor higher than 5, a generally respected sign of scientific excellence. The Centre's exceptional position in basic research at the national level is also demonstrated by its involvement in two projects of the Centre of Excellence of the Czech Science Foundation targeting biomolecules and the interaction of food supplements with medications and nutrigenetics. Aside from basic research, RCPTM also focuses on leading applied research. Applied research products and patented technologies developed at RCPTM are in successful operation in numerous destinations around the globe. Nanoiron production technology, to which RCPTM employees have contributed, has become an everyday application used by remediation companies to treat groundwater at dozens of locations within the Czech Republic, Europe and Asia. High-energy cosmic radiation detectors developed at the Centre in collaboration with the ASCR Institute of Physics are a key component in the world renowned Pierre Auger Observatory's study of elementary particles in Argentina. Mössbauer spectrometers characterizing the iron content of substances are in use in South Africa, England, Sweden, Germany and the USA, while special cameras for observation of the night sky have been installed in Namibia, Mexico, the USA and on the Canary Islands. Borescopes used as sensors for flame temperature have been distributed to a number of European countries, as well as to South America and Asia. Other environmental and medical technologies are in the pilot plant phase or in clinical testing. Leading global companies have also ordered contracted research from RCPTM, among them Procter & Gamble (USA), which has provided long-term support for research into the permeability of substances through the skin using computer chemistry and Waters (Germany), which makes use of the Centre's comprehensive analytical abilities. More testimony to the quality of applied research produced by RCPTM is given by its role in coordinating management of the eightyear Competence Centre project of the Technology Agency of the Czech Republic, focused on environmentally friendly nanotechnologies and biotechnologies for treating water and soil which has also seen the involvement of large domestic companies active in remediation and water treatment.

RCPTM's analytical facilities are exceptional in many respects, partly thanks to the support from the European Regional Development Fund. For example, the microscopic laboratory has high-resolution transmission electron microscopy available for working with low temperatures, scanning probe microscopy, atomic force microscopy, magnetic force microscopy, fluorescence and confocal microscopies, represents one of the leading microscopic labs in Europe. Similarly, we have a laboratory allowing the measurement of the physical properties at large magnetic fields (PPMS), the measurement of magnetism using SQUID, NMR spectroscopy and Mössbauer spectroscopy in fields of up to 10T, which is one of the best equipped magnetic laboratories in Europe.

From the above mentioned, it might be seen that RCPTM has only a bright future ahead of it. But as a director, I also see many problems associated with sources of funding and national support for science and research at the state administration level. RCPTM grew under the wing of an operational programme announcing massive support for applied and industrial research with the requisite high level of funding for the centre provided by non-public sources. Over time it has become evident that such a level of supplementary funding is difficult to obtain for a number of centres and may also be impermissible from the standpoint that it allows unique facilities to be overused by the private sphere. Basic research is clearly preferred, at least from a funding viewpoint, in the national sustainability program designed to ensure funding for RDI centres. This approach (from one extreme to the other) is unfortunately typical for the funding of the Czech research. Ensuring the sustainability of large research centres is thus a highly demanding enterprise.

RCPTM indeed has the makings of a significant international research centre, founded on three pillars, which in my judgment form the basis of sustainability for any research institution. The first of these is a high quality of applied research growing out of an excellent basic research. The second pillar is the multisource funding consisting of balanced income streams from publication, grants, technology transfer and educational activity. The final pillar is the internationalization at all levels emphasizing the high research quality of foreign and returning researchers.

Setting aside the rules of the game, which I am not able to influence, I believe that by maintaining above mentioned philosophy, RCPTM will continue to increase and improve the quality of its research, the transfer of new technologies and educate a new generation of researchers who will contribute in the future to the good name and international prestige of RCPTM, as well as the City of Olomouc, the Olomouc Region and the Czech Republic.

Olomouc, September 30, 2013 Prof. RNDr. Radek Zbořil, Ph.D.



# **2** RCPTM IN BRIEF

THE REGIONAL CENTRE OF ADVANCED TECHNOLOGIES AND MATERIALS (RCPTM) is a scientific and research centre connected to the Faculty of Science, Palacký University, Olomouc. Its chief objective is to produce superlative research and to transfer high-tech products and technologies to medical, industrial and environmental practice with a pronounced emphasis on connecting the Centre to international networks and collaborations.

The Centre is based upon an internationally established research team which has taken part in a number of past projects at the level of Research Plans and Research Centres. Since 2010, the research team has been substantially expanded and internationalized thanks to support from the Operating Programme Research and Development for Innovation (OP RDI). This support totalled almost CZK 500 million, 400 million of which was invested in unique technology and constructing of the new Centre building. The remaining funding was used to support young researchers and internationalization. Today, RCPTM has approximately 100 scientific team members, 25% of whom are foreign specialists.

RCPTM focuses primarily on chemical, material and optical research. Priority research areas include metal oxide nanoparticles for catalytic, magnetic and biomedical applications, carbon nanostructures based on graphene and carbon quantum dots, metal nanoparticles for antimicrobial treatments and water treatment technologies, medical, computational and coordination chemistry, photonics and the development of instrumental techniques for applications in optics and analytical chemistry. Each year, the Centre publishes more than 200 original publications in prestigious foreign journals (average IF  $\sim$  4.0) and collaborates with more than 30 leading world institutions.

The Centre has had long-term success in getting both national and international grants. During the three years

of RCPTM's existence, Centre employees have successfully submitted 55 projects, bringing CZK 520 million in funding to RCPTM. The most important projects are those done under the Competence Centres of the Technology Agency of the Czech Republic, the Centre of Excellence of the Czech Science Foundation and the EU Seventh Framework Programme. The Centre is involved in prestigious international cooperation with institutions like the Pierre Auger Observatory and CERN-ATLAS.

The Centre also has a long tradition of collaboration with industrial and public organizations in the applied research area. RCPTM collaborates with approximately 50 domestic and foreign industrial partners. In addition to hightech approaches and technologies, it also offers modern equipment for use in contract research and implementing joint projects.

Centre employees also guarantee a number of masters and doctoral programmes in the disciplines of physical chemistry, nanotechnology, applied physics and optics and optoelectronics. During RCPTM existence, almost 70 master students and almost 20 doctoral students have successfully concluded their studies under the supervision of Centre employees. While still engaged in their studies, PhD students receive financial support in the form of part-time positions and exceptional scholarships. The best doctoral graduates subsequently gained positions in individual research departments at the Centre.



## Nanocrystal Metal Oxides

#### Head of the group: Assoc. Prof. RNDr. Libor Machala, Ph.D.

The group focuses on research in the field of nanocrystalline metal oxides, chiefly for biomedical applications and environmental technologies. The primary focus is on developing magnetic iron oxide nanoparticles used as a contrast agent for magnetic resonance imaging, drug carriers for targeted transport in cancer therapy and in the magnetic separation of biomolecules and cells. In the environmental chemistry area, the group works on developing new types of magnetic sorbents, environmentally friendly oxidants based on ferrates of alkali metals, and on magnetically separable catalysts. Also of importance is the study of biogenic iron oxide nanoparticles for biotechnological applications, thin oxide films for direct solar water splitting technology and magnetic nanoparticles as electrochemical biosensors.



## Carbon Nanostructures, Biomolecules and Simulations



## Biologically Active Complexes and Molecular Magnets

Head of the group: Prof. RNDr. Zdeněk Trávníček, Ph.D.

The group focuses on novel complex compounds of transitional elements, particularly on the development of novel types of biologically active compounds with medical application potential (e.g. substances with tumour-fighting, anti-inflammatory or antidiabetic effects), the preparation and study of molecular magnets and molecular switches which may be used, e.g. for sensors, high density memory or recording media, research on hybrid molecular-crystalline nanostructures with functionalized nanocrystalline iron oxides bound to a coordination compound. Head of the group: Prof. RNDr. Michal Otyepka, Ph.D.

Graphene and its derivatives (fluorographene, graphene oxide) belong to extensively studied compounds within the framework of our research. The research includes the development of novel methods for the functionalization and chemical modification of graphene and its derivatives. We benefit from a tight connection between both theoretical and experimental approaches. Other research directions include explorations of fluorescent carbon quantum dots and their application for cell imaging, along with the study of porous carbon nanostructures for environmental and catalytic applications. The group develops theoretical methods and tools for the study of biomacromolecules and nanomaterials. The focus is on the structure and dynamics of biomacromolecules and their functional components, on the interaction of biomacromolecules with membrane bilayers, on enzyme and RNA catalysis.



## **Optical and Photonic Technologies**

#### Head of the group: Prof. RNDr. Miroslav Hrabovský, DrSc.

The group focuses for a long time on research into optical quantum and nonlinear phenomena, as well as quantum information, research on nonstandard detection systems based on optics with sensitivity to individual photons, special micro/nano optical surfaces and corresponding optical technologies and measurement methods. Other directions include the development of methods for the deposition and characterization of thin films using plasma and vapour deposition. The group develops optical contactfree measurement methods based upon interferometry in coherent speckle fields and white-light and moiré topography. The group also participates in prestigious international projects such as CERN-ATLAS (research on the nature of matter at the LHC accelerator at CERN in Geneva) and the Pierre Auger Observatory (research on high energy cosmic radiation).





## **Metal Nanomaterials**

Head of the group: Assoc. Prof. RNDr. Libor Kvítek, CSc.

The group works on nanocrystalline metals, particularly those based on iron and noble metals. The chief applied focus includes the use of nanoiron for in situ groundwater treatment technologies (as part of the EU Seventh Framework Programme "Taking Nanotechnological Remediation Processes from Lab Scale to End User Applications for the Restoration of a Clean Environment FP7-NMP" - 2011108), as well as the use of nanosilver in antimicrobial technologies and the application of metal nanoparticles in catalysis. The group also develops materials and composites for application in surface enhanced Raman spectroscopy, particularly for determining substances of medicinal value. In the basic research area, the group is working on a comprehensive description of nanometal toxicity, the mechanism responsible for the antibacterial effect of nanosilver and the mechanism of interaction between nano-iron and selected pollutants.

## Nanotechnology in Analytical Chemistry

#### Head of the group: Prof. RNDr. Karel Lemr, Ph.D.

The group focuses on describing and modelling analytical processes during the transition to the nanoscale (the ionization of substances, nanoseparation beds, the influence of nanoparticles on the interaction of radiation and the analyte, electrochemical conversions) and characterizing nanomaterials using the methods of analytical chemistry (e.g. capillary electrophoresis). The group also works on the development of new analytical tools (ion sources, separation systems, sensitive detection systems) and advanced analytical methods (lower detection thresholds, accelerated analyses). Other favoured directions include the development of methods for observing the conversion of toxic and pharmacologically interesting substances, and the description of the interactions of these substances with living organisms. The group is also concerned with basic research on ionization and fragmentation in mass spectrometry, preconcentration, and chromatographic and electrophoretic separation. The knowledge obtained serves as a basis for e.g. analyzing foods or in forensic analysis.



## Technologies and Research Infrastructure

The Regional Centre of Advanced Technologies and Materials in Olomouc is today one of the best equipped facilities in Europe and throughout the world for research in the fields of materials science, nanotechnologies, chemistry and optics. The construction of a top research infrastructure was initiated with the help of several projects by the Ministry of Education (Research Plans and Centres). Later, the available technology was significantly expanded due to a desire to get involved in large international collaborative efforts. The latest and, to this point, largest expansion in technology has taken place over the last three years, during the course of the implementation phase of the OP RDI project.

RCPTM has a broad spectrum of synthetic and analytic techniques at its disposal, not only because of the wide-ranging research aims of the Centre, but also because of the highly multidisciplinary nature of research in nanotechnologies whose application potential extends into medicine, ecology, biotechnology, energy and a number of other areas. In putting together the Centre's technological facilities, a path was chosen that involves creating several specialized laboratories utilizing related techniques.

Two laboratories (the microscopic technology laboratory and the laboratory for the analysis in external magnetic fields) are unique at the European and global levels, offering a gigantic potential for utilization in collaborative research and international cooperation. For example, the high resolution electron microscope is currently the most powerful microscope in the Czech Republic.

## Microscopic Laboratory

This laboratory contains a collection of microscopic techniques whose composition covers a broad range of required analyses. The flagship of this laboratory and the Centre as a whole is the high resolution transmission electron microscope (resolution 0.08nm), capable of measurements under low temperatures (cryoHRTEM) and possessing chemical mapping technology such as EDX and EELS. This microscopic technique is further complemented by a standard transmission electron microscope (TEM), a scanning electron microscope (SEM) utilizing the EDX system, an atomic and magnetic force microscopes (AFM/MFM), as well as a scanning tunnelling microscope (STM). Other microscopic techniques include fluorescent and confocal optical microscopes.



## Laboratory of Techniques for Analyses in External Magnetic Fields



This laboratory covers some spectroscopic techniques, as well as tools for measuring the physical and chemical properties of materials in external magnetic fields. There is a SQUID magnetometer (Superconducting Quantum Interference Device) working in external fields of up to 7T and allowing the measurements of the FC/ZFC curves, hysteresis loops, temperature dependence and susceptibility, and Mössbauer spectrometry for measurement in a wide range of temperatures and external magnetic fields of up to 10T. Among the newest equipment belong a system for the measurement of physical properties (Physical Property Measuring System -PPMS) permitting the measurement of electrical, magnetic, optical and transport properties in external fields of up to 9T, as well as an NMR spectrometer (600MHz) with the ability to analyze samples in the solid phase.

## X-ray Laboratory for Structural and Phase Analysis

This group of techniques includes spectroscopic and diffraction methods employing X-ray radiation for the complex structural, phase and chemical analysis of materials. Available techniques include an X-ray powder diffractometer enabling phase analysis and the processing of samples at high temperatures (XRD), an X-ray single crystal diffractometer and an X-ray fluorescence spectrometer (XRF) capable of analyzing solid and liquid samples composed of elements in the range from sodium to uranium. A new approach is XPS (X-ray Photoelectron Spectroscopy), which may be used to analyze solid samples composed of elements in the range from lithium to uranium with a depth of up to 10nm.



## Laboratory of Spectroscopic, Chromatographic and Thermal Methods



Principally the laboratory contains devices based on mass spectrometry and other spectroscopic techniques, but also includes chromatographic techniques, methods of thermal analysis and calorimetry. Among the equipment used in the laboratory is a high-definition mass spectrometer, an inductively coupled plasma mass spectrometer (ICP-MS) with laser ablation, capillary electrophoresis with tandem mass spectrometer, gas or liquid chromatography, atomic absorption spectrometer and elemental analyzer (CHNS). Other techniques which may be used include IR/Raman spectroscopy, a Raman scattering microscope, micro-Raman spectroscopy and electron paramagnetic resonance (EPR).

