CATRIN

Czech Advanced Technology and Research Institute

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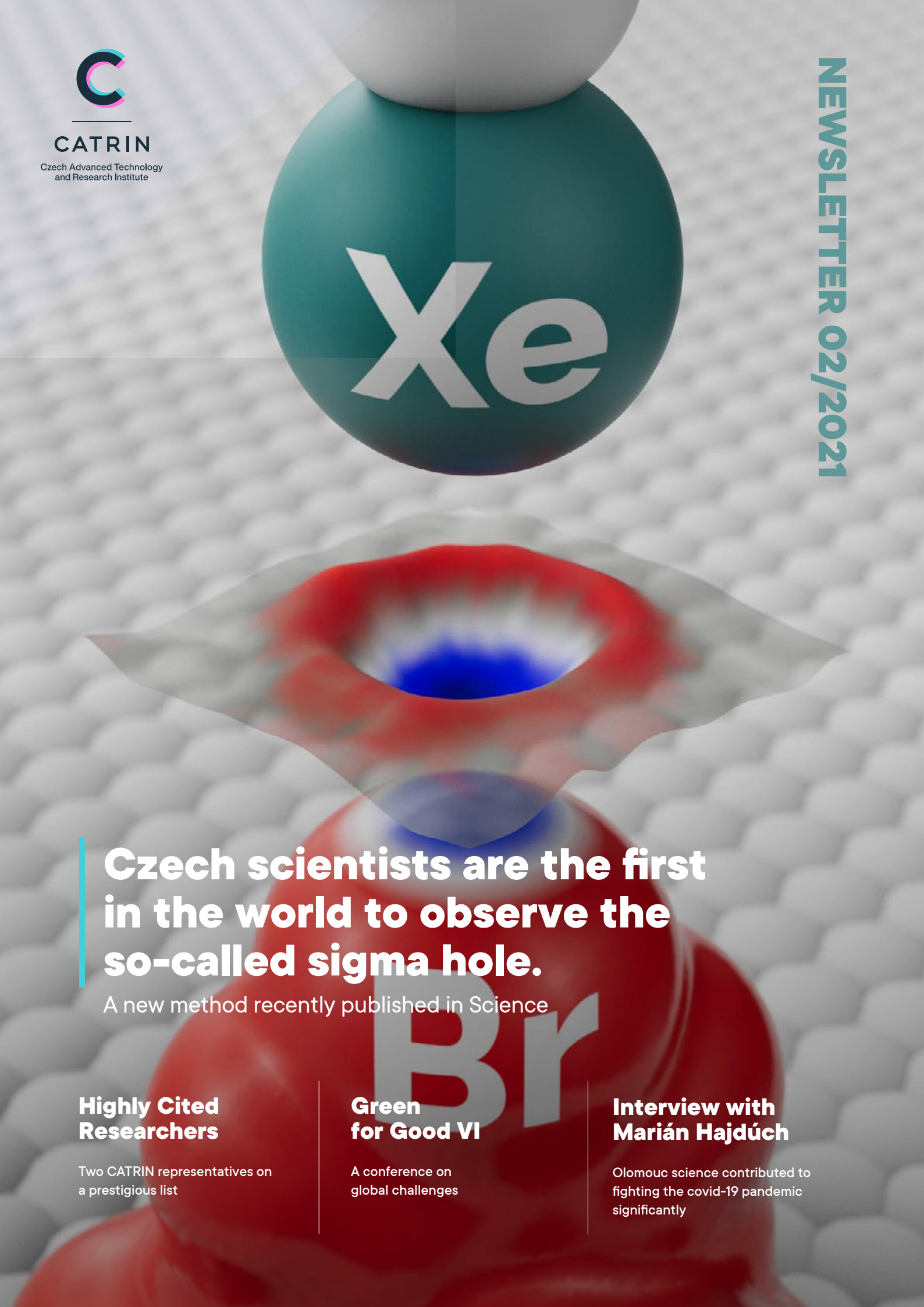


Czech scientists are the first in the world to observe the so-called sigma hole.

A new method recently published in Science

Highly Cited Researchers

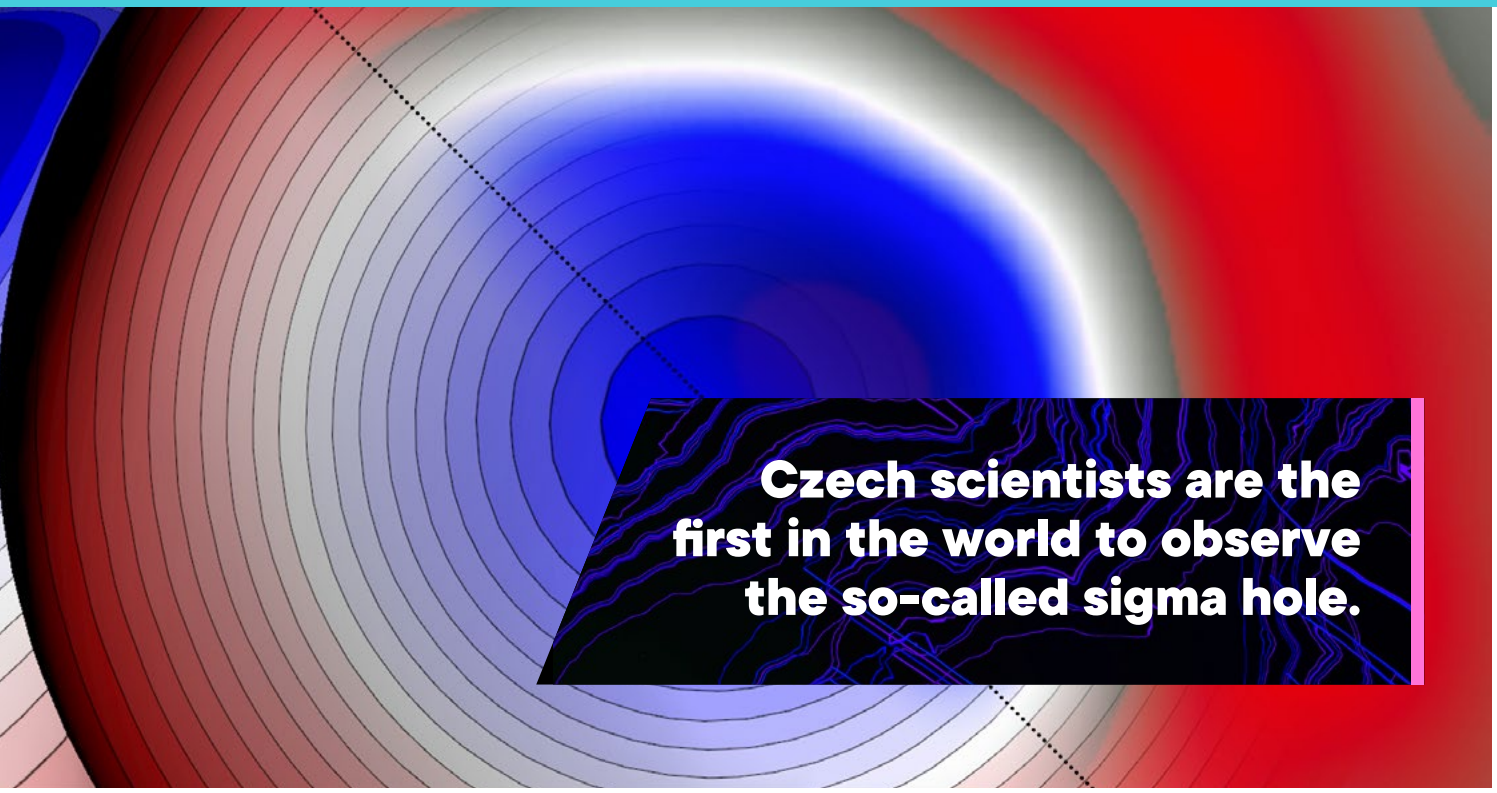
Two CATRIN representatives on a prestigious list

