2022

hpc focus

EURO
SLOVAKIA

Editorial

Dear HPC users and HPC fans,

It was a busy year for us at the **National Competence Center for HPC** and the **National Supercomputing Center**. I hope we have come closer to building an active HPC community in Slovakia – a complex, vital, and sustainable ecosystem.

The first and long-awaited step was the infrastructure renewal, and we were successful even though complications occurred. The new HPC system Devana will be available in autumn 2022. In December 2022, we plan to launch the first call for applications for specific projects.

The HPC was not forgotten in the Slovak Recovery and Resilience Plan either, investment of approximately 70 million is in the plan. Those are good news for Slovak science, research, and innovation. I am convinced that we can fully utilize the investment potential only if we create a nationwide HPC ecosystem and actively support all of its parts. It will require the cooperation and coordination of many partners at different levels, and it will certainly not be easy – but it is high time for Slovakia to star.
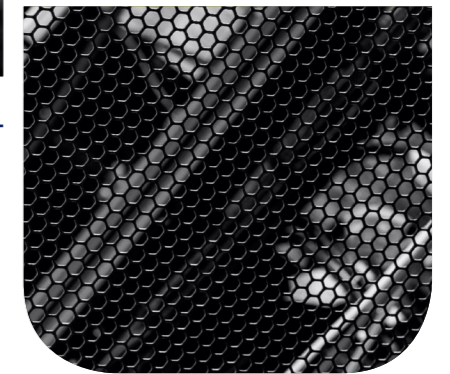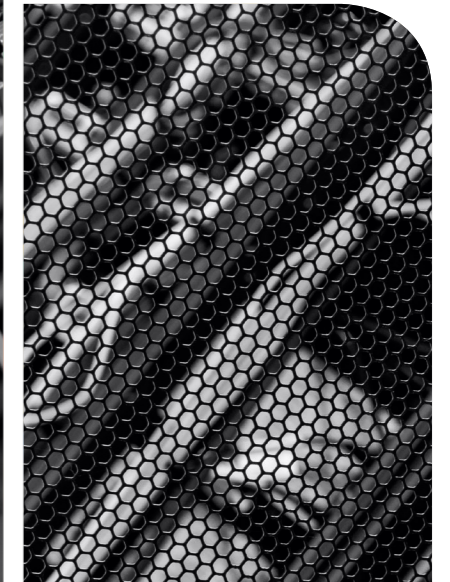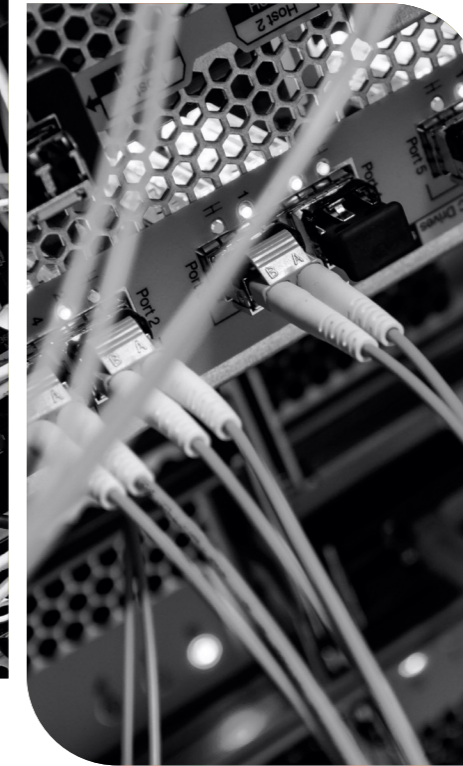
hpc focus
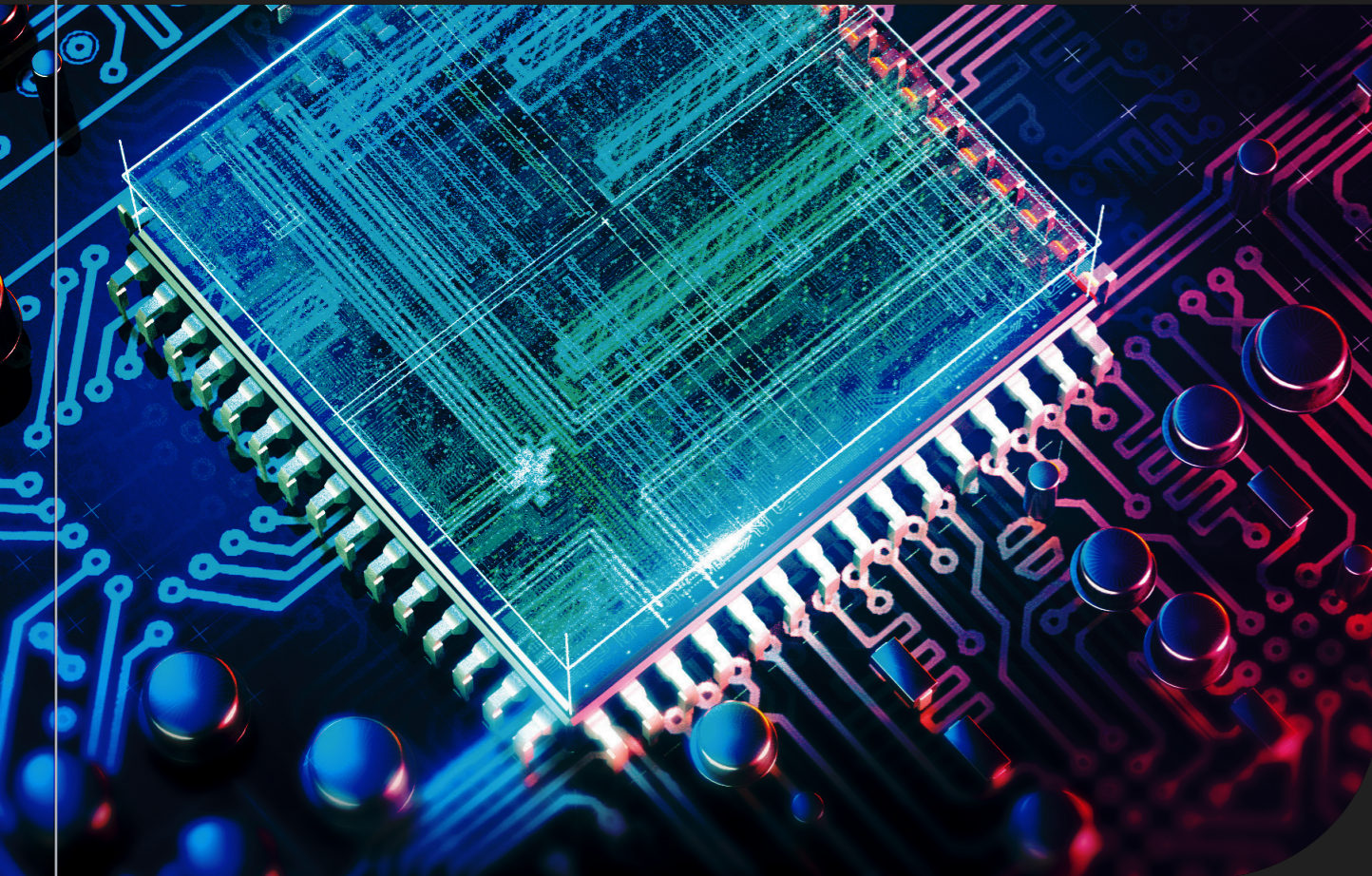
Today is difficult to find a field or segment where advanced technologies such as artificial intelligence, big data, or advanced simulations are not applied. These technologies are relevant not only to academic research and development, which may seem far from real-life applications to many but the adoption by private companies or the public sector is also increasing as HPC is increasingly accessible. These technologies became the basis of innovative processes and advanced digital solutions, for example, the optimization of city traffic, the automated evaluation of medical images, climate models, or digital twins.