Available techniques for the thermal analysis of materials include a simultaneous thermal analyzer with analysis of evolved gases (TG/DSC/EGA) and an isothermal titration calorimeter.

## Laboratory for the Analysis of Size and Surface Properties of Materials

This laboratory relies on a group of techniques permitting the qualitative and quantitative evaluation of surface and size properties of materials, including surface area, surface energy, material porosity, service wettability and particle size distribution. Included is a BET analyzer for the measurement of surface area and material porosity, facilities to measure chemisorption and specific surface area with the capability to perform analyses up to 450°C, a DLS (Dynamic Light Scattering) analyzer for measuring the distribution of particle sizes and zeta potential, and SEA (Surface Energy Analyzer) facilities for measuring surface energy using the inverse gas chromatography method. And last but not least, the wettability of surfaces may be measured using the contact angle method with the option to designate surface tension or the free surface energy of solids.

![](_page_10_Picture_9.jpeg)

## **Optical Laboratory**

The optical laboratory possesses unique laser and deposition systems, along with system for machining (nano)surfaces. The laboratory has a picosecond laser system with a high repetition rate, a pulse femtosecond laser system with amplifier and optical parametric amplifier, a pulse femtosecond system featuring "cavity dumping" and generator of the second and third harmonic frequencies, a nanosecond laser and several intensified CCD cameras with high quantum efficiency. Surface and film preparation may be carried out in centres where surfaces are first ground and then polished to be prepared for optical and non-optical use with a roughness value below 10nm. These surfaces may be subsequently processed using a vacuum steam apparatus for the deposition of thin films, a plasma system for the deposition of functional nanocluster structures, and then tested by measuring the composition of gradient films, scatterometry and using optical spectroscopy techniques.

![](_page_11_Picture_2.jpeg)

![](_page_11_Picture_3.jpeg)

## **Computational Chemistry Laboratory**

The laboratory is equipped with computer clusters for simulating the properties of novel materials, biomacromolecules and hybrid complex systems. The existing software and hardware facilities allow mechanical and electronic properties in the solid phase to be predicted, along with a broad range of the physical-chemical properties of molecules, the conformational behaviour of biomacromolecules, and permit the effectiveness of catalytic processes to be studied and mutual affinities between materials to be evaluated.

The laboratory's computer clusters contain roughly 3,100 CPUs and 7.3TB of RAM, along with data centres with a total capacity of more than 80TB. Quantum chemical calculations are carried out using Gaussian, Molpro, Turbomole, VASP, Molcas, Abinit softwares. AMBER, CHARMM, NAMD and GROMACS softwares are used, among others, for molecular dynamics simulations.

## Synthesis Laboratory

Not all the techniques possessed by the Centre are intended for the characterization of materials. The Centre also possesses a wide range of techniques and facilities for the preparation and processing of materials under laboratory and pilot plant conditions, such as reaction autoclaves, laboratory ovens, microwave systems for material preparations, nanoparticle dispersion units, a jet and ball mill for homogenizing particles, centrifuges, ultrasound equipment and deposition systems employing cold plasma. Large-scale nanomaterial preparation methods developed in the laboratory may be tested using pilot plant fluid and rotation furnaces for working in inert, oxidation and reducing atmospheres.

![](_page_11_Picture_9.jpeg)

![](_page_12_Picture_0.jpeg)

# **3** RCPTM - RESEARCH HIGHLIGHTS

## THE KINGDOM OF GRAPHENE – MATERIALS WITH LIMITED DIMENSIONS AND UNLIMITED POSSIBILITIES

Unusual forms of carbon have fascinated scientists since the early 1990s. Fullerene, made up of 60 carbon atoms shaped like a soccer ball, is harder than diamond. Carbon nanotubes are harder than steel and are becoming an everyday component in a number of commercial products. But it is graphene, a honeycomb twodimensional sheet of carbon atoms, which is perhaps the most studied material at present. Andre Geim and Konstantin Novoselov received the 2010 Nobel Prize in Physics for its discovery. Graphene is a material with a truly huge range of potential uses. It conducts electricity better than copper and the electrons contained in its structure move at almost the speed of light. It is also transparent, exceptionally hard and the best-known conductor of heat.

#### **Fluorographene and Related Derivatives**

The world of graphene, its derivatives, properties and interactions has become one of the key foci of RCPTM researchers. Back in 2010, the Olomouc group was present at the discovery of the first stoichiometric graphene derivative – fluorographene, the thinnest known insulator. In the preparatory phase, a group led by Prof. Otyepka and Prof. Bourlinos (University of Ioannina, Greece) started from three-dimensional graphite fluoride, which they chemically etched using the organic solvent sulfolane. It is interesting to note that fluorographene was simultaneously discovered by a group of researchers at the University of Manchester led by Geim and Novoselov, who used a mechanical preparation technique. The work of both groups came out in the prestigious journal Small at the same time (*Small* 2010).

Fluorographene, a material whose characteristics are similar to those of Teflon<sup>®</sup>, has opened the path to further graphene derivatives with controlled electronic properties such as band gaps. The Olomouc researchers predicted the electronic and optical properties of these fluorinated, chlorinated and brominated derivatives, taking a significant step toward the construction of future two-dimensional semiconductors. The work was even featured on the cover of a prestigious theoretical and computer chemistry journal published by the American Chemical Society (*J. Chem. Theory Comput.* 2013). Not long ago, RCPTM researchers also published the first comprehensive systematization of all existing halogenated graphene systems, including their properties and potential applications, in the ACS Nano journal (ACS Nano 2013).

![](_page_13_Picture_6.jpeg)

![](_page_13_Picture_7.jpeg)

## The Functionalization of Graphene and its Applications

Aside from halogenated graphene derivatives, RCPTM has intensively devoted itself to covalent and noncovalent functionalized graphene, as well, involving chemical modifications to improve certain properties, particularly dispersibility in water, and to modulate electronic and magnetic properties. The first systematization of all possible approaches to the functionalization of graphene, including a description of the properties of its chemical cousins – graphane with covalent bonded hydrogen atoms and graphene oxide with various bondings of oxygen atoms (*Chem. Rev.* 2012) – was published by an international team last year under the leadership of Prof. Zbořil in cooperation

with colleagues from South Korea (Pohang University) and Greece (NCSR Demokritos).

The Chemical Reviews paper, which had already been cited more than 100 times in the first six months after its publication, also focuses on the use of graphene for DNA sequencing and the development of new sensors, among other applications. Above all, it should inspire research teams in the search for further applications of graphene. RCPTM researchers have also been able to measure the extent of mutual interaction between graphene and various organic solvents (*J. Am. Chem. Soc.* 2013) and metals (ACS Nano 2013). Work done with colleagues from Aarhus University in Denmark demonstrated, among other things, the exceptional affinity between graphene and copper. This "love affair" between two excellent conductors may be highly significant in the future for the construction of a new generation of electronic components and sensors.

![](_page_14_Picture_2.jpeg)

![](_page_14_Figure_3.jpeg)

Some of the greatest challenges currently facing RCPTM researchers looking into graphene chemistry include targeting functionalization toward magnetic graphene, the development of novel two-dimensional derivatives with semiconductor properties, preparing new types of graphene quantum dots and understanding the interaction of graphene with RNA, DNA and other biomolecules. In meeting these challenges, RCPTM researchers will be able to avail themselves of a unique high-resolution transmission electron microscope with the capability of highly sensitive chemical mapping of nanostructures and working in a cryogenic regime. This microscope is the first of its kind in the Czech Republic.

#### **Selected Publications:**

- Zbořil, R.; Karlický, R.; Bourlinos, A.B.; Steriotis, T.A.; Stubos, A.K.; Georgakilas, K.; Šafářová, K.; Jančík, D.; Trapalis, Ch.; Otyepka, M.: Graphene Fluoride: A Stable Stoichiometric Graphene Derivative and its Chemical Conversion to Graphene. *Small* 6, 2885–2891, 2010.
- Karlický, K.; Otyepka, M.: Band Gaps and Optical Spectra of Chlorographene, Fluorographene and Graphane from G0W0, GW0 and GW Calculations on Top of PBE and HSE06 Orbitals. J. Chem. Theory Comput. 9, 4155–4164, 2013.
- Karlický, F.; Datta, K.K.R; Otyepka, M.; Zbořil, R.: Halogenated Graphenes: Rapidly Growing Family of Graphene Derivatives. ACS Nano 7, 6434–6464, 2013.
- Georgakilas, V.; Otyepka, M.; Bourlinos, A.B.; Chandra, V.; Kim, N.; K. Kemp, Ch.; Hobza, P.; Zbořil, R.; Kim, K.S.: Functionalization of Graphene: Covalent and Non-Covalent Approaches, Derivatives and Applications. *Chem. Rev.* 112, 6156–6214, 2012.
- Lazar, P.; Karlický, F.; Jurečka, P.; Kocman, M.; Otyepková, E.; Šafářová, K.; Otyepka, M.: Adsorption of Small Organic Molecules on Graphene, *J. Am. Chem. Soc.* 135, 6338– 6344, 2013.
- Lazar, P.; Zhang, S.; Šafářová, K.; Li, Q.; Froning, J.P.; Granatier, J.; Hobza, P.; Zbořil, R.; Besenbacher, F.; Dong, M.; Otyepka, M.: Quantification of the Interaction Forces between Metals and Graphene by Quantum Chemical Calculations and Dynamic Force Measurements under Ambient Conditions. ACS Nano 7, 1646–1651, 2013.

Grant Support: Centre of Excellence, Czech Science Foundation P208/12/G016, 2012-2018. Controlling Structure and Function of Biomolecules at the Molecular Scale: Theory meets Experiment. Principal Investigator: Prof. Ing. Pavel Hobza, DrSc., FRSC; Centre Director: Prof. RNDr. Michal Otyepka, Ph.D.

## PHOTONS - MESSENGERS IN STUDIES OF SPACE AND THE NATURE OF MATTER

The mystery of the beginning of the universe. The fundamental properties of the smallest particles of matter. The spooky (in Einstein's view) action-at-a-distance in the quantum world. What do all these enigmas have in common? Actually, more than you would think at first glance. All of them reveal the truth about themselves only very reluctantly and all stand at the edge of our comprehension. They will not leave us in peace and we sense that somewhere beyond the horizon of our consciousness, they are somehow connected. And so we build larger and larger accelerators and the large international research efforts that go with them in the attempt to look a step further into the interior of matter. And particles fly to us from outer space brimming with energy many orders of magnitude higher than elsewhere around us, whose origin for the time being remains shrouded. In all these cases we try to pull back that veil with the help of tiny, diligent messengers – particles of light – photons, whether they come to us from the depths of space or speak of encounters with other travellers, or whether indeed we ourselves send them out to bring back news of the great and small at remote distances. And here and there, unexpectedly, we also obtain new tools for our everyday lives.

RCPTM contributes to one such examination of the depths of space by taking part in the construction and operation of the Pierre Auger Observatory constructed in the Argentinean Pampa to study the tiniest particles of matter arriving from space with huge amounts of energy. When these particles encounter the Earth's atmosphere, they produce an extensive shower composed of billions of secondary particles. The character and origin of these primary particles represent a great unknown for scientists and that is what the observatory is seeking to clarify. These particles may originate in the decay of supermassive dark energy particles, or by being gradually accelerated by astrophysical objects. Another study direction is aimed at events caused by high-energy neutrinos. Centre researchers took part in building the optical part of the observatory and are currently contributing to its successful operation and the collection of data. Another project looking into the world of high-energy particles in space is the Cherenkov Telescope Array observatory project, to which the Centre is currently contributing.

By contrast, the CERN-ATLAS project peers into the innards of matter. Its most important task is undoubtedly to confirm the existence of the Higgs boson – an elementary particle predicted by the standard model of particle physics to explain why other elementary particles (such as quarks and electrons) have mass. Such a particle has actually been observed in the anticipated energy region around 126GeV

![](_page_15_Picture_4.jpeg)

(*Science* 2012). This is the greatest discovery in particle physics in the last thirty years, that is, since the discovery of the W and Z bosons thirty years ago, confirming the structure of the standard model of particle physics. Other noteworthy areas in which CERN-ATLAS is currently involved include the search for supersymmetric particles, exploring proton-proton interactions (*Nature Commun*. 2011) and the search for further signs of the new physics, such as extra dimensions, the production of microscopic black holes and axions. RCPTM's collaboration with CERN-ATLAS has focused especially on the modelling of optical detection processes.

![](_page_15_Picture_6.jpeg)

#### **Quantum Information**

Exploring the properties of the quantum microworld has led to the rise of a new area of scientific inquiry – that of quantum information. Quantum information processing enables faster computational algorithms to be implemented, as well as faster methods of searching databases and safer methods of communication than are achievable with the methods of classical physics. The quantum optics group at RCPTM studies quantum algorithms and protocols with the aim of bringing the field closer to practical applications. In the RCPTM laboratories individual photons are employed as carriers of quantum information and with the help of single- and two-photon interference, information processing takes place. Among the most significant results recently achieved in this area is the implementation of a tuneable phase gate (Phys. Rev. Lett. 2011). It is a prominent member of the family of elementary quantum-information tools. It may be used as a building block for a broad range of quantum information tasks. In addition, this implementation was the first to offer full tunability and the maximum efficiency permitted under the laws of quantum physics. Another RCPTM product in this area is a multifunctional quantum cloning device, the analogue of a classic copier but controlled by the laws of quantum physics. It is capable of duplicating an unknown quantum state with a maximum level of precision allowed by quantum physics. Such a device may be used for efficient eavesdropping on quantum cryptography (*Phys. Rev. Lett.* 2013). Experimental testing of the resistance of quantum cryptography contributes to determining the limits of its security.

In addition to the design and construction of elements for the quantum processing of information, RCPTM also focuses on the design of original detection schemes for analyzing the properties of two-photon states of light and designing new elements and structures for the generation of photon pairs. The group has designed new methods for analyzing the quantum state of paired fields applicable for absolute calibration of detectors at the level of individual photons (*Opt. Lett.* 2012). These methods are also capable of generating multiphoton nonclassical states of light (*Opt. Express* 2013) which are unparalleled in classical physics and are distinguished by lower noise levels than would be achievable within classical physics.