Green for Good VI

A conference on global challenges

Interview with Marián Hajdúch

Olomouc science contributed to fighting the covid-19 pandemic significantly



Czech scientists are the first in the world to observe the so-called sigma hole.

Until recently, subatomic structures were beyond the resolution of direct imaging methods, but a new method recently published by scientists in the journal Science represents a crucial breakthrough. They dramatically increased the resolution of raster microscopy from the atomic to subatomic phenomena.

They were the first in the world to observe the inhomogeneous distribution of electron charge around a halogen atom and confirmed the existence of a phenomenon called the sigma-hole. This was theoretically predicted 30 years ago, but no experimental proof was available. This discovery will make it easier to understand chemical reactions and interactions between individual atoms and molecules, opening avenues to amend the material and structural properties of diverse physical, biological, and chemical systems.

This was achieved as part of extensive interdisciplinary collaborative activities of scientists from the Czech Advanced Technology and Research Institute (CATRIN) of Palacký University Olomouc, the Institute of Physics of the Czech Academy of Sciences (FZU), the Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences (IOCB Prague), and the IT4Innovations Supercomputing Center at VSB – Technical University of Ostrava.

> When I saw the sigma-hole for the first time, I was certainly sceptical, because it implied that we had overcome the resolution limit of the microscopes down to the subatomic level.
>
> **Bruno de la Torre**

"Confirming the existence of the theoretically predicted sigma-holes can be compared to observation of black holes, whose existence was predicted in 1915 by the general theory of relativity but only seen two years ago. Viewed in that way, it's not much of an exaggeration to say that the imaging of the sigma-hole represents a similar milestone at the atomic level," explains Pavel Jelínek from FZU and CATRIN.

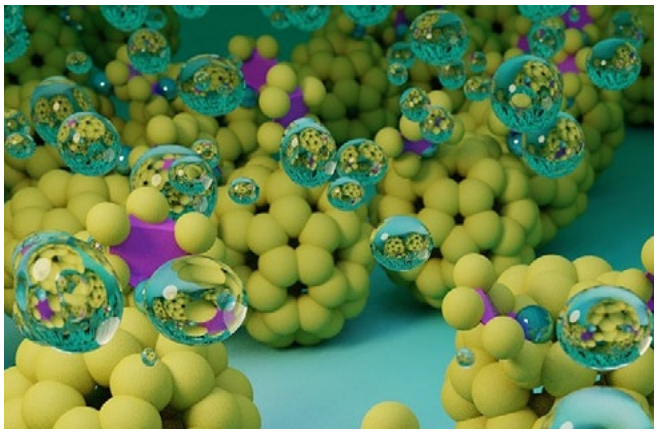
Previously, the existence of the sigma-hole phenomenon has only been indirectly demonstrated by X-ray structures of halogen-bound crystals. These revealed the surprising fact that chemically bonded halogen atoms of one molecule and nitrogen and oxygen atoms of another molecule, which should repel one another, can be in close proximity and therefore attract one another. This observation clearly conflicts with the assumption that these atoms carry a homogeneous negative charge and are repelled by electrostatic force. So scientists decided to investigate the subatomic structure of halogen by Kelvin probe force microscopy. First, they developed a theoretical description of the Kelvin probe's atomic resolution mechanism, which allowed them to optimize the experimental conditions for imaging a sigma-hole. Subsequent combination of experimental measurements and advanced quantum-chemical procedures led to the first experimental visualization of the uneven distribution of electron density, i.e. the sigma-hole, and definitive confirmation of the concept of halogen bonds.

"We improved the sensitivity of our Kelvin probe force microscopy by functionalizing the tip probe with a single xenon atom, which allowed us to visualize the inhomogeneous charge distribution in a bromine atom within a molecule of brominated tetraphenylmethane, that is, a sigma-hole in real space, and confirm the theoretical prediction," says Bruno de la Torre from CATRIN and FZU.

"It's a great satisfaction that we can now observe something that we could previously only 'see' in theory and that the experimental measurements precisely confirm our theoretical prediction of the existence and shape of the sigma-hole," says computational chemist Pavel Hobza from IOCB Prague, who performed the advanced quantum chemical calculations using the supercomputers at IT4Inovations in Ostrava.

Mallada B., Gallardo A., Lamanec M., de la Torre B., Špirko V., Hobza P., Jelínek P.:. Real-space imaging of anisotropic charge of -hole by means of Kelvin probe force microscopy. Science 2021, 374 (6569), 863-867. IF = 47,728

A special bond enhances fullerene's solubility



Scientists from CATRIN, IOCB and VSB-TUO have discovered more details about the reaction between the nanomaterial fullerene and piperidine, in which it dissolves. In two studies, published in prestigious journals, JACS and Angewandte Chemie, they scrutinized the reactions between secondary amines (piperidine) and fullerene containing 60 carbon atoms by both theoretical calculations and experimentally.

Fullerene was the first nanomaterial that opened the door to nanotechnology. It is one of the most widely studied materials due to its unique properties. Its wider application is still hindered by relatively low solubility, but one solvent that can be used successfully with fullerene is piperidine.

"Fullerene was known to be soluble in piperidine, but we never knew why. We have found, using theoretical calculations and experimental methods, that this is a very specific bond whose character is affected by the presence of oxygen," said Pavel Hobza (a theoretical chemist from IOCB and VSB-TUO). When the reaction occurs without oxygen, a complex with a N→C dative bond forms, while in the presence of oxygen the reaction continues to produce addition reaction products. The electronic structures of dative bond complexes and addition reaction products are fundamentally different.

These findings may contribute to further applications of fullerene. "As described in both articles, the results raise the possibility for controlled functionalization of one of the most well-known nanomaterials. Understanding the interaction of fullerene with organic molecules opens the door to the applicability of fullerene in energy storage facilities, for example," said another author, Radek Zbořil from CATRIN and VSB-TUO.