Through ecosystem development, we want to accomplish cross-disciplinary and cross-sectorial cooperation to help Slovak companies take the next step in digitalization and support them in the development and implementation of HPC solutions, and last but not least, raise new experts in Slovakia. Therefore, let's not view investing in the HPC ecosystem as a luxury. Let's consider it a necessity.

Lucia Demovičová

CONTENT

01

NSCC
DEVANA
EUROCC

Slovak National supercomputer centre

A PLATFORM FOR COOPERATION & DEVELOPMENT OF HPC IN SLOVAKIA

In the last issue of HPC Focus, we presented the **Slovak National Supercomputing Centre** (SK NSCC), established in November 2020 as an association of the state, academic and private sectors. We introduced a rather ambitious goal of building HPC infrastructure with the extreme performance provided by a supercomputer that would put Slovakia at the top, at least within Europe. To achieve this, Slovakia will use funds from the Recovery and Resilience Plan of approximately 70 million euros. A comprehensive feasibility study is currently being prepared, based on which we plan to define the exact investment implementation and schedule.

If we talk about significant infrastructure procured with public funding, expecting benefits for national science, society, and the economy is fair enough. It is the opportunity to increase Slovakia's knowledge and skills in HPC and related technologies (AI/ML, HPDA, advanced simulations). We can achieve increased use of digital solutions based on HPC among the companies, educate experts while retaining talents, and make Slovak scientists and researchers equal partners to their European colleagues in solving complex problems in various fields.

The current Recovery and Resilience plan defines the Slovak National Supercomputer Centre as an operator of this infrastructure. Considering environmental responsibility and current energy prices, SK NSCC strongly suggests building an investment strategy for the long-term sustainability of the operation with the wide possible use of green technologies, for example, photovoltaics and usage of waste heat, which the supercomputer produces during its operations.

Whether the new supercomputer will have a performance of tens or hundreds of petaflops, it is undoubtedly necessary to prepare a user community and establish a supporting ecosystem. HPC infrastructure is its foundation, but installation and commissioning alone are far from ensuring the full realisation of the potential of such an investment. Based on experience from abroad (Luxembourg, Spain or Japan) and our own experience, we know this can only be achieved by systematic and long-term support of experts in individual application areas working at universities and the Slovak Academy of Sciences. We also need to support software developers, as well as build expert user support teams and a network of regional intermediaries. It is also necessary to support small and medium-sized enterprises, large industry, and public administration in various forms, from consultancy to grant schemes to cooperation on research and development projects.

Building the HPC ecosystem in Slovakia is a natural task for SK NSCC, which profiles itself as a national platform for cooperation and development in this area. At the same time, SK NSCC is a full-featured institution able to implement individual activities in the field of HPC, coordinate them at the national level, and participate in creating a strategy for the long-term development of HPC. However, SK NSCC won't do it alone, active involvement of its members and partners is necessary to boost the project implementation leading to cooperation and synergies instead of competition. A united community of SK NSCC, universities, SAS, and other relevant institutions is the best way to ensure sufficient weight in the future for HPC development requirements beyond the horizon of the Recovery and Resilience Plan.

It is the opportunity to increase Slovakia's knowledge and skills in HPC and related technologies (AI/ML, HPDA, advanced simulations) and we can achieve increased use of digital solutions based on HPC among the companies, educate experts while retaining talents.

The New DEVANA Supercomputer

The compute section of the supercomputer will consist of 140 universal nodes for classical HPC and 8 accelerated nodes for artificial intelligence and machine learning tasks (AI/ML).

The New HPC system "Devana" (Development and enabling), which was procured as a replacement for Aurel within the Operational Programme Integrated Infrastructure (OPII-2020/7/55-NP, **National Competence Center for High Performance Computing project**, code 311071AKF2) is currently being setup for its users.

Lenovo technology prevailed among a number of other competing offerings. Lenovo is a well-established company in the field of building high performance computers and although it does not have any entries in the top ten of TOP500 highest performing computers in the world, it built 161 systems from the rest of the list (data from June 2022). Our system does not have the parameters to compare even to the last system on the list, however it will still contribute significantly to the restrictive resources of our academic community. We also expect users from the private sector and public administration. This was one of the reasons why we managed to incorporate additional hardware platforms and thereby extend the portfolio of problems that can solved by the supercomputer.