In the particle physics area, RCPTM is striving to become even more broadly involved in international collaboration efforts. In addition to the Cherenkov Telescope Array project noted above, there also appears to be some promise of RCPTM involvement in the CBM Compressed Baryonic Matter project, which will employ the collisions of atomic nuclei to research highly compressed nuclear matter. Another challenge the RCPTM optical group is currently working on is improving the method of generating, manipulating and detecting quantum information in a manner which would open doors to the broader practical use of quantum information science and metrology.

![](_page_16_Picture_4.jpeg)

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- ATLAS Collaboration: A Particle Consistent with the Higgs Boson Observed with the ATLAS Detector at the Large Hadron Collider. Science 338, 1576, 2012.
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- Bartkiewicz, K.; Lemr, K.; Černoch, A.; Soubusta, J.; Miranowicz, A.: Experimental Eavesdropping Based on Optimal Quantum Cloning. *Phys. Rev. Lett.* 110, 173601, 2013.
- Peřina, J. Jr.; Haderka, O.; Michálek, V.: Sub-Poissonian-Light Generation by Postselection from Twin Beams. Opt. Express 21, 19387, 2013.
- Peřina, J. Jr.; Haderka, O.; Michálek, V.; Hamar, M.: Absolute Detector Calibration Using Twin Beams. *Opt. Letters* 37, 2475, 2012.

Grant Support: Involvement in International Collaboration with CERN-ATLAS and the Pierre Auger Observatory

## ENVIRONMENTALLY FRIENDLY NANOTECHNOLOGIES FOR WATER TREATMENT

Securing an adequate supply of safe water is a policy priority for governments around the globe. However, 80% of the world's population lives in the areas where water resources are highly problematic. According to the World Health Organization and Deutsche Bank Research, which regularly monitor the global water market, average water consumption per inhabitant of Earth has doubled over the past 50 years, particularly as a consequence of the radical growth in water consumption by industry, agriculture and related applications. This trend goes hand-in-hand with growth in the pollution of all water sources, including drinking water. Chlorinated hydrocarbons, heavy metals, radioactive compounds, arsenic, cyanides, phosphorus, herbicides, chemical warfare agents and cyanobacteria are just some examples of highly toxic compounds polluting water around the world.

#### Nano Iron for In Situ Treatment of Groundwater

RCPTM research groups are, on a long-term basis, focused on the development of new environmentally friendly technologies for treating water and soil. It is a technology based upon zero-valent iron for in situ treatment of contaminated groundwater. Elementary iron in the form of surface stabilized nanoparticles is capable of "floating" in groundwater and by virtue of its reduction and precipitation effects converting highly toxic solutes to a much less toxic or completely nontoxic phases. RCPTM researchers participated in the development of a method for the large-scale production of nanoiron (EP 2164656, 2013), which has found wide use in the remediation of groundwater, particularly water contaminated with chlorinated hydrocarbons, nitro-compounds, chromium, uranium and other heavy metals. Nanoiron, s.r.o., which uses the technology is currently the largest European producer of nanoiron.

In addition to developing technology for the production and stabilization of nanoiron, RCPTM is intensively involved in studying the mechanisms of degradation of selected pollutants. Last year, RCPTM researchers, together with colleagues from Brno, uncovered a unique selective toxicity of nanoiron towards cyanobacteria (*Environ. Sci. Technol.* 2012). They discovered that nanoiron is a multifunctional weapon in the fight against cyanobacteria, because it is capable of degrading cyanobacteria cells and at the same time it binds toxic microcystine, preventing its release into the water column. And finally, nanoiron also plays a preventive role because it eliminates phosphorus from water – a key nutrient needed by cyanobacteria.

Groups at the Centre are also working on the development of new hybrid systems based on nanoiron and nanosilver enabling the elimination of phosphorus combined with a

![](_page_17_Picture_6.jpeg)

strong antimicrobial effect (*Environ. Sci. Technol.* 2013). A principal advantage of such composite is possibility of its magnetic separation and repeated use.

In the area of nanoiron applications and research, RCPTM is involved in a prestigious European project coordinated by colleagues from the University of Stuttgart. Within this project, Centre researchers are responsible for developing nanoiron and optimizing its surface and migration properties for applications in a wide range of locations throughout Europe.

![](_page_17_Picture_9.jpeg)

#### High Valence Iron States in Oxidation Technologies

Apart from advanced remediation technology employing nanoiron, RCPTM is also involved in developing environmentally friendly oxidative technologies based upon the application of iron compounds in high valence states (ferrate(IV), ferrate(V), and ferrate(VI) compounds). As a part of long-term collaboration with colleagues at the Florida Institute of Technology, Olomouc researchers have demonstrated, among other things, the effectiveness of ferrate(VI) in eliminating chemical warfare agents (J. Hazard. Mater. 2012) and in the process of eliminating cyanide and heavy metals (Chem. Eur. J. 2011). A recent study published in the Environmental Science & Technology journal has demonstrated huge application potential of potassium ferrate(VI) in removing arsenites and arsenates present in water. Arsenic currently poses a serious ecological problem in a number of Asian countries, as well as in the USA and Europe. Studies demonstrate that very low concentrations

of ferrate(VI) are capable of eliminating arsenic even when concentrations of the latter are large. The key, however, lies in the elimination mechanism in which pentavalent arsenic becomes firmly embedded in the secondary formed iron oxide structure, thereby preventing its secondary release into the environment (*Environ. Sci. Technol.* 2013).

RCPTM also works on optimizing and commercializing arsenic elimination technology and on dozens of other environmental activities within the framework of the national Competence Centre entitled "Environmentally Friendly Nanotechnologies and Biotechnologies for Water and Soil Treatment". In addition to RCPTM role as the coordinating facility for the eight-year project, which is supported by TACR funding of CZK 316 million, other academic partners from the Technical University of Liberec and the Institute of Microbiology at ASCR Prague are involved. Six leading industrial partners in the water remediation market (AECOM CZ, s.r.o., AQUATEST, a.s., DEKONTA a.s., GEOtest, a.s., LAC, s.r.o., MEGA a.s.) have taken part in the development and commercialization of the technology.

![](_page_18_Picture_2.jpeg)

Future challenges which RCPTM wishes to meet in the environmental technology area include completing the development of large-scale production of ferrate(VI) and their commercial use in the treatment of wastewater, surface water, and drinking water. Centre researchers also work intensely on developing large-scale technology for the removal of cyanobacteria for realworld on-site testing. Technology for the antimicrobial treatment of filters and membranes using nanosilver is also very close to commercial use, allowing the lifetime of materials used in water filtration processes with a high incidence of microorganisms to be extended. Finally, the Centre works on combining biotechnology and nanotechnology for the degradation of hormonally active substances and drugs which enter the water as a consequence of the widespread use of hormonal contraception and analgesics. Existing technology for the elimination of these toxic substances are either ineffective, very expensive or environmentally unfriendly.

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- Maršálek, B.; Jančula, D.; Maršálková, E.; Mašláň, M.; Šafářová, K.; Tuček, J.; Zbořil, R.: Multimodal Action and Selective Toxicity of Zerovalent Iron Nanoparticles against Cyanobacteria. *Environ. Sci. Technol.* 46, 2316-2323, 2012.
- Marková, Z.; Šišková, K.; Filip, J.; Čuda, J.; Kolář, K.; Šafářová, K.; Medřík, I.; Zbořil, R.: Air Stable Magnetic Bimetallic Fe-Ag Nanoparticles for Advanced Antimicrobial Treatment and Phosphorus Removal, *Environ. Sci. Technol.* 47, 5285-5293, 2013.

![](_page_18_Picture_8.jpeg)

- Zbořil, R.; Andrle, M.; Oplustil, L.; Machala, L.; Tuček,
   J.; Filip, J.; Marušák, Z.; Sharma, V.K.: Treatment of Chemical Warfare Agents by Zero-Valent Iron Nanoparticles and Ferrate(VI)/(III) Composite, J. Hazard. Mater. 211, 126-130, 2012.
- Filip, J.; Yngard, R.A.; Šišková, K.; Marušák, Z.; Ettler, V.; Sajdl, P.; Sharma, V.K.; Zbořil, R.: Mechanisms and Efficiency of the Simultaneous Removal of Metals and Cyanides by Using Ferrate(VI): Crucial Roles of Nanocrystalline Iron(III) Oxyhydroxides and Metal Carbonates, *Chem. Eur. J.* 17, 10097-10105, 2011.
- Prucek, R.; Tuček, J.; Kolařík, J.; Filip, J.; Marušák, V.K.; Zbořil, R.: Ferrate(VI)-Induced Arsenite and Arsenate Removal by In Situ Structural Incorporation into Magnetic Iron(III) Oxide Nanoparticles, *Environ. Sci. Technol.* 47, 3283-3292, 2013.

#### Grant Support:

TACR Competence Centre TE01020218, 2012-2019. Environmentally Friendly Nanotechnologies and Biotechnologies for Water and Soil Treatment. Centre Director: 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.

## NANOMEDICINE – NEW OPTIONS FOR DIAGNOSTICS AND THERAPY

In spite of the tremendous progress made by contemporary medicine, researchers still face dozens of challenges in developing advanced diagnostic and therapeutic approaches. There are many examples, among them the discovery of new methods in the fight against bacteria which are becoming even more resistant to antibiotic treatment. In terms of the success of treatment, it has become more and more important to develop procedures to precisely and timely diagnose illnesses, often with the use of novel types of contrast agents. However, the biggest challenge is to find the ways to increase the effectiveness of anticancer therapy and, at the same time, reduce the incidence and severity of side effects. In all these areas, nanomaterials offer an interesting, highly effective solution and a number of medical nanotechnologies are already undergoing various phases of clinical trials. A special attention is devoted to the use of nanosilver for antimicrobial applications and iron oxide nanoparticles for the targeted magnetic transport of drugs and improving contrast characteristics in magnetic resonance imaging.

#### Nanosilver – a New Tool in the Fight against Bacteria

Studies of nanosilver and its biological activity have been the focus of the RCPTM group led by Prof. Kvítek since 2005. Its advantage over antibiotics lies in the fact that bacteria have not yet developed defence mechanisms against it. In 2006, working with colleagues from the UP Medical Faculty (Prof. Milan Kolář), the group published groundbreaking work in the Journal of Physical Chemistry B quantifying the antibacterial activity of silver nanoparticles against a broad range of bacteria. In September 2013, this work had already been cited almost 500 times and dozens of other groups around the world have based their own work upon it. RCPTM researchers were the first to determine the antifungal activity of nanosilver, which they described in a 2009 article in the Biomaterials journal (with more than 100 citations).

Recent research at RCPTM concentrates on understanding the acute and chronic toxicity of nanosilver toward higher organisms such as *Drosophila melanogaster* (*Environ. Sci. Technol.* 2011), and on developing a method for the magnetic transport of nanosilver for targeted antimicrobial applications (*Biomaterials* 2011). Other significant results include a description of the hemocompatibility of nanosilver in collaboration with colleagues from Tübingen (*Acta Biomater.* 2013). An overview covering the issue of mechanism of nanosilver effects, its biological activity, the preparation of composites using biopolymers and future prospects was published by Prof. Zbořil in collaboration with colleagues from the Cornell University and the Florida Institute of Technology in the Advances in Colloid and Interface Science journal (2011).

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#### Magnetic Nanoparticles for the Transport of Drugs and Diagnostics

Magnetic nanoparticles of iron oxide (maghemite) represent a highly progressive material for biomedical applications. Because of its non-toxic, biocompatible and biodegradable properties, nanomaghemite has been approved for clinical use by the US FDA (US Food and Drug Administration). Superparamagnetic iron oxide nanoparticles are used to improve contrast characteristics in magnetic resonance imaging. Another application includes targeted antitumor therapy, in which the large specific surface of magnetic nanoparticles binds the cancerostatic substance which is targeted using the external magnetic field directly at the location of the tumour and released with the change in physiological conditions or field parameters. In this way, a dramatic reduction in the scale of side effects associated with classic antitumor therapy is brought about.

RCPTM has a long history in exploring magnetic nanosystems for biomedicine. In 2009, the Centre patented a new peroral contrast agent for the MRI diagnosis of illnesses affecting the abdominal cavity, based upon incorporating iron oxide nanoparticles into the porous structure of aluminosilicate bentonite. This substance was successfully clinically tested in subsequent years on more than 100 patients with a wide range of diseases of

![](_page_19_Picture_9.jpeg)

the gastrointestinal tract. Admirable recent successes include the development of magnetic nanoparticles functionalized with terephthalic acid which have set a new record in contrast effectiveness. This is the first example of improved contrast characteristics thanks to the specific surface design of nanoparticles (*Chem. Commun.* 2013). RCPTM has a long history of collaboration with colleagues from the University of Patras in Greece in the area of targeted drug delivery. The most interesting result of this collaborative research has been the preparation of magnetic nanoclusters using a self-organization process in a suitable biopolymer environment. Among other things, these magnetic nanosystems demonstrate record capacity for binding doxorubicin used in chemotherapy (*Small* 2012).

RCPTM's future activity in nanomedicine primarily targets the possibility of in vivo clinical testing, also in collaboration with colleagues from the Institute of Molecular and Translational Medicine (BIOMEDREG) of the UP Medical Faculty. In the field of nanosilver challenges involve a comprehensive description of the biodistribution of silver independence on the method of application and surface treatment of nanoparticles. Another challenge involves research of the synergistic effect of nanosilver and antibiotics in combined treatment, particularly what regards renewing the effectiveness of antibiotics against resistant bacteria. Technologies for the surface modification of the tracheostomy cannula with covalently bound nanosilver are already in the clinical testing phase (Patent CZ 303502, 2012). Research on magnetic ironoxide-based nanoparticles will focus on developing the complex materials known today as theranostics (from therapy and diagnostics).