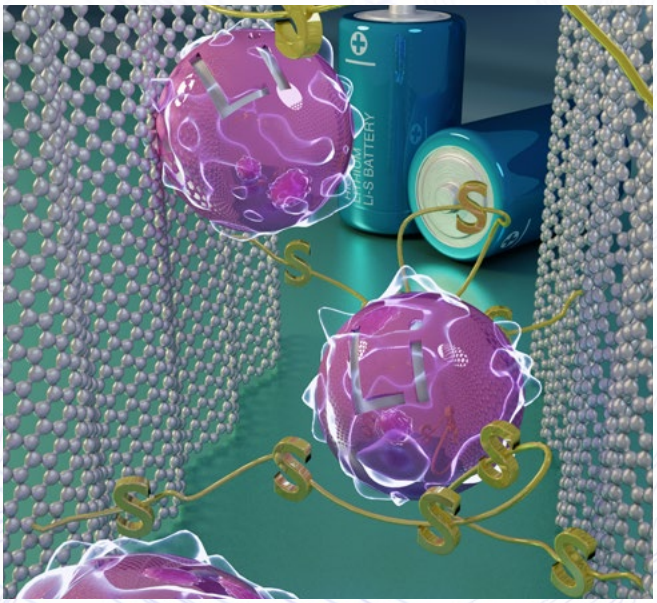
Lo R., Manna D., Lamanec M., Wang W., Bakandritsos A., Dračínský M., Zbořil R., Nachtigallová D., Hobza P.: Addition Reaction between Piperidine and C60 to Form 1,4-Disubstituted C60 Proceeds through van der Waals and Dative Bond Complexes: Theoretical and Experimental Study. Journal of the American Chemical Society 2021, 143 (29), 10930-10939. IF = 15,419

Lamanec M., Lo R., Nachtigallová D., Bakandritsos A., Mohammadi E., Dračínský M., Zbořil R., Hobza P., Wang W.: The Existence of a N→C Dative Bond in the C60–Piperidine Complex. Angewandte Chemie 2021, 60 (4), 1942-1950. IF = 15,336

New material provides a way to use sulphur in lithium batteries

Favourable price, high performance, stability and long life—these are the benefits of a new material designed for lithium battery cathodes developed by CATRIN scientists. The composite, which has great potential for practical applications, was formed by combining the properties of modified fluorographene and sodium polysulphides. The material has already been submitted to the European Patent Office.

Sulphur has great potential for storing energy in lithium batteries, and it is a cheap, environmentally friendly material. However, its practical use has been hampered by its low conductivity and release of sulphur during repeated charges/discharges, which reduces the batteries' capacities. "Therefore, we shifted our focus onto this bottleneck. We applied our extensive expertise in fluorographene chemistry it to prepare a completely new type of electrode with a covalently bonded sulphur compound," said one of the authors, Aristides Bakandritsos.
Using a simple method that could be very efficient in production of lithium-sulphur batteries, they removed some fluorine atoms from fluorographene then tightly bonded polysulfides to the vacant sites. In addition, the properties of polysulfides enable linkage of different layers of graphene. "We've formed strong covalent bonds between the carbon backbone of graphene and sulphur. This prevents the gradual release of sulphur during batteries' charging and discharging cycles," explained the first author of an article in Advanced Functional Materials, Iosif Tantis.



Tantis I., Bakandritsos A., Zaoralová D., Medveď M., Jakubec P., Havláková J., Zbořil R., Otyepka M.: Covalently Interlinked Graphene Sheets with Sulfur-Chains Enable Superior Lithium–Sulfur Battery Cathodes at Full-Mass Level. Advanced Functional Materials 2021, 31 (30), 2101326. IF = 18,808

Combining phenomics and metabolomics gives new possibilities in biostimulant research

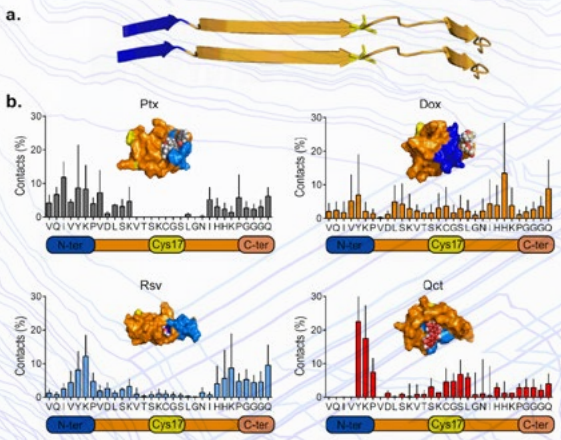
Biostimulants obtained by hydrolysis of plant waste material and their effect on the model plant Arabidopsis thaliana have been studied by researchers from CATRIN, Palacký University, PSI and several Italian universities. By combining automated large-scale plant phenotyping with non-targeted metabolomics, they not only described the functions of individual biostimulants but also revealed their mechanisms of action.

The researchers used a high-throughput screening approach based on simple RGB imaging combined with non-targeted metabolomics. They investigated the effect of biostimulants on Arabidopsis thaliana grown under optimal conditions as well as under salt stress. The traits related to growth and development were evaluated by experts during and at the end of the growth period. Of the 11 biostimulants, they identified two highly effective growth regulators that alleviated plant stress.

"This is a demonstration study where we have tried the procedures on a model plant. Subsequently, we intend to apply this approach to specific agricultural crops," explained Spíchal. According to him, this link is not yet very common in the world of biostimulants. It is mostly used by scientists from the Czech Republic and Italy. Both countries are pioneers in this field. The research is also a continuation of a long-term collaboration with Photon Systems Instruments within the CzPPN (Czech Plant Phenotyping Network). The use of plant biostimulants contributes to sustainable agriculture and their extraction by recycling waste products from industrial crop processing is in line with the concept of circular economy.

Sorrentino M., De Diego N., Ugena L., Spíchal L., Lucini L., Miras-Moreno B., Zhang L., Rouphael Y., Colla G., Panzarová K.: Seed Priming With Protein Hydrolysates Improves Arabidopsis Growth and Stress Tolerance to Abiotic Stresses. Frontiers in Plant Science 2021, 12:626301. IF=5,753

Anti-tumour drugs may have beneficial effects for Alzheimer's patients



The potential use of some commonly available and experimental anti-tumour drugs to fight Alzheimer's disease has been explored by CATRIN scientists alongside colleagues from IMTM and other labs at Palacký University, the Mario Negri Institute for Pharmacological Research in Italy, and IT4Innovations VSB-TUO, Ostrava. In a study published by The FEBS Journal, they showed that some anticancer agents can effectively block, at an early stage, formation of aggregates of so-called TAU proteins, which are present in brain tissues of patients with Alzheimer's disease.