The compute section of the supercomputer will consist of 140 universal nodes for classical HPC and 8 accelerated nodes for artificial intelligence and machine learning tasks (AI/ML). The system also contains a new distributed data array, which is standardly divided into two separate parts, one used to store permanent data and the other for temporary data generated by simulations. Apart from this, the compute nodes have their own local storage. The service nodes are configured for high availability, like those of Aurel super-

computer (all critical components are duplicated in case of a failure). These include nodes used for user login into the system and its management on different levels. We also introduced a new module consisting of four servers, which provides some internal and especially external services (e.g. OpenOnDemand, graphical interface, specific tailored services, ...). Spatially, Devana consists of six compact 42U racks, of the LeSI technological series (**L**enovo **S**calable **I**nfrastructure). Compared to Aurel, the water-cooling technology is also considerably different,

deploying rack door cooling (so called indirect water cooling). This type of cooling simplifies maintenance and faulty component replacement significantly.
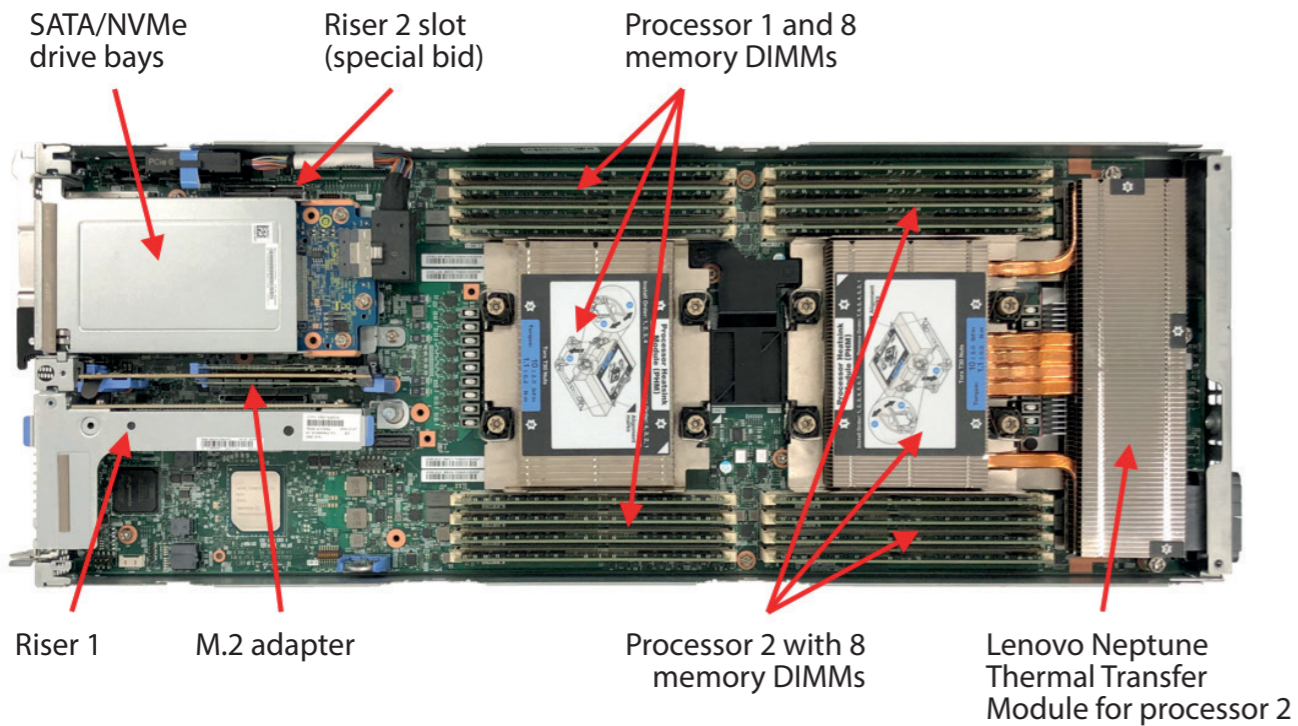
HPC Compute Node

The main unit of a universal compute module contains format 0.5U server SD630 v2. Four of these servers are placed in a single 2U unit DA240 (Fig. 1). This platform is optimized for maximum performance per area/volume of a datacenter while preserving maintenance and operation simplicity. The configuration of a compute node itself consists of two powerful yet efficient processors Intel Icelake 6338 32C/2.0GHz/205W, 256GB operating memory and a 100Gb HDR InfiniBand adapter to connect to the compute network (Fig. 2). As far as Hard drives are concerned, the compute nodes are split into two cathegories, based on performance a local storage capacity. However, in both cases the technology consists of SSD NVMe connected through a PCI express bus.