![](_page_20_Picture_2.jpeg)

![](_page_20_Picture_3.jpeg)

HO HO Iron Oxide Cluster

#### **Selected Publications:**

- Panáček, A.; Prucek, R.; Šafářová, D.; Dittrich, M; Richtrová, J.; Beničková, K.; Zbořil, R.; Kvítek, L.: Acute and Chronic Toxicity Effects of Silver Nanoparticles (NPs) on Drosophila melanogaster. *Environ. Sci. Technol.* 45, 4974-4979, 2011.
- Prucek, R.; Tuček, J.; Kiliánová, M.; Panáček, A.; Kvítek, L.; Filip, J.; Kolář, M.; Tománková, K.; Zbořil, R.: The Targeted Antibacterial and Antifungal Properties of Magnetic Nanocomposite of Iron Oxide and Silver Nanoparticles. *Biomaterials* 32, 4704-4713, 2011.
- Krajewski, S.; Prucek, R.; Panáček, A.; Avci-Adali, M.; Nolte, A.; Straub, A.; Zbořil, R.; Wendel, H. P.; Kvítek, L.: Hemocompatibility Evaluation of Different Silver Nanoparticle Concentrations Employing a Modified Chandler-Loop in vitro Assay on Human Blood. *Acta Biomater.* 9, 7460-7468, 2013.
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- Maity, D.; Zoppellaro, G.; Šeděnková, V.; Tuček, J.; Šafářová, K.; Poláková, K.; Tománková, K.; Diwoky, C.; Stollberger, R.; Machala, L.; Zbořil, R.: Surface Design of Core-Shell Superparamagnetic Iron Oxide Nanoparticles Drives Record Relaxivity Values in Functional MRI Contrast Agents. *Chem. Commun.* 48, 11398-11400, 2012.
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Grant Support: Nanotechnology for Society GA ASCR – KAN115600801, 2008-2012. New Technologies of the Preparation and Use of Iron Oxide Based Nanoparticles for Environmental, Industrial and Medical Applications. Principal Investigator: Prof. RNDr. Radek Zbořil, Ph.D.

## COORDINATION COMPOUNDS IN BIOMEDICAL AND MATERIALS RESEARCH

By their nature, coordination compounds of transition metals represent a broad group of substances whose physical properties, and thereby their application potential, may be modified by the right combination of transition metal and ligand. The scientific focus of the RCPTM research division is thus concentrated on the study of compounds with realistically applicable properties in the fields of biomedicine and advanced materials, i.e. on the preparation of compounds applicable e.g. for the treatment of various oncological and inflammatory diseases on one hand, and on the preparation of materials technologically usable in recording technology, sensors and medical diagnostics on the other.

#### **Medicinal Chemistry**

In the field of medicinal chemistry, the research team led by Prof. Zdeněk Trávníček has been in the long term focused on the rational design, synthesis and detailed physical-chemical characterization of coordination compounds of selected transition metals exhibiting significant biological activity. The research has been primarily focused on antitumour complexes of platinum, copper, iron, ruthenium and zinc on the in vitro, in vivo and ex vivo models, including investigations of the mechanism of action on the cellular and molecular levels. In the course of these studies, several groups of compounds have been identified as significantly more antitumour active than the chemotherapeutics used in the oncological practice, e.g. cisplatin (patents CZ 303009, CZ 303417, CZ 303560, CZ 304045), and moreover, they do not exhibit so severe side effects as the conventional chemotherapeutic agents. Furthermore, these compounds are able to effectively overcome intrinsic or acquired resistance of multiple types of tumours to clinically used drugs (J. Inorg. Biochem. 2012). Additionally, further research activities of the team resulted

![](_page_21_Figure_4.jpeg)

in the preparation of complexes of gold (patent CZ 303649, *J. Med. Chem.* 2012) and zinc (*PLoS One* 2013) whose antiinflammatory activity exceeds that of many currently used drugs. The prepared complexes are also studied for their influence on healthy human cells, on the pathways of drug metabolisms, and also for the potential of their targeted delivery to tissues by binding to suitably functionalized iron oxide nanoparticles or by the formation of liposomes.

## Molecular Magnets and Spin-Crossover Complexes

In the research of magnetically interesting systems, our primary focus involves particularly iron complexes showing spin-crossover as well as compounds with large magnetic anisotropy, which thus have the potential to behave as single-molecule or single-chain magnets (*CrystEngComm* 2013). Systematic studies based on targeted optimization of selected structural types of compounds have resulted in the preparation and detailed characterization of several groups of complexes exhibiting spin-crossover. The influence of the presence and type of co-crystalized solvent and other covalent and non-covalent bonded ions on magnetic properties of the prepared compounds have also been studied (*Inorg. Chem.* 2011).

The most interesting results in the research of single-molecule magnets have been achieved with heterobimetallic complexes of iron in combination

![](_page_21_Picture_10.jpeg)

with lanthanides (*Dalton. Trans.* 2012). Additionally, the team systematically works on the preparation and characterization of hybrid systems of complexes with iron oxide nanoparticles and study of magnetic and transport properties of such systems.

![](_page_21_Figure_12.jpeg)

The challenge for biomedically oriented research teams lies, in general, in the preparation or identification of highly biologically active compounds with only minor side effects for the healthy human tissues. All the activities of the research team in the fields of the preparation and optimization of antitumour and anti-inflammatory complexes of various metals address this challenge. The promising compounds also undergo preclinical studies, whose positive results could serve as stepping stone for their entry into the clinical phase. Further, the preparation of hybrid systems of nanoparticle-small molecular drug, which could be applied in the targeted drug delivery, represents another challenge. The current activities will be expanded by the studies concerning the changes in the materials functionalizing nanoparticles with the aim to bind active compounds as effectively as possible and enable their subsequent controlled release in the target tissue. In the field of magnetically interesting compounds, the challenge for the research team lies in the preparation and development of compounds, or hybrid materials, which combine significant optical and magnetic properties, which could consequently result in generational innovation of the existing systems and could expand their application potential. The above mentioned aims could be achieved also thanks to new unique equipment, such as Physical Property Measurement System (PPMS) and 600 MHz NMR spectrometer for the study of compounds in the solid and solution phases.

![](_page_22_Picture_1.jpeg)

#### **Selected Publications:**

- Štarha, P.; Trávníček, Z.; Popa, A.; Popa, I.; Muchová, T.; Brabec, V.: How to Modify 7-Azaindole to Form Cytotoxic Pt(II) Complexes: Highly in vitro Anticancer Effective Cisplatin Derivatives Involving Halogeno-Substituted 7-Azaindole. J. Inorg. Biochem. 115, 57–63, 2012.
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- Herchel, R.; Trávníček, Z.; Zbořil, R.: Tuning of the Critical Temperature in Iron(II) Spin-Crossover Materials Based on Bridging Polycyanidometallates: Pentacyanidonitrosylferrate(II) and Hexacyanidoplatinate(IV). *Inorg. Chem.* 50, 12390–12392, 2011.
- Nemec, I.; Machata, M.; Herchel, R.; Boča, R.; Trávníček, Z.: A New Family of Fe2Ln Complexes Built from Mononuclear Anionic Schiff Base Subunits. *Dalton Trans.* 41, 14603–14610, 2012.

Grant Support: Centre of Excellence P303/12/G163, 2012-2018. Centre of Drug-Dietary Supplements Interactions and Nutrigenetics Centre Director: Prof. RNDr. Zdeněk Dvořák, DrSc. Et Ph.D.

Czech Science Foundation P207/11/0841, 2011-2014. Functionalized iron oxide nanoparticle-based magnetic carriers with bound biologically active and/or magnetically interesting compounds Principal Investigator: Prof. RNDr. Zdeněk Trávníček, Ph.D.

## THE WORLD OF BIOMOLECULES AND THEIR INTERACTIONS AS SEEN BY SUPERCOMPUTERS AND NANOSENSORS

Biomacromolecules, especially proteins and nucleic acids (DNA and RNA) are the building blocks of living organisms, where they play their essential roles. Although biomacromolecules have been subject to intensive research in recent decades, we still have no answers for a number of questions connected to their function and new questions are arising all the time. Among the questions which remain unanswered are those to do with how the unique three-dimensional structure of biomacromolecules originates. This is an important problem connected with Levinthal's Paradox, which says that although biomolecules are capable of folding into an uncountable number of shapes, they are able to fold into the correct shape in just fractions of a second. The folding to the right and biologically relevant shape originates in physical and chemical interactions precisely tuned by evolution. It is of utmost importance that only the correct fold of a biomacromolecule is able to carry out a biological function of the respective biomacromolecule. A number of serious illnesses is known such as cystic fibrosis, Creutzfeldt-Jakob, Alzheimer's and Parkinson's disease, which stem from the improper folding of biomacromolecules. Similarly, mechanisms of interaction of biomolecules with nanosystems are the focus of a significant area in contemporary research - nanosensorics. Properly prepared nanoparticles are capable, for instance, of monitoring enzymatic processes, marking pertinent biomolecules or permeating cells and "listening" to the activity inside living cells.

#### Noncovalent Interactions and the Structure of Biomolecules from a Computer Chemistry **Standpoint**

 ${\sf RCPTM}$  researchers have also spent much time investigating the role played by noncovalent interactions in the world of biomacromolecules and Prof. Hobza is a renowned world-class leader in the area (Acc. Chem. Res. 2013). RCPTM has developed a broad range of quantum chemistry methods for describing noncovalent interactions which allow very precise values to be obtained for interaction energies. The knowledge acquired is then used to develop methods of molecular mechanics and molecular dynamics. It is molecular dynamics which provides a unique simulation technique, the only such technique to offer fine-grained resolution in both space (atomic) and time (down to femtoseconds) for studying the dynamic behaviour of biomacromolecules. This helps us to understand how metabolism is regulated by RNA switching and the spatial arrangement of RNA is achieved. We have also successfully described the threedimensional structure of small proteins in combined computer-experimental studies with colleagues from the University of Cambridge (Biophys J. 2012).

The three-dimensional structure of proteins in and of itself is, of course, highly complex, thus we find its interior composed of various cavities and channels which may be functionally important. Recent studies by RCPTM researchers have shown that the great majority of enzymes have deeply buried active sites. This has prompted RCPTM to work on the development of novel approaches for seeking out and characterizing cavities and channels in protein structures. In collaboration with colleagues from CEITEC in Brno, MOLE 2.0 (see the online version at mole.upol.cz), a very effective piece of software, was developed to search and characterize these interior spaces (Nuc. Acids Res. 2012). The software is intensively used around the world for applications in protein engineering and understanding medication metabolism of drugs.

![](_page_23_Picture_5.jpeg)

#### **Nanosensors and Carbon Quantum Dots**

Magnetic iron oxide nanoparticles are being successfully used for the separation of DNA and proteins, as well as for the identification and designation of biomolecules including enzymes. RCPTM has enjoyed a long partnership in the area of magnetic biosensors with colleagues from the University

![](_page_23_Picture_8.jpeg)

ACS Publications

of Padua in Italy. Among the things we have recently jointly developed are universal magnetofluorescence sensors based on nanoparticles of maghemite with a specific surface treatment and functionalized using a rhodamine derivative useful for, among other things, determining glucose (Biosens. Bioelectron. 2013), and sensors for electrochemical determining hydrogen peroxide produced by mitochondria. Another interesting group of nanomaterials, used for labelling biomolecules and cells, are carbon guantum dots. Olomouc researchers together with colleagues from Greece and Cornell University were present at the birth of this new type of carbon nanomaterials. Their joint work, published in the journals Small and Chemistry of Materials have been cited today more than 300 times. Carbon dots win out over "classic" metallic quantum dots (CdSe, CdTe) by virtue of their lack of toxicity, their biocompatibility and their utility for biomedical applications. RCPTM researchers have already optimized methods of preparation which allow the surface and fluorescence properties of these carbon dots to be controlled (Chem. Mater. 2012). Current work is moving toward the study of hybrid systems employing gadolinium doped dots and iron oxide composites with carbon dots which have proven to be highly efficient in dual MRI/ fluorescence labelling of stem cells (J. Mater. Chem. 2012).

![](_page_24_Figure_1.jpeg)

New challenges in the study of biomolecules and their interactions, including interactions with nanosystems, are also tied to new possibilities in terms of instruments, thanks to a grant from OP RDI. This means above all the use of a resolution electron microscope capable of working in low temperatures and a new supercomputer. At present, RCPTM possesses computer clusters comprising a total 3026 CPUs and 72 GPUs with 50TB of storage space. Computer simulation is used not only for the study of biomacromolecules but also to study the permeability and accumulation of substances (drugs, antioxidants, etc.) in biological membranes, the structure and properties of new materials (including carbon and graphene quantum dots) and for describing chemical catalysis. In the area of nanosensors, research is focused on the development of new immunosensors based on magnetic nanoparticles, as well as on the use of carbon dots for in vivo fluorescent labelling, and for the study of internal cellular processes. A big challenge remains understanding the origin for the photoluminescent properties of carbon dots and their application in photodynamic anticancer therapy.

#### **Selected Publications:**

- Riley, K. E.; Hobza, P.: On the Importance and Origin of Aromatic Interactions in Chemistry and Biodisciplines. *Acc. Chem. Res.* 46, 927-936, 2013.
- Kůhrová, P.; De Simone, A.; Otyepka, M.; Best, R. B.: Force-Field Dependence of Chignolin Folding and Misfolding: Comparison with Experiment and Redesign. *Biophys. J.* 102, 1897-1906, 2012.
- Berka, K.; Hanák, O.; Sehnal, D.; Banáš, P.; Navrátilová, V.; Jaiswal, D.; Ionescu, C. M.; Svobodová Vařeková, R.; Koča, J.; Otyepka, M.: MOLEonline 2.0: Interactive Web-based Analysis of Biomacromolecular Channels. *Nuc. Acids Res.* 40, W222-W227, 2012.
- Baratella, D.; Magro, M.; Sinigaglia, G.; Zbořil, R.; Salviulo, G.; Vianello, F.: A Glucose Biosensor Based on Surface Active Maghemite Nanoparticles. *Biosens. Bioelectron.* 45, 13-18, 2013.
- Bourlinos, A. B.; Zbořil, R.; Petr, J.; Bakandritsos, A.; Krysmann, M.; Giannelis, E. P.: Luminescent Surface Quaternized Carbon Dots, *Chem. Mater.* 24, 6-8, 2012.
- Marková, Z.; Bourlinos, A. B.; Šafářová, K.; Poláková, K.; Tuček, J.; Medřík, I.; Šišková, K.; Petr, J.; Krysmann, M.; Giannelis, E. P.; Zbořil, R.: Synthesis and Properties of Core-Shell Fluorescent Hybrids with Distinct Morphologies Based on Carbon Dots, *J. Mater. Chem.* 22, 16219-16223, 2012.

![](_page_24_Picture_10.jpeg)

#### Grant Support:

#### Centre of Excellence P208/12/G016, 2012-2018.

Controlling Structure and Function of Biomolecules at the Molecular Scale: Theory meets Experiment. Principal Investigator: Prof. Ing. Pavel Hobza, DrSc., FRSC; Centre Director: Prof. RNDr. Michal Otyepka, Ph.D.