Preventing formation of these protein clusters early on may be an effective approach to deal with Alzheimer's disease, according to scientists. The researchers focused on the part of the TAU protein sequence responsible for the agglomeration. They then tested the hypothesis (based on observations that the risk of Alzheimer's disease was reduced in some

oncology patients) that interaction with anti-tumour drugs may prevent TAU protein formation.

"We complemented our colleagues' experiments with computer simulations. We created protein models and studied their behaviour in the presence of experimentally active substances. TAU proteins can easily agglomerate but some anticancer drugs can prevent this aggregation. In examples of dimeric peptides we showed where the binding sites for anticancer drugs might be. These are found in the areas responsible for the agglomeration. Thus, binding drugs to these sites blocks further growth of the agglomerates. Anti-cancer drugs prevent the formation of TAU aggregates at an early stage and thus potentially protect against Alzheimer's disease," said Martin Šrejber from CATRIN, summarizing the results. Alzheimer's disease is a neurodegenerative disease. It is currently the most common cause of dementia in middle-aged and elderly people. As people gradually prolong their lives, it is becoming a major health and socio-economic problem.

Annadurai N., Malina L., Salmona M., Diomede L., Bastone A., Cagnotto A., Romeo M., Šrejber M., Berka K., Otyepka M., Hajdúch M., Das V.: Antitumour drugs targeting tau R3 VQIVYK and Cys322 prevent seeding of endogenous tau aggregates by exogenous seeds. The FEBS Journal 2021, in press, DOI: 10.1111/febs.16270. IF = 5,542

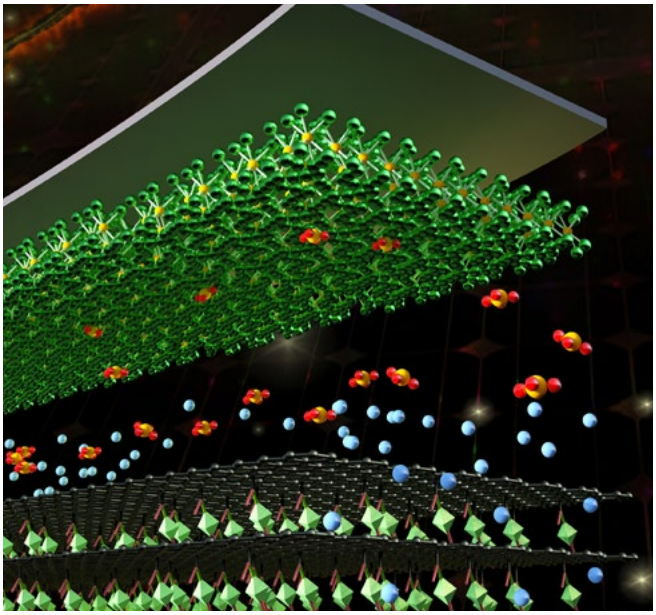
The chemical bonding of graphene and metallic organic networks has great potential for developing supercapacitors

Two unique classes of carbon materials are graphene derivatives and metal organic frameworks (MOFs). Linking their properties to develop new technologies has long been the focus of CATRIN scientific teams in collaboration with colleagues from the Technical University of Munich. Now they have prepared a material that exhibits excellent properties for use in so-called supercapacitors.

"For covalent bonding, we used a graphene acid, a graphene chemically modified by carboxyl groups, and a zircon-based metal organic framework with free amine groups. We applied this hybrid as an anode in a new type of supercapacitor, and used another low-dimensional titanium carbide-based material from the so-called MXene class as a cathode. Such an asymmetrical supercapacitor enables energy densities over 70 Wh/kg, approaching or even surpassing the characteristics of commercially available systems," said one of the corresponding authors, Radek Zbořil.

Advantages of supercapacitors, in addition to high energy densities, include very fast charging/discharging rates and long lifetimes. "It's very encouraging that we're only seeing about a 10% loss rate after 10,000 charging cycles. The designed electrochemical system works similarly to batteries, but allows faster charging. It expands the possibilities for electricity storage," concluded another of the authors, Michal Otyepka, who is dedicated to developing new graphene derivatives and their supercapacitor applications under two ERC grants.

Scientists have also demonstrated hybrid systems' potential by developing new types of superhydrophobic and superoleophilic sorbents that allow removal of oil fractions and organic solvents from polluted waters (e.g., Jayaramulu et al. Adv. Mater. 31, 1900820, 2019), gas sensors (e.g., Jayaramulu et al. J. Mater. Chem. A, 32 (9), 17434-17441, 2021) and lithium batteries (e.g., Jayaramulu et al. Adv. Funct. Mater. 29, 1902539, 2019).



Jayaramulu K., Horn M., Schneemann A., Saini H., Bakandritsos A., Ranc V., Petr M., Stavila V., Narayana C., Scheibe B., Kment Š., Otyepka M., Motta N., Dubal D., Zbořil R., Fischer R. A.: Covalent GrapheneMOF Hybrids for HighPerformance Asymmetric Supercapacitors. Advanced Materials 2021, 33 (4), 2004560. IF = 30.849

Our Recent Reviews

B. Singh, M. B. Gawande, A. D. Kute, R. S. Varma, P. Fornasiero, P. McNeice, R. V. Jagdeesh, M. Beller and R. Zbořil

„Single-Atom (Iron-Based) Catalysts: Synthesis and Applications",

Chemical Reviews 2021, 121 (21), 13620-13697. IF = 60,622

R. K. Sharma, S. Yadav, S. Dutta, H. B. Kale, I. R. Warkad, R. Zbořil, R. S. Varma and M. B. Gawande

„Silver nanomaterials: synthesis and (electro/photo) catalytic applications",

Chemical Society Reviews 2021, 50 (20), 11293-11380. IF = 54,564

Marián Hajdúch is an expert in drug research and molecular oncology, but with the onset of the covid-19 pandemic he is visibly linked to the fight against the disease. The Institute of Molecular and Translational Medicine (IMTM), which he leads, straddles the UP Faculty of Medicine and Dentistry (LF UP) and CATRIN.

Olomouc science has strongly contributed to coping with the covid-19 pandemic

How did you transition from molecular oncology to fighting the covid-19 pandemic?

A number of cancer diseases are of infectious origin, and in the past I have done extensive research on the genetics of infectious diseases. It's one of the areas in which I have contributed numerous scientific papers. We were motivated to test for covid-19 by students who wanted to contribute to dealing with the pandemic. We then very quickly created a large automatic testing platform, probably the largest in the Czech Republic at the time. Thanks to this, and my previous scientific activity, I was placed in charge of the laboratory group for coordinating covid-19 disease tests. I resigned from this post at the end of last year for various reasons, but we have remained very active in this area, both diagnostically and in research. I continue to participate in various advisory bodies to combat the disease.

In the context of covid-19, we observed a great upsurge in scientific activity, leading to extraordinary collaboration across scientific institutions. Scientists now have a lot of media coverage. Has science and the scientific community lived up to expectations regarding the fight against the new type of coronavirus?