FIGURE 1

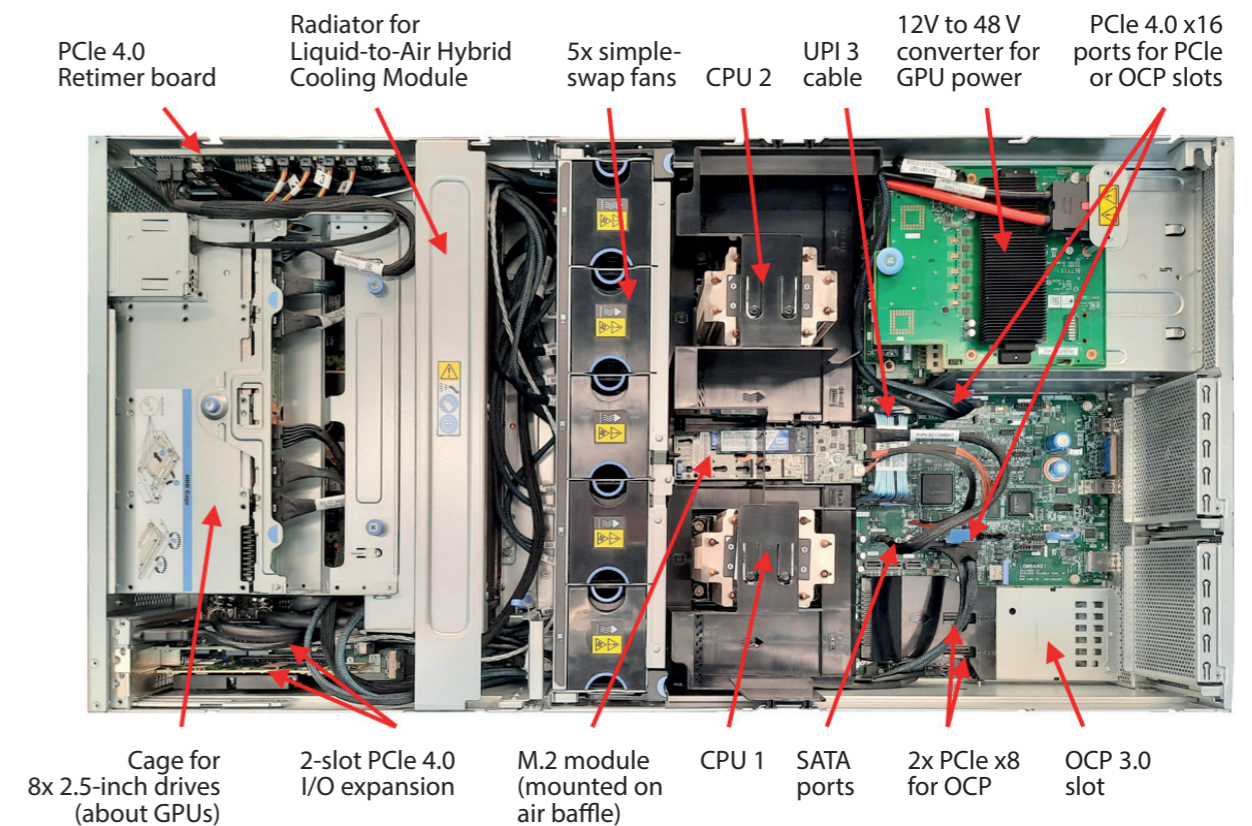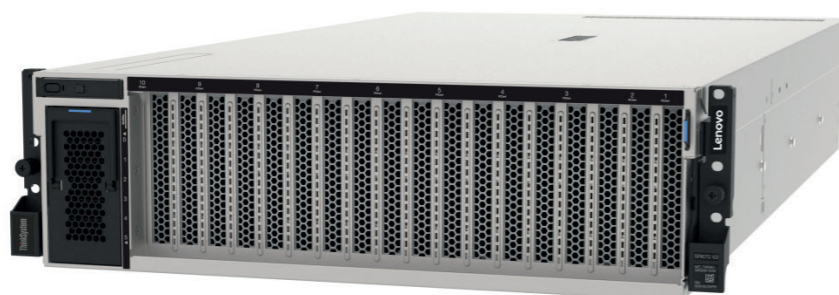Four universal compute nodes Lenovo ThinkSystem SD630 v2 in a DA240 unit.

SATA/NVMe drive bays   Riser 2 slot (special bid)   Processor 1 and 8 memory DIMMs

Riser 1   M.2 adapter   Processor 2 with 8 memory DIMMs   Lenovo Neptune Thermal Transfer Module for processor 2

FIGURE 2

View of SD630 v2 compute node internal system layout.

AI/ML Compute node

An accelerated module of the new supercomputer contains type SR670 v2. The server itself is 3U tall (Fig. 3), with the option of deploying up to eight type GPGPU accelerators. Due to binary and instructional compatibility, the accelerated nodes are of the same type and processor count as the universal nodes. The operating memory and local drives configuration are also the same. (Fig. 4). Unlike in the universal nodes, the connection to the compute network is doubled to 200 Gb/s. The performance portion of the machine learning and artificial intelligence application node consists of four GPGPU accelerators Nvidia A100 40GB in the SXM format (Fig. 5), connected uniformly through the NVlink technology. Every card with its 6912 CUDA and 432 tensor cores provides a respectable computing power even for the most demanding applications from the field of AI/ML.
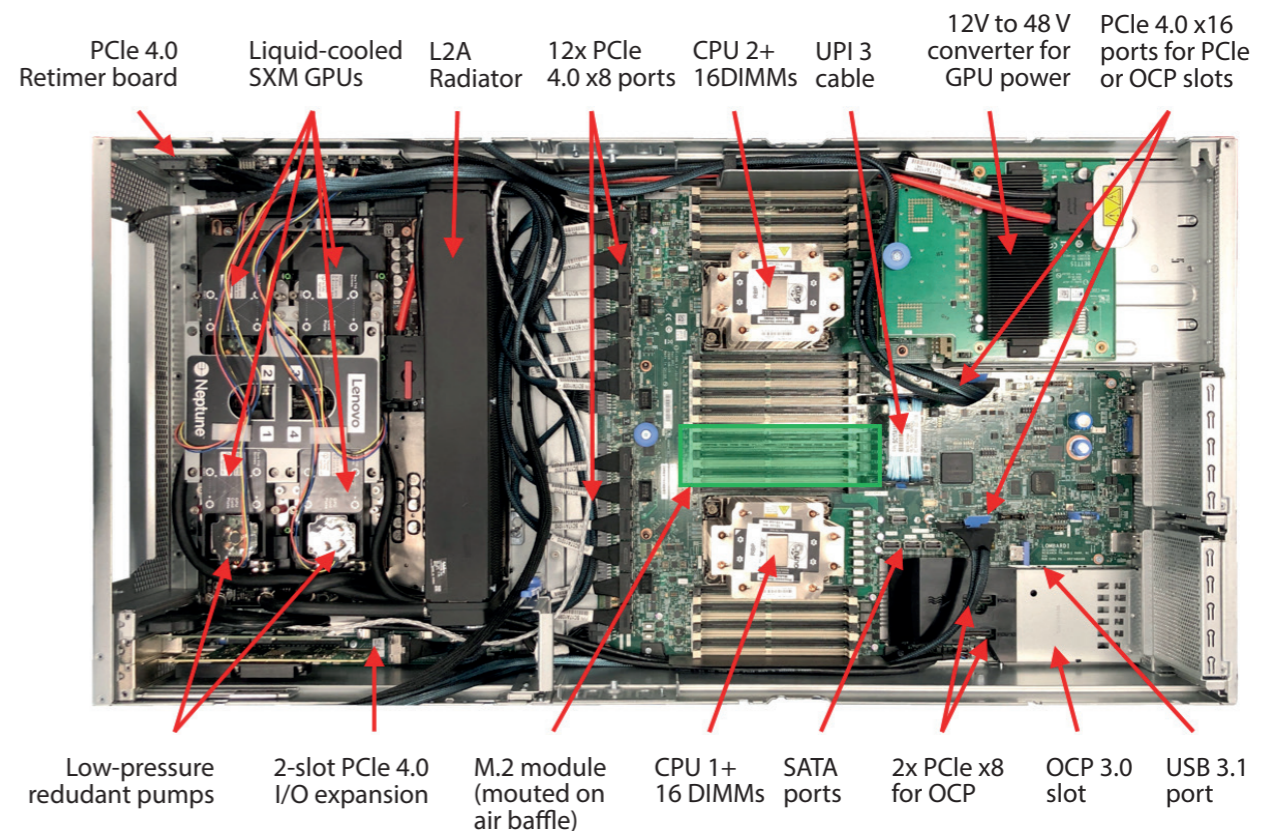
FIGURE 3