## MINIATURIZATION – A NEW CHALLENGE IN ANALYTICAL CHEMISTRY

Miniaturization has accompanied the evolution of mankind since its very beginnings. Today it is primarily connected to the development of new tools and materials which enable us to talk to our near and dear ones via mobile phone from one continent to another or to send cosmic probes to distant planets in our solar system, diligently monitor the quality of foods and produce new medicines. This trend toward miniaturization has also impacted on analytical chemistry. Special attention has been paid to the construction of mobile devices which allow analysis to be carried out in the field, as well as to the development of methods that consume small quantities of reagents and are becoming more economical and more environmentally friendly, methods that permit the analysis of specimens that cannot be weighed. The development of novel materials enables us to reach better analytical results, to achieve higher selectivity, lower detection limits, and to determine or identify small amounts of substances in complex matrices.

![](_page_25_Picture_2.jpeg)

#### **Miniaturized Devices**

The miniaturization of analytical tools or portions of these tools represents a milestone in analytical chemistry. Desorption nanoelectrospray, miniaturized desorption electrospray, is an example of ion source for mass spectrometry developed by a group led by Prof. Lemr. Its potential was demonstrated in the analysis of optical isomers in drugs in whole blood and in the analysis of wine (J. Chromatogr. A 2010). Complex miniaturized devices (so-called micro total analytical systems, µTAS) are capable of carrying out the entire analysis, including extraction processes, derivatization, separation and actual detection, on a single mobile platform which may be used, for example, directly by the patient's bedside. In 2010, a group led by Prof. Ševčík initiated collaboration with a leading global institution in this area, the Korea Institute of Science and Technology in Germany, led by Prof. Andreas Manz, one of the fathers of these technologies. At RCPTM, this collaboration is being nurtured by Assoc. Prof. Maier and Assoc. Prof. Petr. The development of miniaturized devices using superheated liquids has led to new ways to

break up and analyze bacterial spores with the potential for application in the fight against bioterrorism. Work in this area has culminated in a publication in the flagship journal of miniaturization, Lab on a Chip (2013). Review articles focusing on the analysis of microorganisms have also been published in the prestigious journals Trends in Analytical Chemistry (2012) and Analytical Chemistry (2013). Complex, costly analytical tools uncover the secrets of substances and processes in living organisms but the need to find gualified operators and economics present certain limitations. The analytical chemistry group has not overlooked the issue of low-cost devices based, for example, on paper (so-called micro paper-based analytical devices, µPAD). Miniaturized devices have been developed to monitor environmental pollution which allow analysis directly on-site and perform evaluations by sending images via mobile phone. Aside from collaboration with the group led by Prof. Manz, joint work has also been carried out in these areas with other foreign teams (e.g. Prof. Kevin Schug, University of Texas at Arlington, USA).

#### **Novel Analytical Methods**

The analytical chemistry group is also involved in the development of a wide variety of new methods, for example, for clinical and forensic analysis and the analysis of foods. The group works with clinical specialist from the Faculty Hospitals in Olomouc and Ostrava. Some interesting areas are the study of potential drugs (J. Med. Chem. 2013) and problems connected with the rejection of joint replacements, for which the distribution of released metals in the organism is monitored. Close cooperation with the Institute of Forensic Medicine of the Faculty Hospital of Olomouc has led to new approaches to determine mushroom intoxication and the identification of so-called "new designer drugs". A group led by Assoc. Prof. Bednář has had a long-term focus on analyzing wines and their properties with potential uses in detecting adulteration (J. Chromatogr. A 2011). A somewhat new direction is the development of methods characterizing nanoparticles in solutions and monitoring their interaction with biologically active substances, such as proteins or DNA (Assoc. Prof. Petr). Nanoparticles are used for the development of sensors or in preparing sorbents with required selectivity. Special analyses include the identification of pigment in historical painting samples which cannot be weighed (J. Mass Spectrom. 2013).

![](_page_26_Picture_2.jpeg)

![](_page_26_Picture_3.jpeg)

One of the greatest challenges RCPTM researchers in miniaturization and analytical chemistry are currently working on is the development of low-cost devices for medicinal applications, the development of stable ionization techniques for mass spectrometry for the rapid analysis of complex samples and the development of novel electrode materials and stationary phases using nanomaterials. All of this hinges on the study of fundamental processes, including the creation and fragmentation of ions, surface chemistry and exchange equilibrium in nanoparticles. Research benefits from sophisticated instrumentation such as the combination of separation methods with mass spectrometry or mass spectrometry combined with inductively coupled plasma.

#### Selected Publications:

- Papoušková, B.; Bednář, P.; Hron, K.; Stávek, J.; Balík, J.; Myjavcová, R.; Barták, P.; Tománková, E.; Lemr, K.: Advanced Liquid Chromatography/Mass Spectrometry Profiling of Anthocyanins in Relation to Set of Red Wine Varieties Certified in Czech Republic. J. Chromatogr. A 1218, 7581-7591, 2011.
- Petr, J.; Maier, V.: Analysis of Microorganisms by Capillary Electrophoresis. TrAC Trends Anal. Chem. 31, 9–22, 2012.
- Havlíček, V.; Lemr, K.; Schug K.A.: Current Trends in Microbial Diagnostics Based on Mass Spectrometry. Anal. Chem. 85, 790-797, 2013.
- Přibylka, A.; Almeida, A.V.; Altmeyer, M.O.; Petr, J.; Ševčík, J.; Manz, A.; Neužil, P.: Fast Spore Breaking by Superheating. Lab. Chip. 13, 1695–1698, 2013.
- Li, L.; Yang, S.H.; Lemr, K.; Havlíček, V.; Schug, K.A.: Continuous Flow-Extractive Desorption Electrospray Ionization: Analysis from "Non-Electrospray Ionization-Friendly" Solvents and Related Mechanism. Anal. Chim. Acta 769, 84– 90, 2013.
- Knob, R.; Breadmore, M.C.; Guijt, R.M.; Petr, J.; Macka, M.: Porous Layer Open Tubular Monolith Capillary Column: Switching-off the Reaction Kinetics as the Governing Factor in their Preparation by Using an Immiscible Liquid-Controlled Polymerization. *RSC. Adv.* 2013, in press (doi: 10.1039/C2RA23417C)

Grant Support: GA CR, P206/12/1150, 2012-2016. Sampling and efficiency of atmospheric pressure desorption/ionization in mass spectrometric experiment in Mass Spectrometry Experiments. Principal Investigator: Prof. RNDr. Karel Lemr, Ph.D.

![](_page_27_Picture_0.jpeg)

# 4 RCPTM AND TECHNOLOGY TRANSFER

## LOOKING INTO HEAVEN AND HELL

A number of scientific and industrial facilities which do their work under the open sky are dependent upon the state of the atmosphere or the amount of precipitation and cloud cover. Long-term monitoring of the atmosphere at often remote locations targeted for the construction and future operation of such facilities is essential in selecting a location effectively. To ensure the functioning of a number of operations and facilities which require clear skies, the ability to monitor the level of cloudiness both day and night is crucial.

All-sky cameras developed by both the RCPTM and the Institute of Physics of the Academy of Sciences of the CR are a by product of the Centre's involvement in large international scientific collaboration projects. Currently, they are in use as part of two projects - at Pierre Auger Observatory (in Argentina, four camera systems installed) and at Cherenkov Telescope Array (a total of seven systems installed in Namibia, Mexico, USA and the Canary Islands). A reference system has also been installed near Olomouc. These are autonomous cameras, highly flexible and capable of many different uses. They are capable of monitoring the intensity of light of the night sky background with an angular resolution of around 1.5°. They can also be used for long-term monitoring of day and night cloud coverage levels and the brightness of the night sky. This is highly useful, for example, in planning the location of future observatories, registering the effects of light pollution near urban agglomerations and increasing the efficiency of operation of systems and facilities which are dependent upon a clear sky.

![](_page_28_Figure_4.jpeg)

Map of camera systems installed.

![](_page_28_Picture_6.jpeg)

Examples of nighttime cloud coverage and the brightness of the night sky.

Increasing the efficiency of combustion processes in various industries (power plants, heating plants, cement plants, chemical plants, waste incinerators, mining) is currently not possible without facilities capable of monitoring the combustion process in real-time. Based upon a knowledge of the physics of flame, combustion can be influenced to minimize air pollution while achieving maximum efficiency.

For this reason, RCPTM has designed a method of videocomputer monitoring of flame spectrum temperature during the combustion process using a CCD camera. This method of measurement takes advantage of the sharp differences between the spectral reduction image (yellow prevails) and oxidizing flame (blue prevails). One of the key conditions for successful solution to this problem entails the development and implementation of an optical device which will allow a high-quality imaging of the flame on the CCD chip of a colour camera used under various types of combustion operations with various types of furnaces. The RCPTM Department of Optical and Photonic Technologies is responsible for the development and production of the optical portion of the device, a technical borescope, in close collaboration with several companies. Based upon validation tests of functional samples and prototypes provided by INDEL s.r.o. (Slovakia), the borescopes are distributed

to POWITEC (Germany) which introduces them into manufacturing processes in Europe (mainly Germany, Austria, the CR and Slovakia), South America (Argentina) and Asia (India, Malaysia and Turkey).

![](_page_28_Picture_11.jpeg)

Coloration of the reduction and oxidizing flames.

![](_page_28_Picture_13.jpeg)

Photographs of the borescopes developed.

## LOOKING INSIDE MATERIALS

To understand the structure and properties of materials, first-rank techniques are currently in use capable of monitoring the tiniest interactions. Mössbauer spectroscopy is one these techniques. Rudolf Ludwig Mössbauer won the Nobel Prize in Physics for its discovery in 1961. This method, based upon the interaction between atomic nuclei and electrons (so-called hyperfine interactions), is particularly suitable for the study of materials containing iron. It allows the various structural forms of iron to be identified and quantified, along with various valence and spin states, all directly in the solid phase with no need to destroy the specimen. A great advantage of this method lies in its element selectivity, which allows both qualitative and quantitative information to be obtained even with very low levels of iron compounds. It has been widely used not only in chemistry and physics but also in mineralogy, archeology, medicine, and space research. Only a few companies currently provide this technique on a commercial basis (e.g. Wissel, Germany).

Researchers in Olomouc have been focusing on the construction of Mössbauer spectrometers since the 1990s, as well as on the development of equipment for the movement of radioactive sources, gamma radiation detectors, electronic synchronization units and software control. Prof. Miroslav Mašláň, Palacky University Rector, was present when these devices came into being. Advantages of the spectrometers developed at RCPTM include their compactness and simple design, not requiring great technical knowledge on the part of the user, along with the fact that they are relatively simple to install and operate (on a plug-andplay basis), are user-friendly and may be operated by remote control. Another highly important feature is the spectrometer compatibility with systems working at low and high temperatures or in large external magnetic fields (furnaces, cryomagnetic facilities).

Olomouc spectrometers have been installed in a number of laboratories all over the world. These include the University of Johannesburg, University of Lund, University of Tokyo, University of Derby,

![](_page_29_Picture_4.jpeg)

"Cover arts" by RCPTM authors on the covers of journals published by the American Chemical Society

![](_page_29_Picture_6.jpeg)

The Mössbauer spectrometer in combination with a cryomagnetic system

University of Uppsala and this year, installation at the Florida Institute of Technology is underway. In terms of commercial entities, the spectrometers have been installed at SASOL Ltd., the largest chemical company in the Republic of South Africa and, more recently, at Forschungszentrum Jülich GmbH, Germany.

Aside from these commercial uses, RCPTM scientists use them for their own research activities, particularly to describe the structural and magnetic properties of various structural forms of iron(III) oxide nanoparticles. Their review articles on the use of Mössbauer spectroscopy studying the properties and applications of iron oxides have been published on the cover of Chemistry of Materials, a prestigious journal published by American Chemical Society.

## LOOKING UNDER THE SKIN

The skin is the largest organ of our body, protecting it from the direct impact of the external environment, preventing dehydration of the organism and limiting permeation of substances from the environment directly into the organism. However, many substances are known to permeate the skin. This characteristic of the skin is advantageous for local treatment using ointments and other transdermal applications. On the other hand, we have to protect our skin from permeation by some types of undesirable substances (for instance, herbicides, fungicides, organic solvents such as alcohols or petrol and many other toxic compounds). This is why new substances present in cosmetics, detergents and cleaning products which come into contact with skin have to be tested for their permeability through the skin and how they will impact upon the skin's permeability as a whole. Because experiments testing the permeation of substances are neither trivial nor cheap and require a source of human skin, the method by which the interaction and permeability of substances through the skin can be described effectively is computational chemistry.

RCPTM has realised this research, thanks to significant support from Procter & Gamble Company. Computer simulations are used to model the permeability of various commercially significant substances through the top protective layer of the skin (the so called stratum corneum). Currently, simplified models of the lipid bilayer are studied. Computer simulations allow to determine how substances accumulate in the lipid bilayer and how easily they are able to pass through it. RCPTM works on the development of stratum corneum model at the same time, but this task is complicated by the fact that it is a highly comlex structure created by ceramides, free fatty acids and cholesterol.

![](_page_30_Figure_3.jpeg)

A simple model of the interaction between the membrane (colourful spheres represent lipid polar heads, light blue chains non-polar lipid chains and grey dots represent water) with a model caffeine molecule (the lighter molecule). The free caffeine energy profile (red line) allows us to determine how caffeine accumulates in the membrane (depending upon the depth of the profile) and where it may be found most frequently (at the deepest point of the free energy profile).

The simplest model stratum corneum – on the left a pure bilayer of ceramides (water molecules are depicted in grey, lipids in blue-grey, polar sections are blue spheres, yellow and orange spheres represent the position of the lipid chain ends) and on the right a mixture of ceramide, free fatty acid, and cholesterol. In both cases the gel phase is visible in which the ceramide chains are ordered in a very regular manner. This structure significantly limits the permeability of the ceramide layers.

![](_page_30_Picture_6.jpeg)

## **GROUNDWATER TREATMENT**

Today, groundwater is contaminated by dozens of toxic substances in a number of locations all over the world. These enter the environment as the result of environmentally unfriendly industrial production, industrial accidents and armed conflicts. In the Czech Republic, dealing with old ecological burdens is a significant economic and technological issue. These include the elimination of toxic substances which have entered the environment during the activities of the Soviet Army, or past environmentally unfriendly industrial processes such as uranium mining. Groundwater contaminated with chlorinated hydrocarbons, nitro-compounds, arsenic and heavy metals thus represents a real, high risk of contamination of drinking water. Researchers all over the world are seeking for new environmentally friendly methods for groundwater remediation.