In medical terms, it certainly has. Science has provided the tools to manage this pandemic—diagnostic, preventive, and curative. A great deal of work has been done in that direction. However, the pandemic has taken on a more social dimension, and in that respect, perhaps we scientists have not always done the best work. Unfortunately, some doctors and researchers have been involved in spreading disinformation that does not contribute to handling the pandemic effectively and polarizes society very significantly.

How do you assess the contribution of Olomouc scientists?

Olomouc science has contributed very significantly both within the Czech Republic and internationally. First, at a very early stage, we were instrumental in developing new diagnostic procedures. As part of the cooperation between the IMTM and RCPTM we created magnetic balls to isolate RNA, which are still used in diagnostic kits. Further, we designed self-sampling kits and created a large diagnostic centre for covid-19 testing in cooperation with the University Hospital in Olomouc. We programmed several IT solutions that became part of the Smart Quarantine system. We have provided more than 2.5 million test results with these solutions. Individuals are using self-reporting tools in our systems, alongside other parts of Smart Quarantine. We provided all of this through the hospital, the scientific institutes, CATRIN, in particular the IMTM and RCPTM, as well as through major research infrastructures including EATRIS. As a result, we have been involved in a wide range of international research projects.

At a recent conference in Olomouc, you described covid-19 as a disease full of surprises. What surprised you most?

In fact, in the context of SARS-CoV-2, in a relatively short time, we are witnessing the course of evolution—the evolution of natural selection, as described by Darwin. We see how the SARS-CoV-2 virus, which, although it does not have the ability to mutate quickly (and unlike other viruses, even has some repair mechanisms built into it) does mutate and mutants are rapidly selected. Since more and more people around the world are being infected, we are creating a huge opportunity for the virus to evolve. It can adapt very quickly to the situation and bypass the immune system. That is what surprises me most.

You are extensively researching Covid-19, are you planning further research in that direction?

We are continuing with a study on the prevalence of the disease in the population, which will be complemented by consideration of a number of other factors. We'll start next year, after this wave of the epidemic, when we'll find out to what extent the population has been affected. The study will be open to two and a half to three thousand candidates, primarily those who participated in the Preval I study. We will test both antibody and cellular immunity parameters and detect the presence of virus on the mucous membranes of these individuals. The goal is to get information about how vaccinated people or people with post-infectious immunity can resist SARS-CoV-2 infection.

Besides covid-19, what are you working on at the institute now?

We are implementing a number of drug development and diagnostic projects, particularly in the areas of cancer and infectious diseases. We are developing a project to screen lung cancer through exhaled-air biomarkers. We have completed a project dedicated to new methods for estimating the ageing process. We published a paper describing the senolytic effect of one substance and we are working on others. We want to bring two candidate anti-cancer drugs into clinical testing. One of them is a nanoparticle formulation that we developed in collaboration with Professor Zbořil's group and tested in both CATRIN and LF UP. It is one of several promising substances that has provided such good results in preclinical tests that we believe is worth continuing with a clinical trial.

How much has the pandemic affected your teams' research work?

Very significantly. At least at the beginning of the pandemic, research capacities at our institute were significantly concentrated on providing diagnostic processes for the covid-19 disease. But the big problem with research in general is that material deliveries have been dramatically delayed. There are still shortages of some plastics and chemicals. There are bottlenecks in transport between countries, with delivery times being incredibly extended. This negatively impacts the day-to-day work of both researchers and administrative staff.

doc. MUDr. Marián Hajdúch, Ph.D.
(*1969)

He graduated from LF UP Olomouc. Earlier in his studies he focused on science and research, first in the fields of immunology and then oncology. His activities in molecular and translational medicine resulted in establishment of the Institute of Molecular and Translational Medicine of Palacký University, which he now leads. He is vice chair of the Cancer Research Foundation CR and a member of the management committee of Early Cancer Detection Europe.

He has been involved in running the European Research Infrastructure for Translational Medicine (EATRIS-ERIC) for eight years and is still its national director. In 2020, he managed the covid-19 Laboratory Group at the Ministry of Health—he was one of the authors of the National Testing Strategy. He has published a number of papers, mainly in the fields of clinical, experimental, and molecular oncology as well as on research and development of anticancer drugs and diagnostics. He is an author of more than 40 patents of pharmaceuticals and diagnostics.

Nuria De Diego
In CATRIN we can carry out complex studies with valuable results

Nuria De Diego originally came to Olomouc on a short internship that turned into an almost 9-year career at Palacký University. She has fallen in love with the city and found new challenges within her research interests. As an important member of the Phenotyping group, she is devoted mainly to studying plants' stress responses.

"I think that the response of plants to different types of stress, such as drought, weather fluctuations and so on, is a very important topic that needs to be addressed with regard to ongoing climate change. Understanding of it will allow us to find important markers for identifying new genotypes of interest," the scientist explained.

She completed a Master's degree in Biotechnology at the Public University of Pamplona and her doctoral thesis focused on pine trees' physiological responses to drought at the University of the Basque Country. She combined her doctoral studies with work as a technician, working on in vitro cultures of pine trees. "I thought that I could improve my knowledge of plant metabolism here in Olomouc, which fits very well with my physiological training. However, I gradually became more interested in plant stress responses, so I started working on this topic with the phenotyping group," she revealed. The opportunities for systematic interdisciplinary collaboration were the main reason she joined CATRIN. Here she also benefits from the rich international contacts and interdisciplinary collaborations within the research centre.

"We can conduct very complex studies with valuable results. I consider my greatest achievement so far is to have become a respected scientist in the plant phenotyping community. In addition, the review article in which we described plant stress responses in a very comprehensive way two years ago has had a great impact in the scientific community with more than 100 citations. This makes me very happy," she added.

Martin Mistrík
Breakthrough discoveries emerge at frontiers of disciplines

The path to science is not always straightforward, as illustrated by Martin Mistrík, who initially made his living in marketing and as a woodworker. Following a later lab visit during ecological studies at PřF UP he switched direction and obtained a PhD in biochemistry. He now works at the Laboratory of Genome Integrity, focusing on cancer.

"We're investigating tumour growth, the mechanisms of tumour cell transformation, and their causes. At the molecular level, we study different kinds of DNA damage—how they occur and how the cells cope with them. One of the newest topics is protein stress at the cellular level. We study the factors that cause or amplify it, as well as cells' ability to discard the damaged proteins or reduce their effect," he said.
In some cases results of fundamental research can have important medical applications. For example, using a fundamental approach he and his colleagues found that use of cannabinoid substances may reduce the efficacy of some chemotherapy. Another study revealed anti-cancer effects of the drug disulfiram, which is used to treat alcohol addiction. He also participated in development of a ground-breaking method to investigate cell stress, combining targeted protein damage in individual cells using silver nanoparticles and a laser beam with parallel microscopic analysis. This can help efforts to investigate and prevent degenerative diseases.
"It feels good to know that your work has a positive effect on human health. But I don't do science with the desire to save the world. A lot of scientific activities don't have such an impact, but that doesn't necessarily make them less important," said the scientist. He considers multidisciplinarity to be very important. "This can be offered by joint institutes such as CATRIN, where there are interesting opportunities to link together the research of individual groups. Breakthrough discoveries tend to arise at the frontiers of the disciplines."