Lenovo ThinkSystem SR670 v2 accelerated node with up to 8 PCIe GPGPU cards capacity.

PCIe 4.0 Retimer board   Radiator for Liquid-to-Air Hybrid Cooling Module   5x simple-swap fans   CPU 2   UPI 3 cable   12V to 48 V converter for GPU power   PCIe 4.0 x16 ports for PCIe or OCP slots

Cage for 8x 2.5-inch drives (about GPUs)   2-slot PCIe 4.0 I/O expansion   M.2 module (mounted on air baffle)   CPU 1   SATA ports   2x PCIe x8 for OCP   OCP 3.0 slot

FIGURE 4

Two levels view of SD670 v2 internal system layout.

PCIe 4.0 Retimer board   Liquid-cooled SXM GPUs   L2A Radiator   12x PCIe 4.0 x8 ports   CPU 2+ 16DIMMs   UPI 3 cable   12V to 48 V converter for GPU power   PCIe 4.0 x16 ports for PCIe or OCP slots

Low-pressure redudant pumps   2-slot PCIe 4.0 I/O expansion   M.2 module (mounted on air baffle)   CPU 1+ 16 DIMMs   SATA ports   2x PCIe x8 for OCP   OCP 3.0 slot   USB 3.1 port

FIGURE 5

SXM format GPGPU accelerator Nvidia A100.
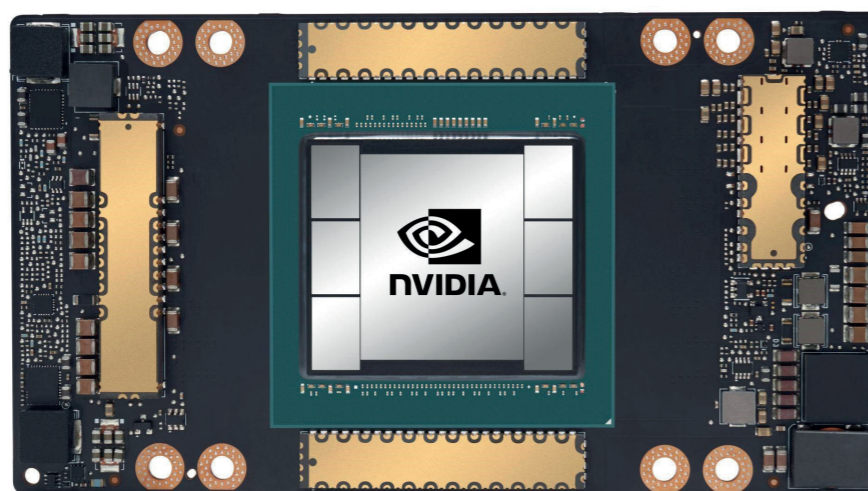
Compute network

The internal communication network of the supercomputer, which provides communication between the nodes and access to the data on the shared storage, uses HDR InfiniBand (implicit RDMA technology deployment) with a 100 Gb/s throughput and a maximal latency of 10 microseconds. Reinforced double throughputs are available to accelerated module nodes and severs providing data access to shared storage. The network uses a tree topology – nonblocking network (i.e. the blocking ratio is 1:1). It consists of two levels of switches, L1 switch level (so called "leaf" switches) is used to connect the endpoints, L2 switch level (so called "spine" switches) connects the L1 switches to each other.

Shared data storage

Data storage module contains two independent physical clusters, a HOME cluster and a SCRATCH cluster. The first is designed as a secure file storage designated primarily for permanent user data. It is a complex hardware solution usable for NFS protocol distributable file system deployment (NFSv4.0 or higher version is planned). Two NFS service nodes will be configurable in the active-active or active-passive mode. SCRATCH is a high-performance file storage for short term temporary data storage generated during job execution. The final configuration includes two metadata servers and four data servers (Aurel had data and metadata distributed uniformly across all data servers). An open source solution BeeGFS is used on the file system level, which allows simple bandwidth increase by adding more data servers.

LAUNCH OF THE FIRST GRANT COMPETITION FOR PROJECTS IS SCHEDULED IN DECEMBER 2022.

TABLE

Comparison of technical parameters of the AUREL supercomputer with its successor – the DEVANA supercomputer.

	AUREL	DEVANA
PLATFORMA	IBM Power 775	Lenovo ThinkSystem SD630 v2 + SR670 v2
OS	AIX 7.x	CentOS 7.x
ARCHITECTURE	Power7	x86_64
CPU NODES	122	140
GPU NODES	0	8
CPU CORES	4096	9472
GPU CORES	0	221184 CUDA + 13824 Tensor
THEORETICAL PERFORMANCE	~130 TFlops	~800 TFlops
RAM	32 TB	38 TB
DATA STORAGE	600 TB + 300 TB	1 PB + 600 TB + 400 TB
FILE SYSTEM	GPFS	BeeGFS + Linux native
COMPUTE NETWORK	IBM HFI Interconnect	HDR Infiniband
NETWORK TOPOLOGY	Fat tree (non-blocking)	Fat tree (non-blocking)
POWER CONSUMPTION	220 kW	130 kW

We spoke with **Tomáš Karásek** from IT4Innovations in Ostrava about cooperation with non-academic entities in the field of HPC and the functioning of the competence center in the Czech Republic.