As part of a joint project with the Technical University of Liberec, RCPTM researchers took part in developing a method using iron nanoparticles for in situ remediation of contaminated groundwater in which nanoiron soaks into the groundwater and eliminates toxic soluble organic and inorganic pollutants, while the nontoxic iron oxide based products remain underground. In the past, the chief problem with broader application of this environmentally friendly technology lay in the lack of adequate nanomaterials at a reasonable price on the global market. RCPTM researchers working together with colleagues from LAC s.r.o. began development of large-scale production technology of nanoiron and its surface stabilization, since pyrophoric iron ignites on contact with air. This effort has resulted in a patented technology which employs a thermally induced solidstate reaction (EP 2164656, 2013). After production, nanoiron is further treated by a polymer layer providing good migration properties when applied in groundwater, thus allowing the long-distance use of the reductionprecipitation decontamination effect. Nanoiron, s.r.o, which uses the technology, is the largest European producer of nanoiron, which is commonly used by both

Czech and European remediation companies for treating groundwater contaminated by chlorinated hydrocarbons, arsenic and heavy metals in particular. Pilot applications have also been carried out in the USA.

![](_page_31_Picture_4.jpeg)

High-temperature furnaces and accessories for working in a reducing atmosphere enable the large-scale production of nanoiron

## RAPID QUALITY CONTROL

The introduction of automated visual systems (also called machine vision systems) for monitoring goods and products is a problem frequently faced in assembly line production. If visual checks are carried out by humans, the monotonous work inevitably leads to gradually failing concentration, which subsequently increases errors. For this reason, sensing cameras for technological operations have been offered and put to use. Upon being connected to a control computer with the requisite programme, they are capable of controlling manipulators and providing status signals to technological systems.

![](_page_31_Picture_8.jpeg)

Launch of the system on the Mubea, s.r.o. technological assembly line and an image of coloured markers on the surface of an automobile spring.

In this area, RCPTM researchers participated in the design, development and implementation of an inspection device for monitoring the quality of a process involving the spraying of coloured markers on the surface of automobile springs. The springs are monitored on a technological assembly line located in a production hall environment typical for mechanical engineering. The monitored objects consist of coloured markers sprayed on the surface of automobile springs. The number of markers and their colours indicate the spring class; there may be several classes for each type of spring. The entire cycle of scanning and evaluating an image may not exceed 6 seconds, which is dictated by the speed of the technological assembly line. In addition to designing the device, RCPTM researchers participated in the production itself, including development of the requisite software.

## **5** RCPTM – INTERNATIONAL CENTRE FOR SCIENCE AND EDUCATION

The aim of the RCPTM management has been a strong internationalization of the research teams since the very beginning of RCPTM existence. Challenging topics, first rank instrumental equipment and motivating social environment allow the foreign scientists to work in the Centre at the "Distinguished Scientist" positions, the young researchers to apply for the "Junior Researcher" positions or to attract the excellent Czech researchers back to the Czech Republic. Not only due to the supporting RCPTM projects from the "Operational Programme Education for Competitiveness" the Centre was successful in employing 25 excellent international scientists. The Centre thus represents an interesting place for building up research teams and starting a scientific career.

## Leading Foreign Researchers at RCPTM

![](_page_32_Picture_3.jpeg)

One of TOP 25 authors in Nanotechnologies (about 21,000 citations, H-58).

*Scientific profile:* Nanocomposites, Nanoparticle Fluids, Flexible Electronics, Nanobiohybrids, Nanohybrid Membranes for Fuel Cells

Joint research with RCPTM in the field of carbon quantum dots and their applications for cell labeling, e.g. Chemistry of Materials, 24, 6-8, 2012.

"From my first encounter with Prof. Zboril several years ago, I realized that we share the same passion for science and for research. These shared interests have formed the foundation for our long standing personal friendship and inspired our collaborative research. One of the dreams of Radek, which he shared with me many years ago, was to establish an interdisciplinary research centre to advance the frontiers of science and inspire and train the next generations of Czech students. The Regional Centre of Advanced Technologies and Materials that has emerged since is already regarded as a premier research center in central Europe. The Centre is not only open to Czech students and researchers, but has become a home for many international scientists. It has established a worldwide network of collaborations tackling cutting-edge research projects. Despite that the Centre is only 3 years old and the youth of the research team, the average age of the researchers is less than 33, the output is very impressive with more than 200 publications per year. Clearly the Centre under the leadership of Prof. Zboril has come a long way from his early dream and is well positioned for many successes in the future. I am honored to have known and worked with Radek and be part of this inspiring and impressive Centre."

![](_page_32_Picture_8.jpeg)

Director of Center of Ferrate Excellence, holder of the "Outstanding Chemist Award"- American Chemical Society.

*Scientific profile:* Ferates Research, Fundamental Chemistry, Environmental Chemistry – Pharmaceuticals, Endocrine Disruptor Chemicals, Photocatalytic Oxidation of Pollutants

*Joint research with RCPTM* in the field of antimicrobial applications of nanosilver and environmental applications, e.g. *Advances in Colloid and Interface Science*, 166, 119-135, 2011.

"A collaborative team of Florida Institute of Technology and RCPTM is indulgently pursuing innovative research on ferrate applications and synthesis and antibacterial activities of silver nanoparticles. The focus of collaborative research is on the mechanism of the reactions involved in performing superior environmental remediation of contaminants (e.g. arsenic) by ferrates. The synthesis of silver nanoparticles by organics present naturally was demonstrated for the first time. The collaboration has resulted in high quality results and a team published their results in high impact journals such as Environmental Science & Technology and Advances in Colloid and Interface Science. This could be possible because of unique instrumental capability of the RCPTM. Interestingly, RCPTM continues to strengthen the capability by obtaining state-of-the art instruments. More importantly, the RCPTM has a pool of young researchers who are enthusiastic to take this opportunity to generate high quality research to accomplish the goals of the RCPTM. This approach of the young researchers with high level of knowledge is imperative to sustain the high quality research growth of the RCPTM."

#### Prof. Andrey L. Rogach

![](_page_33_Picture_1.jpeg)

City University of Hong Kong, China

One of TOP 10 most cited authors in Nanocrystals and TOP 50 in Materials Science (more than 15,000 citations, H-66).

Joint research in nanosystems based on  $SnO_2$  and quantum dots, e.g. *Nanoscale*, 5, 9101-9109, 2013.

#### Prof. Shin-ichi Ohkoshi

![](_page_33_Picture_6.jpeg)

University of Tokyo, Japan

World recognized expert in the field of magnetic materials (about 9,000 citations, H-49). Holder of IBM Japan Science Prize and Japan Academy Medal.

Joint research in the field of iron oxides with new magnetic properties, e.g. *Chemistry of Materials*, 22 6483-6505, 2010.

#### Prof. Aharon Gedanken

![](_page_33_Picture_11.jpeg)

Bar-Ilan University, Israel

One of the pioneers of sonochemistry, expert in applications of metallic nanomaterials (almost 18,000 citations, H-68). The holder of President of Israel Achievement Award.

Joint research in the field of applications of nanometals and iron oxides, e.g. *Journal of Physical Chemistry B*, 111, 4003-4018, 2007.

![](_page_33_Picture_15.jpeg)

#### University of Patras, Greece

World recognized expert in chemistry of new carbon allotropes (more than 3,500 citations, H-29). Co-author of significant papers in Chemical Reviews and Journal of the American Chemical Society.

Joint research in the field of functionalization of graphene, e.g. *Chemical Reviews*, 112, 6156-6214, 2012.

#### Prof. Mingdong Dong

![](_page_33_Picture_20.jpeg)

Aarhus University, Denmark

Leading scientist in AFM imaging of biomolecules. Co-author of several papers in the most prestigious journals Nature, Nature Communications, Nature Nanotechnology.

Joint research in the field of description of the interaction of graphene with metals and biomolecules, e.g. ACS Nano, 7, 1646-1651, 2013.

![](_page_33_Picture_24.jpeg)

![](_page_33_Picture_25.jpeg)

EPFL Lausanne, Switzerland

Holder of prestigious award Prix Zeno Karl Schindler/EPFL. Head of the Laboratory for Molecular Engineering of Optoelectric Nanomaterials. Publications for example in Nature Materials, JACS, Angewandte Chemie.

Joint research in the field of thin films of iron oxide for direct solar splitting, e.g. *Journal of Materials Chemistry*, 22, 23232-23239, 2012.

#### Dr. Rajender S. Varma

![](_page_34_Picture_1.jpeg)

#### U.S. Environmental Protection Agency

Recognized expert in the field of environmental chemistry and catalysis (more than 14,000 citations, H-63). Holder of prestigious award Visionary of the Year 2009 - Green Technology.

Joint research on magnetically separable catalysts.

![](_page_34_Picture_5.jpeg)

University of Ioannina, Greece

Expert in the field of porous materials and their applications (about 3,000 citations), investigator of several prestigious NATO projects.

Joint research in the field of hybrid silicate and carbon nanomaterials for environmental and optical applications, e.g. *Carbon*, 61, 640-643, 2013.

#### Prof. Martin Pumera

![](_page_34_Picture_10.jpeg)

Nanyang Technological Univ. Singapore

Expert in the field of graphene and its derivatives (about 5,700 citations, H-40). Principal investigator of the prestigious ERC grant.

Joint research in the field of covalent functionalization of graphene and electrochemical nanosensors.

Prof. Fabio Vianello

![](_page_34_Picture_14.jpeg)

#### University of Texas Arlington, USA

Expert in the field of chromatography and mass spectrometry. Holder of prestigious NSF CAREER Award.

Joint research in the field of mass spectrometry, e.g. *Anal. Chem.* 85, 790-797, 2013.

Dr. Athanasios B. Bourlinos

University of Ioannina, Greece

Expert in the field of carbon nanostructures. Publications for example in Chemical Reviews or Journal of the American Chemical Society.

Joint research in the field of carbon quantum dots and graphene derivatives, e.g. *Journal of Materials Chemistry*, 2, 23327-23330, 2012.

![](_page_34_Picture_22.jpeg)

University of Padua, Italy

Expert in the field of biochemistry and magnetic sensors. Publications for example in Cancer Research and Biosensors & Bioelectronics.

Joint research in the field of electrochemical biosensors based on magnetic nanoparticles, e.g. *Biosensors & Bioelectronics*, 45, 13-18, 2013.

33

## The rising generation at RCPTM

The Regional Centre of Advanced Technologies and Materials (RCPTM) employs not only experienced scientists, but also graduates of master degree and PhD study programmes. RCPTM has a broad base of younger generation due to close links to several departments of the Faculty of Science at Palacký University. It guarantees a large number of study programmes in the fields of physical, inorganic, analytical and materials chemistry, applied physics, optics, optoelectronics and nanotechnology. Since the foundation of RCPTM dozens of students have become involved in research at RCPTM, some of whom have gained research positions at the Centre. For this reason, too, the average age of employees is very low (33 years). RCPTM endeavours to maintain the trend of a high degree of internationalization amongst the rising generation of scientists, too, which manifests itself in the number of PhD students from abroad and the number and quality of employees in post-doc positions. Here are the responses of some representatives of the rising generation of scientists when being asked the question: "Why did you choose the RCPTM for your scientific career?"

#### Dr. Jason Permar

![](_page_35_Picture_3.jpeg)

## "Why am I doing research in Olomouc?

I began my scientific endeavors in mv hometown of Tampa, Florida at the University of South Florida. After completing my bachelor's degree, I decided to continue my education and training to become a chemist under the supervision of Professor Michael J. Zaworotko in the

fields of supramolecular, inorganic, and green chemistry. After completing and defending my Ph.D. in chemistry in 2011, I wanted to explore other avenues of science. An opportunity presented itself with Josef Michl at the Institute of Organic and Biochemistry ASCR in Prague, where I developed new skills as a post-doctoral fellow. The research and the facilities were very high and the city of Prague is very beautiful and full of life. This was a wonderful place to start in Europe for both research and cultural enrichment. Recently, I have made a big leap to join as a Junior Research at RCPTM in Olomouc where I can work with an excellent group of researchers and professors. RCPTM is directed by Radek Zboril who is very supportive of many ideas I have and the future of the Centre and how it can be transformed to something great with the right group of researchers. Currently, we have an amazing and new facility with top of the line equipment and great collaborations' within the Czech Republic, Europe and abroad.

#### Previous places of work:

- University of South Florida, USA;
- Institute of Organic Chemistry and Biochemistry AS CR.

#### Scientific profile:

Synthesis of advanced organometallic materials, organic chemistry, solid-state reactions, carbon nanostructures. *Selected publications:* 

*Chem. Soc. Rev.* 38, 1400-1417, 2009; *Angew. Chem. Int. Ed.* 47, 8460-8463; 2008; *JACS* 130, 1560 – 1561, 2008; *JACS* 132, 12796-12799, 2010.

"I am Dr. rer. nat. Giorgio Zoppellaro, and I received my first Master degree in Industrial Chemistry from University of Milan (1997, Italy) and a second Master degree in Pharmacology from University Kanazawa (2000, Japan). I obtained the Ph.D. degree in Synthetic Physical/ Organic Chemistry from The Johannes Gutenberg University

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of Mainz (2004, Germany) with research work carried out at The Max Planck Institute for Polymer Research in Mainz (Prof. K. Mullen Group). I covered a post-doctoral position at the Institute of Nanotechnology (Prof. Nobel laureate J.-M. Lehn Group) in Karlsruhe (2005-2007, Germany) and then from 2008 I became researcher at the Department of Biosciences, University of Oslo with a Marie-Curie FP7 IEF grant. Since 2011 I covered a senior research position at RCPTM, a research-core institution that is well on its way to become highly internationally recognized. In my opinion, there are three key factors that lay the basis for the RCPTM successful journey into the future; first key, the vision behind its establishment, where cutting edge research and knowledge suitable for transfer into industrial practice are merged together, in a single research-body. Second key, RCPTM offers a dynamic working architecture combined with excellent infrastructures (administrative and instrumental facilities). Third key, RCPTM embraces a highly trained pool of scientists, people that share vibrant passion for research. Therefore, let's the journey begin, welcome to RCPTM."

#### Previous places of work:

- Max Planck Institute for Polymer Research, Germany;
- University of Milan, Italy; University of Oslo, Norway;
- Institute of Nanotechnology, FZK, Karlsruhe, Germany. *Scientific profile:*

Organic/inorganic synthesis, chromatography, quantum chemical calculations, magnetic nanosystems.

#### Selected publications:

Nature Chem. 2, 131-137; 2010; Coord. Chem, Rev. 257, 3-26, 2013; Angew. Chem. Int. Ed. 46, 710-713, 2007; Nano Lett. 7, 3813 – 3817, 2007.

#### Ing. Veronika Urbanová, Ph.D.

![](_page_36_Picture_1.jpeg)

"Why did I choose Olomouc as my place of work?