Veronika Šedajová
It's important to be able to explain our work to the public and children

As a scientist in CATRIN's Magnetic Nanostructures group, Veronika Šedajová is mainly involved in the preparation of new materials (graphene derivatives) and their subsequent use in energy storage, especially in supercapacitors.

She has also completed a five-month research internship at the laboratory of the world's leading expert in materials chemistry, Yury Gogotsi, at Drexel University in Philadelphia, where she has acquired very valuable knowledge as well as practical experience in synthesizing and applying MXenes. These are 2D materials with myriads of applications, for example, in various kinds of sensors, energy storage technologies, water purification, optoelectronics, and medicine.

"I learnt how to synthesize MXenes, their further processing, the preparation of flexible electrodes and consequently composites with our graphene derivatives from Olomouc. I also tried new ways of testing supercapacitors. I tremendously benefitted from the opportunity to work in another research group and gain experience in a different workplace. I'm truly grateful for the time my colleagues in the US invested in my training, and I must also thank my supervisors, who gave me this chance. The equipment at CATRIN was also helpful, as it enabled me to assess various techniques and I had experience of different measurements.

Alongside the research activities in the experimental part of her doctoral studies, preparation of publications, and collaboration with other colleagues, she welcomes opportunities to bring CATRIN's research closer to the public, e.g., through events such as the Night of Scientists, Science Camp, and Children's University. "There is a lot of work, and of diverse nature, which makes me happy—especially the popularization events that I regularly get involved in. I think it's very important to be able to explain to children or the general public what we do."

CATRIN and Bar Ilan Institute have a cooperation agreement

CATRIN and the Bar-Ilan Institute of Nanotechnology & Advanced Materials (BINA) have agreed to a mutual scientific cooperation in a memorandum signed in Israel in October. The aims are to strengthen links between the two institutions, facilitate exchange of scientific and technical knowledge, and strengthen scientific and technological developments in materials science and nanotechnology.

"The Bar-Ilan Institute is a leading nanotechnology research institute in Israel and a world leader in many fields. This mutual cooperation, which has already produced a tangible result in the preparation of a joint project, is highly appreciated and I am pleased that we have formally confirmed it with a memorandum," said CATRIN Director Pavel Banáš. The memorandum covers five years, which may be subsequently extended.

In further comments, he said that BINA connects scientists with interests in technical sciences, life sciences, physics, chemistry, and computer science. The institute's laboratories are among the most modern in the world and offer the highest standards of scientific performance. Its instrumentation includes equipment for microscopy of charged particles, surface analysis, and nanotechnological manufacture.

Green for Good VI will focus on global challenges

The sixth conference in the Green for Good series, this time with the subtitle Global Challenges, will take place from 12 to 15 September 2022 in Olomouc. CATRIN, in cooperation with the European Federation of Biotechnology (EFB) and Institute of Experimental Botany of the Czech Academy of Sciences, is involved in its preparation. The organisers are already promising new features in the programme.

As always, the central theme of the conference will be plant biotechnology, genome editing of economically important crops, etc. "New topics will include the bioeconomy and circular economy, the European Commission's Green Deal, energy capture and storage in biological systems, and a section on women in agriculture. The programme's structure corresponds to the global shift towards more sustainable agriculture and cannot ignore the fight against climate change. The aim is to invite experts in these fields to share their latest scientific results and discuss possible solutions to global challenges in the pursuit of a more sustainable future," said Karolina Zavoralová, a member of the organising team.

Green for Good VI was originally scheduled to take place this year, but it was postponed due to the covid-19 pandemic. More information will be available at https://www.efbiotechnology.org/g4g.

Two CATRIN scientists among Highly Cited Researchers

The chemists Radek Zbořil and Rajender Varma are on the Highly Cited Researchers 2021 list, and they have both repeatedly been members of this elite group The list comprises about 6600 scientists from 70 countries, including 24 Nobel laureates.

Clarivate Analytics annually rewards personalities who are pioneers in their fields. Their research during the past decade has resulted, among other things, in high-profile publications ranking in the top one percent of the most cited papers on the Web of Science in their respective fields in a year.

"I am very pleased to be included for the fifth time in this elite list, which includes 240 chemists from all over the world. I really appreciate such an entirely independent evaluation of my research, with nearly 52,000 citations over the last decade," said Varma, who works at the Environmental Protection Agency in the US and is a member of the Environmental Nanotechnologies group at CATRIN.

For four consecutive years, the Highly Cited Researchers list has included Radek Zbořil, a nanomaterials research expert who focuses mainly on the use of nanomaterials in medicine, chemistry, and environmental cleaning technologies. This year, he's listed in the Chemistry category. He and Varma are the only two representatives in it with domestic affiliations.

"It's not easy at all to secure one's position in this growing competition. The key to success is the right choice of topics and the ability to identify key challenges in the area, and, of course, a great team of scientists who can turn ideas into findings and sell them in the world's best journals. I have people like these around me. My thanks and a part of this award go to every one of my colleagues in Olomouc and Ostrava," said Radek Zbořil in comments on his success. Prof. Zbořil is Scientific Director of CATRIN-RCPTM and active in the Centre for Energy and Environmental Technologies of VSB-TUO..

There are also 10 scientists in this elite group who are affiliated with domestic institutions or universities. The list is available at https://recognition.webofscience.com/awards/highly-cited/2021/.

Pavel Hobza's Jubilee Celebration

One of the most highly cited Czech scientists, computational chemist Pavel Hobza, who is based at Charles University, CATRIN, and the Institute of Organic Chemistry and Biochemistry of CAS (IOCB), is celebrating his birthday today. To mark this occasion, the nation's oldest university awarded him a Gold Medal of Remembrance.

"When I met Professor Hobza, I was a junior researcher at the Department of Physical Chemistry of Palacký University (UP) and later on I became his colleague there. He brought to the university the spirit of world-class science combined with grace and dignity. Over the past 15 years he has shaped students' perspectives through a Contemporary Chemistry lecture series, to which he would invite especially prominent scientists. I believe that Palacký University owes him a lot for its development in the field of physical and theoretical chemistry. Today, Professor Hobza is an invaluable asset, and I feel privileged that he became CATRIN's first employee in September 2020," said CATRIN Director Pavel Banáš.