To begin with, can you tell us something about the Czech competence center - how many partners are involved, and how big is your team?

The National Competence Center (NCC) for HPC within the EuroHPC Joint Undertaking is represented in the Czech Republic by IT4Innovations – the national supercomputer center at the Technical University of Ostrava. More than 45 workers (20 FTE) participate in the activities of the competence center, of which the majority (35) are scientific or technical professionals.

Did you have previous experience in the Czech Republic with providing HPC services to non-academic users even before the start of the EuroCC project? (The project launch was in September 2020.)

IT4Innovations has been co-operating with industry partners for a long time, and not only with small and medium-sized enterprises. Over more than ten years, we have worked with dozens of companies across industries. Our co-operation includes commercial access to computing capacities, contract research, and, in particular, joint research within national and international projects.

Which services from your portfolio are among the most requested?

IT4Innovations offers its partners with industrial practice many years of experience in advanced numerical simulations, virtual prototyping, and Big data analyses.

We offer our partners the execution of simulations of physical processes in fluid flow, structural mechanics, heat transfer, acoustics, and electromagnetism. To solve these problems, we use commercial software packages such as ANSYS Multiphysics, Fluent, CFX, and Comsol Multiphysics and also non-commercial open-source packages, for example, OpenFOAM, etc.

We also offer the development of automated, tailor-made computing tools based on third-party open-source products such as OpenFOAM, Code_Saturne, Code_Aster, Elmer, or Calculix. We can modify these packages to automate solving a specific problem with minimal user requirements. Furthermore, based on the request, we can create a complete methodology for solving the given problem using open-source products. It enables companies to use such open-source products in their R&D activities.

In the field of Big data analyses, IT4Innovations is dedicated to processing and analysing large-scale data and simulations that have various uses in real life. For example, management and decision-making support in emergencies, intelligent navigation, traffic load predictions, flood propagation modeling, smart cities, bioinformatics, and reliability analyses. We also deal with program models for distributed applications and their implementation.

Could you mention some successful collaborations with SMEs and the industry?

Of a large number of successful projects, cooperation with Siemens s.r.o. is worth mentioning. The work consisted of the joint development of an optimal design of a ventilation unit ensuring effective cooling of an asynchronous electric

Dr. Tomáš Karásek works as the Head of the Parallel Algorithms Development Laboratory in the company IT4Innovations in Ostrava.

NATIONAL COMPETENCE CENTER FOR HPC IN THE CZECH REPUBLIC

motor: https://www.it4i.cz/en/industry-cooperation/exam-ples-of-cooperation/fan-section-optimization-in-asynchro-nous-electric-motors. The cooperation subsequently contin-ued within the project "Digital twin of a product within the Siemens production facilities" supported with a grant by the Ministry of Industry and Trade.

Projects with the companies Viderize or Orgrez are among the successful cooperation with SMEs.

Viderize

www.it4i.cz/en/industry-cooperation/examples-of-cooperation/improving-retinal-screenings-of-patients

The joint project „Development of an expert system for the automatic evaluation of pathologies from an eye image" was supported by the Technical Agency of the Czech Republic (TAČR) to develop and validate an expert system using mo-deling and training of neural networks for the detection of pathologies related to diabetic retinopathy on images taken by the so-called fundus camera. Neural networks trained for the classification and segmentation of images from fundus cameras enabled the division of images into categories de-termining the degree of severity of the disease, including de-tailed segmentation of specific defects related to individual degrees. Thousands of high-resolution images used for trai-ning and validation place high demands on computing power. Therefore, the project used specialized accelerated systems of artificial intelligence computation as the Barbora super-computer or NVIDIA DGX-2.

Orgrez

www.it4i.cz/en/industry-cooperation/examples-of-cooperation/computational-simulation-for-pollutant-emission-reduction-in-combustion-plants

The Proof-of-concept (PoC) within the EuroCC project was at the beginning of the cooperation with the company ORGREZ. This PoC aimed to verify the possibilities of numerical mode-ling, specifically the so-called Computational Fluid Dynamics (CFD) for solving the selective catalytic reduction (SCR) pro-cess. Based on the outputs of this PoC, a joint project was

submitted and supported via a call of the Ministry of Industry and Trade to create a software tool for the evaluation effec-tiveness of catalytic processes and comprehensive support in the design of SCR technologies for industrial applications.

In Slovakia, public sector engagement is quite a difficult task. Based on your experience, what is the most effective way to involve this group of stakeholders, and what challenges do you consider are the most significant in this regard?

In the Czech Republic, not many state administration orga-nizations use high-performance computing. It is attributed to lower awareness of the HPC possibilities and the lack of employees within these institutions with the correspond-ing knowledge and experience. From our point of view, the most effective way to increase the use of HPC in this target group appears to be the active search for potential partners and raising awareness of HPC usage via good practices such as the Floreon+ system (https://floreon.eu/mapa/) used to evaluate the information for decision-making support within crisis management processes, mainly floods, with a focus on the Moravian-Silesian region. Other examples are coopera-tion with the Faculty Hospital in Ostrava focused on medi-cal image processing Medical image processing as a service – IT4Innovations or with the Moravian-Silesian Region and the city of Ostrava during the construction of a large-capacity vaccination center, which was put into operation in March 2021 in Ostrava's Černá louka.

In the case of cooperation with the state administration, one of the biggest challenges is to increase the number of users and suitable case studies from this segment

In your opinion, what competencies and activities are yet to be added to the portfolio of competence centers so they can fulfill their role more effectively, especially concerning their sustainability?

Due to the different status of individual competence centers and mainly different needs of communities in each country, it is difficult to determine any general competence that compe-tence centers should introduce into their portfolio of services.