Once I completed my master studies in analytical chemistry at the University of Pardubice, I decided to continue my doctoral studies at the same university and deepen my knowledge in the field of electrochemistry.

During my first year I received a grant from the French embassy in Prague, supporting my parallel studies at both Czech and French universities. I then had the opportunity to undertake scientific activities at the well-established NSYSA electrochemical laboratory, headed by Professor Alexander Kuhn, at the University of Bordeaux 1. Following the successful defense of my thesis at both universities in 2010, I decided to continue my scientific career abroad and accepted the position of research fellow under Professor Alain Walcarius at the LCPME laboratory at the University of Nancy, where I had the opportunity to not only collaborate with true specialists in the field of electrochemistry, but also gain experience of interdisciplinary collaboration with other laboratories through the ERUDESP European project.

After working as part of this group for three years, the time came to consider my future place of work. It was at this time that I found out, through the press, about the RCPTM, a new scientific Centre being developed in Olomouc, which engaged my interest on the one hand because of the high number of international collaborations and second, because of the extraordinarily high level of facilities and equipment available, which you don't always get in even the big European laboratories. So I decided to contact Professor Zbořil, whose fast, helpful response was further evidence of the high standards and professionalism of the Centre. The opportunity to build an electrochemical section, which the RCPTM did not, at the time, have, together with interesting financial aspect, represented a challenge and was the deciding factor in my return to the Czech Republic. I hope that my experience and contacts abroad can aid the further development of the RCPTM in becoming a high-quality, recognized scientific Centre, and also hope that my current position can contribute towards the development of my scientific career in the right direction."

![](_page_36_Picture_6.jpeg)

"Why did I choose the RCPTM? As far back as my student days I felt that my professional career would always be associated with the Palacký University in Olomouc. When I began studies doctorate my in Applied Physics in 2003, I became a part of young people collective where I had, from the very beginning, a clearly defined position, tasks, responsibilities and competencies. This inspired

me and motivated me to further develop my personal scientific focus. I soon realized that such an approach would invoke massive opportunities for me. I easily came into contact with leading global specialists in the field of magnetism and was entrusted with the responsibility of leading major research projects. Today, I successfully maintain 7 international collaborations, which I regularly put to good use in published outcomes. My personal feelings from my time at the Regional Centre for Advanced Technologies and Materials are, and always will be, associated with the fact that I am a member of a big family that can still continue to enrich me."

Mgr. Kateřina Holá

![](_page_36_Picture_11.jpeg)

"The actor Jan Werich once said that people always paid more money for music than for physics, which is why there is no Czech Einstein. The development of the Internet has meant that music isn't what it used to be, whereas science can look forward to a brighter future. One good example of this is our Centre. Even as students we get the opportunity here to

become involved in world-class research, work with stateof-the-art instruments and contribute to the writing and resolution of grants, while having our Ph.D. studies as a fulltime occupation. One great advantage is the opportunity to visit prestigious global laboratories to find out how things work outside the Czech Republic. Fortunately, I'm glad that I never showed any musical talent!"

![](_page_36_Picture_14.jpeg)

"It was just the period that I had started my PhD studies, coming from a country that nowadays faces political serious economic and problems, definetely one of the greatest opportunities in my life. Curious for the unknown and full of expectations on expanding my scientific horizons I came to a country and a scientific centre that тy

supervisor kindly recommended in the context of significant collaboration that was established during the last years. It didn't take much time and I started to feel to be a part of this amazing scientific family. I immediately realized and appreciated the willingness of all the members of RCPTM to collaborate and discuss thoroughly about our work and new ideas. Amazing leadership and management of the institute, expertized and brilliant scientists as members and collaborators, excellent working conditions and facilities, well equipped laboratories, and very interesting and innovative topics that came along here, amplified my knowledge and experience providing me with more skills and promising better future career."

# **6** RCPTM IN NUMBERS

## Grant successes

The grant success rate is the measurable ratio between the number of projects applied and gained. Employees of the Regional Centre of Advanced Technologies and Materials submit project applications in many fields of basic and applied research, not to mention educational projects and projects in support of collaboration with industrial partners. The percentage success rate of the Centre's grant policy is above 80 percent. RCPTM employees are currently dealing with large, long-term projects of the Czech Science Foundation Centre of Excellence, collaborative applied research projects for the Czech Technology Agency – Competence Centre, projects of the 7<sup>th</sup> EU framework programme and projects for the Operational Programme Education for Competitiveness and the Building of Excellent Research Teams. During the Centre's realization phase, that is the last three years, the Centre dealt with or is dealing with 55 projects with the total amount of subsidies of app. CZK 520 million for RCPTM.

#### 7<sup>th</sup> EU Framework Program

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FP7-Collaboration: Taking Nanotechnological Remediation Processes from Lab Scale to End User Applications for the Restoration of a Clean Environment; FP7-NMP 2011108

Principal Investigator at Palacký University: Prof. RNDr. Radek Zbořil, Ph.D.

www.nanorem.eu

![](_page_37_Picture_8.jpeg)

NANOREM is a four-year project coordinated by the University of Stuttgart, where a group of RCPTM researchers works with 28 partners on the development of new methods of water treatment based on nanotechnologies and their transfer from the laboratory to industry.

FP7-SME: Innovative Green Technology for Smart Energy Saving on Existing Residential Buildings with Centralized Heating/Cooling Generators; FP7-INFRASTRUCTURES 315025

Principal Investigator at Palacký University: Mgr. Pavel Tuček, Ph.D.

www.ecothermoproject.com

![](_page_37_Picture_13.jpeg)

ECOTHERMO is a three-year project coordinated by the private company Ingenia srl. (Italy). As part of the project, which involves 8 partners, RCPTM employees work on the development of new technologies for the efficient heating of buildings.

Technology Agency of the Czech Republic

![](_page_37_Picture_16.jpeg)

Competence Centre: Environmentally Friendly Nanotechnologies and Biotechnologies for Water and Soil Treatment; TACR TE01020218.

Centre Director: Prof. RNDr. Radek Zbořil, Ph.D.

www.nanobiowat.com

![](_page_37_Picture_20.jpeg)

This project joins the capacities of three academic and six industrial partners for the development and implementation of environmentally friendly nanotechnologies and biotechnologies applicable for the treatment of a wide spectrum of types of water, including groundwater, waste and surface water, with the possibility of removing organic, inorganic and microbial pollutants.

Czech Science Foundation

![](_page_37_Picture_23.jpeg)

Centre of Excellence: Controling Structure and Function of the Molecular Scale: Theory meets Experiment; P208/12/G016.

Principal Investigator: Prof. Ing. Pavel Hobza, Dr.Sc., Centre Co-investigator: Prof. RNDr. Michal Otyepka, Ph.D.

This project deals with a new methodology for the control of the structure and function of biological systems on the molecular level. The methodology is based on the development of experimental and calculation methods for the quantitative description of non-covalent interactions in large molecular systems. This interdisciplinary approach requires a combination of connection of computational chemistry, medicinal chemistry, biochemistry, organic chemistry and structural biology.

Centre of Excellence: Centre of drug - Dietary Supplements Interaction and Nutrigenetic; P303/12/G163.

#### Centre Co-investigator: Prof. RNDr. Zdeněk Dvořák, Ph.D.

This project looks at the interaction of selected groups of plant substances contained in food supplements with the most important biotransformational enzymes, transporters and nuclear receptors, with regard to their potentially clinically significant interactions with drugs. The project further aims to describe the pharmacological and toxicological properties of selected substances of natural origin and their metabolites. The effect of genetic predisposition on kinetics and undesired side-effects of these substances are also being studied.

## Selected Publications and Patents

Publications are the showcase of every scientific centre, and their number, quality and the team of coauthors frequently tell a lot about the realized research in the Centre and the importance of international collaboration. A list of selected RCPTM publications with an impact factor higher than 5, as well as a list of issued patents are given below.

- 1. V. Georgakilas, M. Otyepka, A.B. Bourlinos, V. Chandra, N. Kim, K.C. Kemp, P. Hobza, R. Zboril, K.S. Kim: "Functionalization of Graphene: Covalent and Non-Covalent Approaches, Derivatives and Applications", *Chem. Rev. 112*, 6156-6214 (2012). IF=41.30
- 2. P.Hobza: "Calculations on Noncovalent Interactions and Databases of Benchmark Interaction energie", Acc. Chem. Res. 45, 663–672 (2012). IF=20.83
- 3. K.E. Riley, P. Hobza: "On the Importance and Origin of Aromatic Interactions in Chemistry and Biodisciplines", Acc. Chem. Res. 46, 927-936 (2013). IF=20.83
- P. Lazar, S. Zhang, K. Safarova, Q. Li, J.P. Froning, J. Granatier, P. Hobza, R. Zboril, F. Besenbacher, M. Dong, M. Otyepka: "Quantification of the Interaction Forces between Metals and Graphene by Quantum Chemical Calculations and Dynamic Force Measurements under Ambient Conditions", ACS Nano 7, 1646-1651 (2013). IF=12.06
- 5. F. Karlicky, K.K.R. Datta, M. Otyepka, R. Zboril: "Halogenated Graphenes: Rapidly Growing Family of Graphene Derivatives", ACS Nano 7, 6434-6464 (2013). IF = 12.06
- T. Zeleny, M. Ruckenbauer, A.J.A. Aquino, T. Muller, F. Lankas, T. Drsata, W.L. Hase, D. Nachtigallova, H. Lischka: "Strikingly Different Effects of Hydrogen Bonding on the Photodynamics of Individual Nucleobases in DNA: Comparison of Guanine and Cytosine", J. Am. Chem. Soc. 134, 13662-13669 (2012). IF=10.68
- 7. P. Lazar, F. Karlicky, P. Jurecka, M. Kocman, E. Otyepkova, K. Safarova, M. Otyepka: "Adsorption of Small Organic Molecules on Graphene", J. Am. Chem. Soc. 135, 6372-6377 (2013). IF=10.68
- 8. K. Berka, O. Hanak, D. Sehnal, P. Banas, V. Navratilova, D. Jaiswal, C.M. Ionescu, R. Svobodova-Varekova, J. Koca, M. Otyepka: "MOLEonline 2.0: Interactive Web-based Analysis of Biomacromolecular Channels", *Nuc. Acids. Res.* 40, W222 (2012). IF=8.28
- 9. L. Machala, J. Tucek, R. Zboril: "Polymorphous Transformations of Nanometric Iron(III) Oxide: A Review", Chem. Mater. 23, 3255-3272 (2011). IF=8.24
- 10. A. B. Bourlinos, R. Zboril, J. Petr, A. Bakandritsos, M. Krysmann, E. P. Giannelis: "Luminescent Surface Quaternized Carbon Dots", Chem. Mater. 24, 6–8 (2012). IF=8.24
- 11. K. Lemr, A. Cernoch, J. Soubusta, K. Kieling, J. Eisert, M. Dusek: "Experimental Implementation of the Optimal Linear-Optical Controlled Phase Gate", Phys. Rev. Lett. 106, 013602 (2011). IF=7.94
- 12. K. Bartkiewicz, K. Lemr, A. Cernoch, J. Soubusta, A. Miranowicz: "Experimental Eavesdropping Based on Optimal Quantum Cloning", *Phys. Rev. Lett.* 110, 173601 (2013). IF=7.94
- 13. R. Zboril, F. Karlicky, A. B. Bourlinos, T. A. Steriotis, A. K. Stubos, V. Georgakilas, K. Safarova, D. Jancik, C. Trapalis, M. Otyepka: "Graphene Fluoride: A Stable Stoichiometric Graphene Derivative and its Chemical Conversion to Graphene", *Small 6*, 2885-2891 (2010). IF=7.82
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- R. Prucek, J. Tucek, M. Kilianova, A. Panacek, L. Kvitek, J. Filip, M. Kolar, K. Tomankova, R. Zboril: "The Targeted Antibacterial and Antifungal Pproperties of Magnetic Nanocomposite of Iron Oxide and Silver Nanoparticles", *Biomaterials 32*, 4704-4713 (2011). IF=7.60
- Z. Markova, K. Siskova, J. Filip, K. Safarova, R. Prucek, A. Panacek, M. Kolar and R. Zboril: "Chitosan-Based Synthesis of Magnetically-Driven Nanocomposites with Biogenic Magnetite Core, Controlled Silver Size, and High Antimicrobial Activity", Green Chemistry 14, 2550-8 (2012). IF=6.83
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- 18. J. Petr, V. Maier: "Analysis of Microorganisms by Capillary Electrophoresis", Trends Anal. Chem. 31, 9–22 (2012). IF=6.35
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- 20. P. Dallas, V. K. Sharma, R. Zboril: "Silver Polymeric Nanocomposites as Advanced Antimicrobial Agents: Classification, Synthetic Paths, Applications, and Perspectives", Adv. Colloid Interface Sci. 166, 119-135 (2011). IF=6.17
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- 22. R. Prucek, A. Panacek, J. Soukupova, R. Novotny, L. Kvitek: "Reproducible Synthesis of Silver Colloidal Particles Tailored for Application in Near-Infrared Surface-Enhanced Raman Spectroscopy", J. Mat. Chem. 21, 6416-6420 (2011). IF=5.97
- 23. A.B. Bourlinos, A. Bakandritsos, A. Kouloumpis, D. Gournis, M. Krysmann, E.P. Giannelis, K. Polakova, K. Safarova, K. Hola, R. Zboril: "Gd(III)-doped carbon dots as a dual fluorescent-MRI probe", J. Mater. Chem. 22, 23327-23330 (2012). IF=5.97
- J. Frydrych, L. Machala, J. Tucek, K. Siskova, J. Filip, J. Pechousek, K. Safarova, M. Vondracek, J. Seo, O. Schneeweiss, M. Gratzel, K. Sivula, R. Zboril: "Facile Fabrication of Tin-Doped Hematite Photoelectrodes: Effect of Doping on Magnetic Properties and Performance for Light-Induced Water Splitting", J. Mater. Chem. 22, 23232-23239 (2012). IF=5.97
- 25. A. B. Bourlinos, K. Safarova, K. Siskova, R. Zboril: "The Production of Chemically Converted Graphenes from Graphite Fluoride", Carbon 50, 1425-1428 (2011). IF=5.87
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- 27. J. Filip, R. A. Yngard, K. Siskova, Z. Marusak, V. Ettler, P. Sajdl, V. K. Sharma, R. Zboril: "Mechanisms and Efficiency of the Simultaneous Removal of Metals and Cyanides by Using Ferrate(VI): Crucial Roles of Nanocrystalline Iron(III) Oxyhydroxides and Metal Carbonates", *Chem. Eur. J.* 17, 10097-10105 (2011). IF=5.83
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- 29. A. Pribylka, A.V. Almeida, M.O. Altmeyer, J. Petr, J. Sevcik, A. Manz, P. Neuzil: "Fast Spore Breaking by Superheating", Lab on a Chip 13, 1695-1698 (2013). IF=5.70
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- 35. J. Rezac, K. E. Riley, P. Hobza: "Extensions of the S66 Data Set: More Accurate Interaction Energies and Angular-Displaced Nonequilibrium Geometries", J. Chem. Theory Comput. 7, 3466-3470 (2011). IF=5.39
- 36. J. Granatier, P. Lazar, M. Otyepka, P. Hobza: "The Nature of the Binding of Au, Ag, and Pd to Benzene, Coronene, and Graphene: From Benchmark CCSD(T) Calculations to Plane-Wave DFT Calculations", J. Chem. Theory Comput. 7, 3743–3755 (2011). IF=5.39
- F. Karlicky, M. Otyepka: "The First Step in the Reaction of Zerovalent Iron with Water", J. Chem. Theory Comput. 7, 2876-2885 (2011). IF=5.39
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- 39. P. Sklenovsky, P. Florova, P. Banas, K. Reblova, F. Lankas, M. Otyepka, J. Sponer: "Understanding RNA Flexibility Using Explicit Solvent Simulations: The Ribosomal and Group I Intron Reverse Kink-Turn Motifs", J. Chem. Theory Comput. 7, 2963-2980 (2011). IF=5.39
- 40. J. Rezac, K. E. Riley, P. Hobza: "S66: A Well-balanced Database of Benchmark Interaction Energies Relevant to Biomolecular Structures", J. Chem. Theory Comput. 7, 2427-2438 (2011), IF=5.39