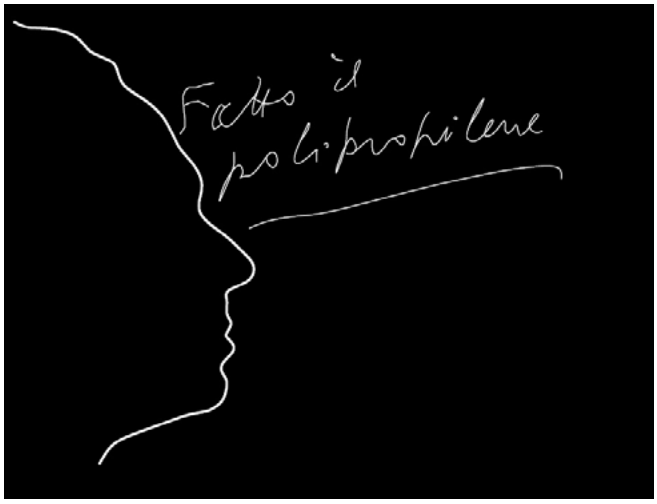
Pavel Hobza is famous for, among other things, discovery of the improper hydrogen bond. Other major scientific feats include elucidation of the role of stacking interactions in DNA and proteins, and explanation of the role of dispersion energy in biomacromolecules. This year, he participated in a breakthrough discovery—confirmation of the existence of a so-called sigma-hole. He is also a winner of the most important Czech science award, Česká Hlava.

Patrik Schmuki received the prestigious Natta Award 2020

World-renowned electrochemistry expert Patrik Schmuki from Friedrich–Alexander University Erlangen–Nürnberg, Germany, who also leads the Photoelectrochemistry group at CATRIN, received the Natta Award 2020. This prize is annually awarded by the Department of Chemistry, Materials and Chemical Engineering "Giulio Natta" of the Polytechnic University of Milan for remarkable accomplishments in areas of the department's scientific interests.

The award ceremony took place on 12 November 2021. During the ceremony, Professor Schmuki gave a lecture on self-organizing electrochemistry entitled Formation and Features of Aligned Oxide Nanotubes.

This prize is named after the Italian chemist Giulio Natta, who, alongside



Karl Ziegler, was awarded the Nobel Prize for discoveries in chemistry and polymer technology. Previous recipients of the Natta Award include Sir J. Fraser Stoddart, the Scottish chemist who, together with colleagues, won the 2016 Nobel Prize for research into molecular machines, Elazer R. Edelman (MIT), and Arvind Varma (Purdue University).

Michal Langer succeeded in the Jean-Marie Lehn competition

The Jean-Marie Lehn Prize competition (organized by the French Embassy and Solvay, a company with activities in diverse scientific sectors) awards the best PhD research by young Czech and Slovak chemists. This year Michal Langer of CATRIN was awarded third place for his research on possibilities of modelling nanoparticles using computational chemistry and work on carbon dots. Michal Otyepka was also recognized in the award, as his supervisor.

"I consider this award a huge success. After all, this is a national competition that all PhD students engaged in research in the field of chemistry from universities and institutions affiliated with the Academy of Sciences of the Czech Republic could enter. I am grateful to my mentor for including me in his excellent team, for the opportunity to work on projects devoted to world-class science and his efforts to push me scientifically further. This experience motivates me to continue working on my professional growth," said Michal Langer. It was also a great experience for him to meet Jean-Marie Lehn, the 1987 Nobel Prize winner in Chemistry, who hosted the award ceremony on 30 September.

Cleaning tablets earn CATRIN scientists first prize on Transfera Technology Day 2021

Scientists from CATRIN were awarded first prize in the national Transfera Technology Day competition for their development of effervescent cleaning tablets, which was judged the best of 13 shortlisted projects by groups from domestic universities and research institutes.

"I believe this success can help us find an investor to finalize the product and bring it to market. Even during the competition we were invited to collaborate with other universities," said one of the product's developers: Jan Filip from CATRIN. It has now been protected by a European patent that came into force in April 2021.

This product, which is based on highly reactive iron nanoparticles, is mainly intended for use in clean-up after environmental accidents. It can remove hexavalent chromium, arsenic, herbicides, pesticides and other pollutants from aqueous environments very quickly and efficiently.

Tomas Malina wins postdoc position at Karolinska Institute

The prestigious Karolinska Institute in Sweden will host Tomas Malina from CATRIN, who competed against another 30 candidates. As a postdoc in Professor Fadeel's team, one of the world's top nanotoxicity groups, he will be involved in starting a new scientific project from February 2022.

"I'm going to deal with the interactions of nanomaterials with immune system cells, which is a fascinating topic, from my point of view. I spent my entire doctoral studies investigating 2D nanomaterials, but I will now study them from a slightly different perspective. I believe it will be a great opportunity to learn new things," said Malina, who works at CATRIN in the Nanomaterials in Biomedicine group and recently received his PhD degree for work supervised by Radek Zbořil.

He looks forward in particular to working with the renowned scientist Bengt Fadeel, Head of the Molecular Toxicology Unit at the Institute of Environmental Medicine. Like Peter Wick from the Swiss science centre EMPA, where this young scientist had an internship last year, Fadeel is an active member of the European cluster for nano-safety and nanotoxicity. "After my stay, I would certainly like to go back to CATRIN and help to integrate our science centre into this international cluster. Its members are top scientists in the field," said Malina.

CATRIN steps onto the science stage

CATRIN symbolically embarked on a journey to join Europe's research elite at an opening ceremony at Palacký University's Rector Office, including cutting a ribbon, on October 1, 2021. Attendees included the university's leadership, representatives of the government and domestic universities, and other important guests.

CATRIN's research aims are to contribute to efforts to address global societal challenges. "Our priority is to focus on new options for harvesting and storing 'green' energy and to participate in the development of sustainable agriculture, environmental protection, and the prevention and treatment of diseases of civilization. In addition to conducting cutting-edge fundamental research, we pay attention to transferring the results of the research into practice," said Pavel Banáš, CATRIN Director.

CATRIN is a result of Palacký University's efforts to integrate research capacities and build a strong institute at both European and global scales, which has been long supported by the Ministry of Education, Youth and Sports of the Czech Republic. CATRIN currently has over 220 employees, about a third of whom are foreigners. Among them are several researchers who regularly appear in the list of the world's most highly cited scientists annually announced by the American company Clarivate Analytics. The team, led by Michal Otyepka, is heavily engaged in research funded by two prestigious European Research Council (ERC) grants on low-dimensional carbon nanomaterials and their applications. CATRIN scientists are also deeply involved in management of the European Federation of Biotechnology and development of new technologies to combat COVID-19. The CATRIN team also includes Marián Hajdúch, the former national coordinator of COVID-19 testing. The Institute collaborates closely with a number of leading international institutes, in countries including Italy, Spain, Switzerland, Germany, the US, and Japan.

CATRIN began operating on 1 October last year, when the statute legally establishing it came into force. The opening ceremony was delayed due to the covid-19 pandemic.