In every country, HPC users' needs define the need for the so-called „hard" competencies. On the other hand, the nec-

In the field of Big data analyses, IT4Innovations is dedicated to processing and analysing large-scale data and simulations that have various uses in real life.

essary „soft" competencies should reflect the needs of the given ecosystem, for example, innovation centers, digital innovation hubs, European digital innovation hubs, union clusters, etc.

Considering the nature and mission, the future sustainability of national competence centers will depend mainly on public funding, most likely a combination of European and national resources. Given the current level of HPC technologies used among SMEs, it is not realistic for national competence centers to be financed only from the income obtained from the services provided.

Have you had problems recruiting or retaining qualified employees for your Competence Center?

Currently IT4Innovations employees are involved in the NCC activities and are engaged continuously when needed. However, getting new reinforcements is not easy. It is mainly because this field requirements demand high competence and experience. There is also strong demand for such candidates in the labor market, which exceeds the supply. Given that IT4Innovations or NCC operates within the university, it is a difficult mission to compete with offers from the private sector in terms of financial compensation.

Given the current level of HPC technologies used among SMEs, it is not realistic for national competence centers to be financed only from the income obtained from the services provided.

Karolina

The petascale system Karolina, acquired as part of the EuroHPC Joint Undertaking, was installed in 2021. In the TOP500 list, which evaluates supercomputers in terms of their performance, it ranked 69th worldwide, 19th in Europe, and in the Green500 list of the most energy-efficient supercomputers, it even ranked 8th in 2021.

The new supercomputer reaches a theoretical peak performance of 15.7 PFlop/s, which corresponds to 15.7 quadrillion operations per second.

HPC
Applications

Professor
Roman Martoňák

PRESSURE, MATTER, & COMPUTER

Prof. Ing. Roman Martoňák, DrSc. works at the Department of Experimental Physics of the Faculty of Mathematics, Physics and Informatics of the Comenius University in Bratislava as a professor of physics.

In this paper we will present a fascinating and generally relatively little-known field of high pressure physics. Our everyday life takes place at atmospheric pressure, and therefore we more often encounter changes caused by temperature (melting of solids or boiling of liquids). However, high pressure can cause much more dramatic changes in matter than temperature. A well-known example is the transformation of soft graphite into superhard diamond, which found practical use in the production of artificial diamonds. Inside the Earth and the planets there are enormous pressures (up to millions of times higher than atmospheric pressure), and to understand what happens there, we need to know how pressure and temperature change the structure of matter. It has recently been shown that at a pressure of 1-2 million atmospheric pressures, superconductivity (conduction of electric current without losses) can exist even almost at room temperature. In addition to experiments, which are complicated, phenomena at high pressures can nowadays be investigated very effectively with the help of computer simulations. These allow us to look inside the crystals and directly observe how the atoms rearrange under the influence of high pressure. Currently, these methods are going through a stage of rapid development.

01 Jumps called phase transitions

At the beginning, we will start from a slightly different problem where our common everyday experience will help us. When we see melting snow, it seems to us that it is something so common that it doesn't even make sense to think about it. Everyone knows that ice melts at a temperature of 0 °C and turns into liquid water. In fact, there are many questions that could occur to us, and we start with the most important ones. The laws of Nature are continuous and therefore it appears natural that a small cause usually induces a small effect. But why doesn't melting produce something that is partly ice and partly water? Why even with a slight increase in temperature above 0° such a dramatic transformation occurs? It seems like in the case of melting the continuity does not work because we see a jump. How is it possible? Of course, in high school it is taught that the melting of a crystal (in this case ice) is an example of the so-called phase transition. It is not a specific property of water and is observed in practically all substances. But mere giving a name to a phenomenon is not its explanation. So how can melting be explained from the point of view of physics?

For the answer, we need an important part of physics called statistical mechanics. It tells us that for given external conditions, the most probable state of the system is realized. The probability of the existence of water and ice depends on the temperature. What happens at 0 °C is simply a reversal of these probabilities – below 0 °C ice is more likely than water, and above 0 °C the opposite is true. A simple principle – the most probable state wins – can generally and naturally explain the existence of a jump or phase transition.

It has recently been shown that at a pressure of 1-2 million atmospheric pressures, superconductivity (conduction of electric current without losses) can exist even almost at room temperature.
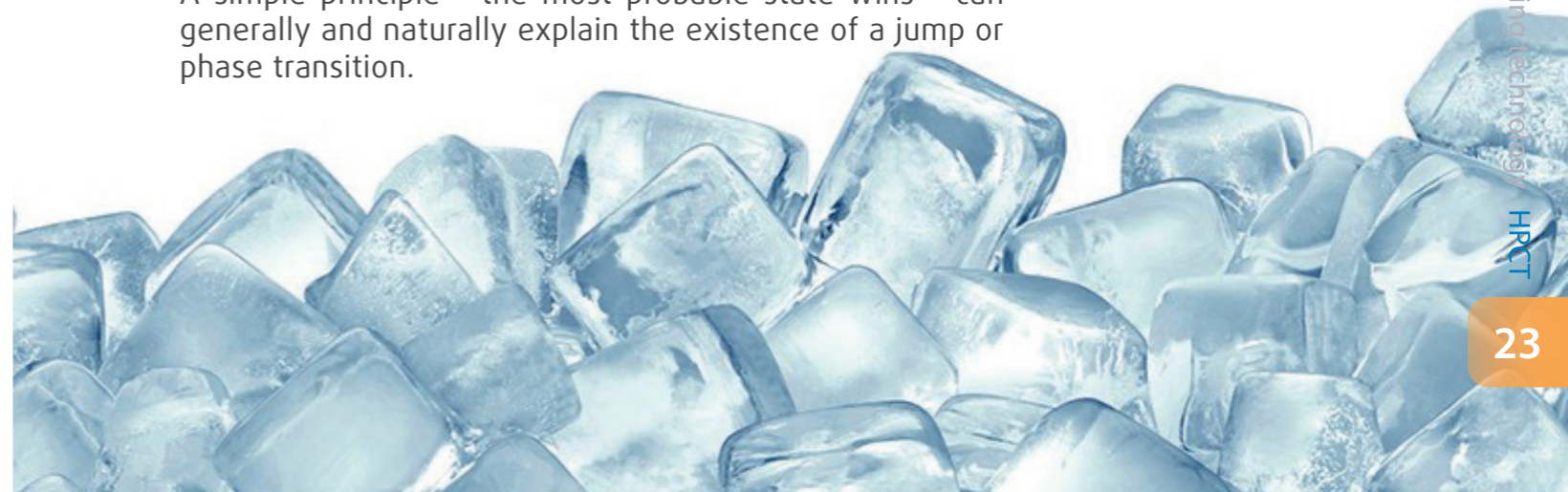
It can roughly
be said that
no less than
thousands
of atmospheric
pressures begin
to represent
values relevant
for the
preparation
of new crystalline
structures.