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- 46. M. Paloncyova, K. Berka, M. Otyepka: "Convergence of Free Energy Profile of Coumarin in Lipid Bilayer", J. Chem. Theory Comput. 8, 1200-1211 (2012). IF=5.39
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- 51. P. Kuhrova, P. Banas, R.B. Best, J. Sponer, M. Otyepka: "Computer folding of RNA tetraloops? Are we there yet?", J. Chem. Theory Comput. 9, 2115-2125 (2013). IF=5.39
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- 53. J. Rezac, L. Simova, P. Hobza: "CCSD[T] Describes Noncovalent Interactions Better than the CCSD Better than the CCSD(T), CCSD(TQ), and CCSDT Methods", J. Chem. Theory Comput. 9, 346-369 (2013). IF=5.39
- 54. A. Panacek, R. Prucek, D. Safarova, M. Dittrich, J. Richtrova, K. Benickova, R. Zboril, L. Kvitek: "Acute and Chronic Toxicity Effects of Silver Nanoparticles (NPs) on Drosophila melanogaster", *Environ. Sci. Technol.* 45, 4974-4979 (2011). IF=5.26
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- 56. Z. Markova, K. Machalova Siskova, J. Filip, J. Cuda, M. Kolar, K. Safarova, I. Medrik, R. Zboril: "Air Stable Magnetic Bimetallic Fe-Ag Nanoparticles for Advanced Antimicrobial Treatment and Phosphorus Removal", *Environ. Sci. Technol.* 47, 5285-5293 (2013). IF=5.26

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# Most significant publications produced through collaboration within ATLAS-CERN and Pierre Auger Collaboration:

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PIERRE

- 1. ATLAS Collaboration: "A Particle Consistent with the Higgs Boson Observed with the ATLAS Detector at the Large Hadron Collider", Science 338, 1576-1582 (2012). IF=31.03
- 2. Pierre Auger Collaboration: "Large-Scale Distribution of Arrival Directions of cosmic Rays detected above 10(18) eV at The Pierre Auger Observatory", Astrophysical Journal Supplement Series 203, 34, (2012). IF=16.24
- 3. ATLAS Collaboration: "Measurement of the Inelastic Proton-Proton Cross-Section at Root s=7 TeV with the ATLAS detector", Nature Commun. 2, 463 (2011). IF=10.02
- 4. ATLAS Collaboration: "Search for the Higgs Boson in the H -> WW -> I nu jj Decay Channel in pp Collisions at root s=7 TeV with the ATLAS Detector", *Phys. Rev. Lett.* 107, 231801 (2011). IF=7.94
- 5. ATLAS Collaboration: " Search for a Standard Model Higgs Boson in the H -> ZZ -> I(+)I(-)v(v)over-bar Decay Channel with the ATLAS Detector", Phys. Rev. Lett. 107, 221802 (2011). IF=7.94
- 6. ATLAS Collaboration: "Search for a Heavy Particle Decaying into an Electron and a Muon with the ATLAS Detector in root s=7 TeV pp Collisions at the LHC. *Phys. Rev. Lett.* 106, 251801 (2011). IF=7.94
- 7. ATLAS Collaboration: "Search for Magnetic Monopoles in √s = 7 TeV pp Collisions with the ATLAS Detector", *Phys. Rev. Lett.* 109, 261803 (2012). IF=7.94
- 8. Pierre Auger Collaboration: "Measurement of the Proton-Air Cross Section at root s=57 TeV with the Pierre Auger Observatory", *Phys. Rev. Lett.* 109, 062002 (2012). IF=7.94
- 9. ATLAS Collaboration: "Search for Dark Matter Candidates and Large Extra Dimensions in Events with a Photon and Missing Transverse Momentum in pp Collision Data at root at root s=7 TeV with the ATLAS Detector", *Phys. Rev. Lett.* 110, 011802 (2013). IF=7.94
- 10. ATLAS Collaboration: "Search for New Phenomena in t(t)overbar Events with Large Missing Transverse Momentum in Proton-Proton Collisions at root s=7 TeV with the ATLAS Detector", *Phys. Rev. Lett.* 108, 041805 (2012). IF=7.94

## Patents

• The method of synthesis of the iron nanopowder with the protective oxidic coat from natural and synthetic nanopowdered iron oxides and oxyhydroxides.

Inventors: R. Zbořil, O. Schneeweiss, J. Filip, M. Mašláň: (EP2164656)

- Universal approach for immobilization of silver nanoparticles onto solid substrates using polyethylenimine with branch structure as adhesive layer and reducing agent.
- Inventors: R. Zbořil, J. Soukupová: (CZ2012000068)
- Use of copper complexes containing 2-phenyl-3-hydroxyquinolin-4(1H)-one and 1,10-phenanthroline derivatives for preparing medicaments intended for the treatment of tumor diseases.
   Inventors: Z. Trávníček, J. Vančo, R. Buchtík, Z. Dvořák: (CZ 304045).
- Complexes of gold with N6-benzyladenine derivatives and phosphine derivatives, method of their preparation and application of these complexes as drugs in anti-inflammatory therapy.
   Inventors: Z. Trávníček, J. Vančo, I. Popa, T. Šilha: (CZ 303649).
- Utilization of the dichlorido complexes of platinum with 7-azaindole halogeno-derivatives for the preparation of drugs for the treatment of tumour diseases.
  - Inventors: Z. Trávníček, P. Štarha, Z. Dvořák: (CZ 303560)
- Dichlorido complexes of platinum with 7-azaindole halogeno-derivatives and application of these complexes as drugs in antitumor therapy.
- Inventors: Z. Trávníček, P. Štarha, I. Popa: (CZ 303417).
- Complexes of copper with 2-phenyl-3-hydroxychinolin-4(1H)-one derivatives, method of their preparation and application of these complexes as drugs in antitumor therapy.
- Inventors: R. Buchtík, Z. Dvořák, Z. Trávníček, J. Vančo: (CZ 303009).
- Platinum oxalate-complexes with N6-benzyladenine derivatives, process of their preparation and use of such complexes as medicaments in antitumor therapy.

Inventors: P. Štarha, Z. Trávníček, I. Popa: (CZ 302623).

 Platinum cyclobutane-1,1-dicarboxylato complexes with N6-benzyladenine derivatives, synthesis and their use in anticancer therapy.

Inventors: Z. Dvořák, Z. Trávníček, I. Popa: (CZ 302618).

## Awards

The Award of the Minister of Education, Youth and Sport for Outstanding Results in Research, Experimental Development and Innovation was received in 2011 by Professor Radek Zbořil.

![](_page_41_Picture_2.jpeg)

Prof. Radek Zbořil won the Award of the Minister of Education, Youth and Sport for Outstanding Results in Research, Experimental Development and Innovation for 2011. He received the award from the Minister on November 10, 2011 in the Lesser Hall of Mirrors of the Ministry.

"I'm delighted to receive this award. I feel that you need, above all, courage to engage in costly, multidisciplinary research in nanotechnologies, which require the involvement of scientists from a wide variety of fields. I believe that I have been able to build such a team in Olomouc, and that I have succeeded in enthusing it for the study of objects whose behavior surprises us every day. I have been lucky not only with the people but, at a certain stage, also with the topics that I have chosen as the main ones in our research nanoiron, carbon nanostructures and nanosilver. It is these materials that today form the basis of research at the Regional Centre of Advanced Technologies and Materials and related results are reflected in dozens of publications, grants and contractbased collaborations every year. Therefore, I sincerely see the Award of the Minister as an appreciation of the ability to build a strong scientific team, give them a financial foundation and themes that can bring breakthrough results."

![](_page_41_Picture_5.jpeg)

The prestigious Galileo Galilei Award was awarded to Prof. Jan Peřina in recognition of his scientific work by the International Commission for Optics.

Prof. Jan Peřina was honoured with the prestigious Galileo Galilei Award of the International Commission for Optics (ICO). The ICO committee for the awarding of the Galileo Galilei Award recognized Jan Peřina with this award for the year 2011 for his 'impressive results in quantum optics and coherence regarding non-classical states achieved under difficult circumstances'. The committee considers it remarkable that he could produce such a considerable volume of work under difficult circumstances that the prevailed in Czechoslovakia during the period when he was at the height of his powers.

The 2012 SIEMENS Award for the best thesis was given to Karel Lemr (author) and Jan Soubusta (supervisor).

![](_page_41_Picture_9.jpeg)

The 2012 Siemens Award for best thesis was given to Karel Lemr (the author of the thesis) and Jan Soubusta (his supervisor). The winning thesis, entitled Experimental quantum processing of information with photon pairs, is a summary of research carried out and published over the previous four years. The common denominator between all experiments described in the thesis is the use of pairs of photons for the quantum processing of information. The Siemens Award is conferred every year in several categories, from basic research to applied research and the recognition of pedagogical activities.

![](_page_41_Picture_11.jpeg)

The award for the best presentation at the prestigious ISIAME 2012 (International Symposium on the Industrial Applications of the Mössbauer Effect) was won by Dr. Jiří Tuček.

![](_page_41_Picture_13.jpeg)

ISIAME is one of the biggest international gatherings of specialists in the field of Mössbauer spectroscopy. Dr. Tuček gave a presentation on issues surrounding the description and application potential of iron oxides from the point of view of Mössbauer spectroscopy. The results presented in the talk represented a summary of three years of research in the field.

The same award, for the best presentation, was won by Dr. František Karlický at ISTCP 2013 (Congress of the International Society of Theoretical Chemical Physics) in Budapest.

![](_page_41_Picture_16.jpeg)

At this conference, Dr. Karlický gave a presentation in front of several experts from all over hundred the world on issues surrounding noncovalent interactions between graphene and various molecules and atoms. "The presentation was based on results which had also been previously published in several prestigious international journals. Apart from graphene models, the presentation also contained information on interactions, experimental methods used for the measurement of atomic forces and absorption energies, as well as the comparison of theories with the results of experiments." Graphene is currently one of the most intensely studied materials in the world of science. The discovery of graphene was associated with the awarding of the Nobel Prize for Physics in 2010.

## CONCLUSION

"Scientific research is possible only around outstanding personalities, who must be supported by all possible means so as to create favourable conditions for research."

During its short existence, the institute, known mainly under the abbreviation RCPTM, has already earned a decent level of respect internationally, indeed the kind of respect that existing, established scientific institutions would not be ashamed of. Therefore it seems that a bright future awaits the Centre, which one cannot but enthusiastically wish upon it. Nevertheless, it must be realized that future success, or even lack of success, (and therefore also whether the RCPTM becomes part of the world elite or not) depends on several basic strategic decisions. Talking about the fact that future success depends on correct or incorrect decisions may, understandably, seem rather trivial. Nevertheless, it does have its own urgency in the globalized world of today, which leads to a great scientific and technological progress.

Nevertheless, one of the other sides of globalization is the incredible level of competition, which is a prerequisite for scientific and technological progress, but also immediately and ruthlessly punishes every wrong decision. Let us not forget what happened to the Finnish company that only a few years ago more or less monopolized the market in mobile phones. The fall of Nokia was the result of nothing less than an incorrect strategic decision concerning so-called smartphones. Many of us today will probably own an iPhone, made by the American company Apple, which took control of this market and is currently the largest company in the world. However, it is a question whether Apple will be able to maintain its position without the brilliant, visionary decisions taken by its founder, Steve Jobs.

This excursion into the world of globalization was essential in order to realize the importance of strategic decisions. Naturally, decisions affecting the RCPTM are fully in the hands of its management and above all the director. It is more than apparent from the achieved results that these decisions are taken with the forethought and competency. Despite this, I would like to make several recommendations for the new institute. These recommendations do not concern anything that RCPTM management would not do or even does not know about; rather they are a kind of support and recognition of the current path being taken.

If we realize that the greatest discoveries over the past 50 years in the Czech science were based primarily on the extraordinary quality of basic research (Wichterle's contact lenses and Holý's antiviral drugs), one cannot but hope that RCPTM does not succumb to current trends and does not devote itself solely to applied research, but also carries on the best traditions of the Czech science and maintains high-quality basic research. Without high-quality or even excellent basic research, it is also not possible to carry out successful applied research.

Successful scientific research is possible only around outstanding personalities, who must be supported by all possible means so as to create favourable conditions for research. Support should not be only financial and economical. A friendly and stimulating atmosphere should

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also be created, because in only such conditions fruitful thoughts and ideas, and the exchange and cultivation of these, can flourish. While healthy competitiveness and competition are beneficial to science, jealousy, envy, selfishness and thoughtlessness are damaging it.

Although the RCPTM was given excellent start-up conditions, it faces some difficult tasks. If it makes the right decisions (and so far everything indicates that it does), then the significance of this regional Centre can achieve European and global level.

Paul Hokace

Prague, September 28, 2013 Prof. Ing. Pavel Hobza, Dr.Sc., FRSC, dr.h.c.

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![](_page_45_Picture_1.jpeg)

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