Scientists from IT4Innovations and CATRIN join forces

Presenting research activities and discussing the possibilities for cooperation were the main goals of a workshop jointly organized by the IT4Innovations National Supercomputing Centre at VSB – Technical University of Ostrava and Czech Advanced Technology and Research Institute (CATRIN) of Palacký University. About 30 scientists attended the event (in Ostrava on November 4), particularly seeking synergies in areas of high-performance computing (HPC) and artificial intelligence.

Representatives of both research centres presented 12 research topics that could be usefully addressed using supercomputers, machine learning and/or artificial intelligence methods. "If we manage to combine our expertise and know-how in the fields of the development of new nanomaterials, methods for their rational design, or computer simulations of biomolecules with the experience of colleagues at IT4I in the fields of artificial intelligence and HPC, we can push the boundaries of knowledge even faster and more efficiently in the future. Together, we want to target important topics such as new functional nanomaterials, efficient energy storage, or the design of systems for targeted drug delivery inside cells," said CATRIN Director Pavel Banáš.

The need for cooperation has been also highlighted by the IT4Innovations Scientific Director Tomáš Kozubek. "Significant advances in science cannot be made in isolation from the rest of the world. Current scientific projects are bringing together dozens and sometimes hundreds of scientists, often from different parts of the world, but mostly from different scientific disciplines. Today's science is all about teamwork—collaborations among scientific workplaces always bear fruit," he said. The workshop in Ostrava will be followed by another mutual meeting.

The British Ambassador discussed possibilities of cooperation at CATRIN

In a recent visit the British Ambassador to the Czech Republic, Nicholas Archer, primarily discussed the possibilities of cooperation between Olomouc and British researchers with the CATRIN management. During his visit to the science centre, he also saw the laboratories and learnt about the main directions of the research here.

"I heard about the cutting-edge research of Palacký University and CATRIN. I came to see this highly reputed research centre for myself, and I was looking forward to seeing the exceptional technologies in advanced materials and agricultural research. The main aim of the visit is to encourage further scientific collaboration between British researchers and scientists from Palacký University," said the British Ambassador.

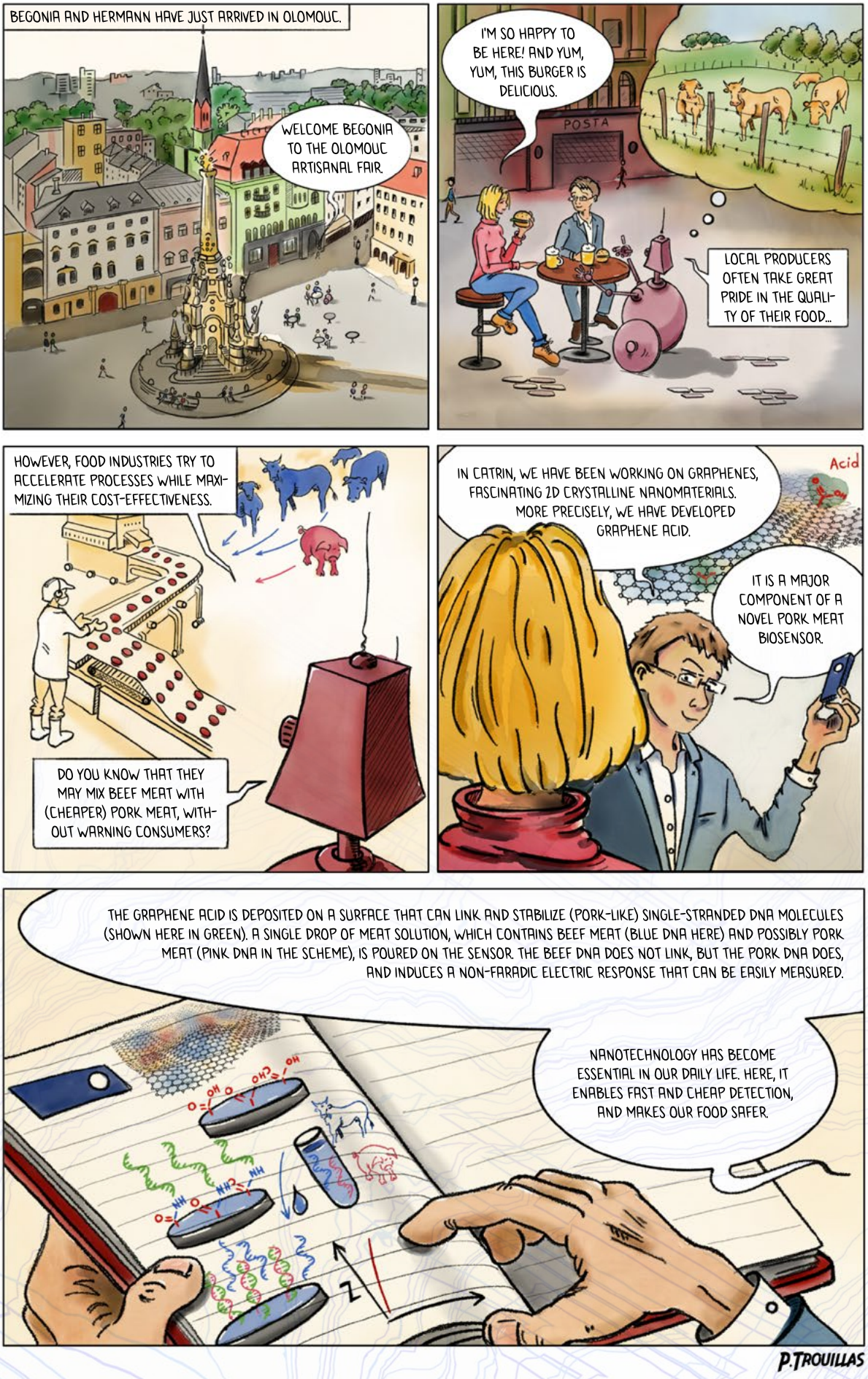
The Director of CATRIN, Pavel Banáš, and other members of the University's management presented the research directions and some results of basic and applied research to this distinguished guest. An important part of the negotiations was discussion of the possibilities of working with partners from Great Britain. "In this country, we are working rather inconsistently with individual colleagues. The ambassador and I have discussed the possibilities of systemic and long-term cooperation with, for example, one of the universities. Among other things, he was interested in how they could help establish or deepen such cooperation," said Banáš.

First Researchers' Night at CATRIN exceeded expectations

Sparking great interest from visitors, CATRIN joined Researchers' Night for the first time on Friday September 24. The rich programme attracted about 500 visitors to the Holice campus, with a five-metre glowing model of the Earth borrowed from the Academia film Olomouc festival being a notable highlight.

A large proportion of visitors, both kids and adults, seized the opportunity to take a look at the centre's laboratories as part of guided tours. Young researchers, in particular, prepared a series of fun experiments and games for visitors. Visitors could learn, for example, how the world's fastest train works and about liquids' viscosity. They also saw a levitating magnet or learned to distinguish between fluorescence and phosphorescence through graphic demonstrations.

The adventure of Hermann and Begonia: Beef or not Beef



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