This could be compared to a model situation in economics where buyers would make a buying decision based on price alone, and there would be only two types of product, A and B. If the price of A is lower than the price of B, everyone will buy A. But if B becomes cheaper and its price falls even slightly below A, everyone will buy B. A small change in prices caused a dramatic change in behavior.

After this introduction we can move from temperature to pressure. The principle is similar and it should not be surprising that pressure also causes discontinuous changes, or jumps. But in a sense, pressure can do more. Temperature, by its very nature, induces chaos and moves the system toward disorder. Therefore, upon melting, the ordered crystal, where the atoms have a precisely defined position, disappears and is replaced by a much less ordered liquid, where each atom can be everywhere. Unlike temperature, however, pressure does not cause chaos, but merely pushes the system towards a smaller volume. Therefore, pressure typically causes a transformation of an ordered crystal structure into another one which has a smaller volume. Volume is determined by how close the atoms are packed together. The higher the pressure, the more important it is to reduce the volume, and the „better" the atoms have to be arranged.

## 02 A new world above atmospheric pressure

Transformation of graphite into diamond and 18 forms of ice

At this point we need to specify more precisely what we mean by high pressure. In everyday life, we encounter higher pressures, e.g. when cooking in a pressure cooker or when inflating tires. From the point of view of crystals such pressures are actually quite low and therefore uninteresting. It can roughly be said that no less than thousands of atmospheric pressures begin to represent values relevant for the preparation of new crystalline structures. At pressures reaching millions of atmospheric pressures, almost all substances change their structure.

It is fascinating that such extreme pressures can be achieved relatively easily in the laboratory today. The story began in 1905, when the American physicist P. Bridgman decided to

systematically investigate what happens to various materials when they are compressed. For his pioneering work in this area, he was in 1946 awarded the Nobel Prize in Physics. Pressure is a force per unit area and therefore the path to high pressure leads through a large force acting on a small area. Currently, the most used method is the so-called diamond anvil cell (DAC - diamond anvil cell, Fig. 1), in which the examined sample is placed between two pointed diamonds that compress it. Of course, there is only a very tiny amount of sample in this cell, but with the help of electromagnetic radiation (from infrared to X-ray), it is possible to directly examine its structure and physical properties (this is most often done at so-called synchrotrons).
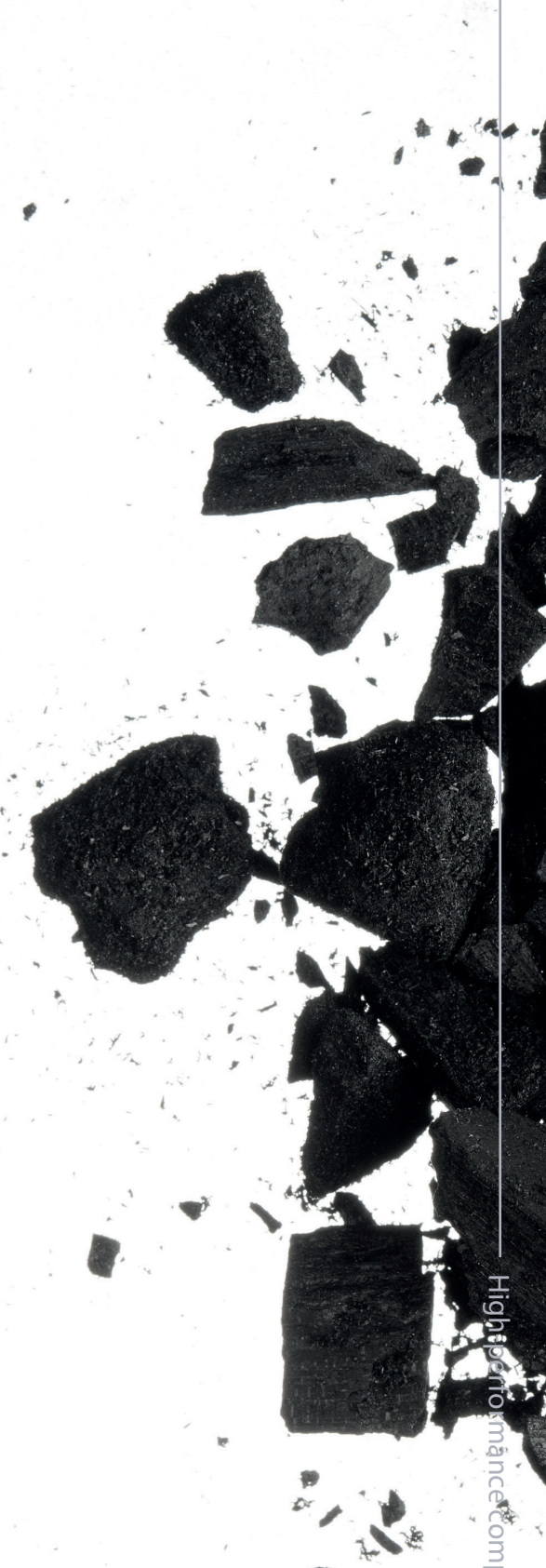
The real possibility of achieving such high pressures in the laboratory opens up a new world. Pressure, via volume reduction, fundamentally changes the structure and chemical bonds. As a result, all the properties of matter will change – density, hardness, color, conductivity, magnetic properties, etc. Semiconductors typically become metals (e.g. silicon), but it can also be the other way around – e.g. metallic sodium turns into an insulator. The existence of a certain substance in different crystalline forms is referred to as polymorphism.
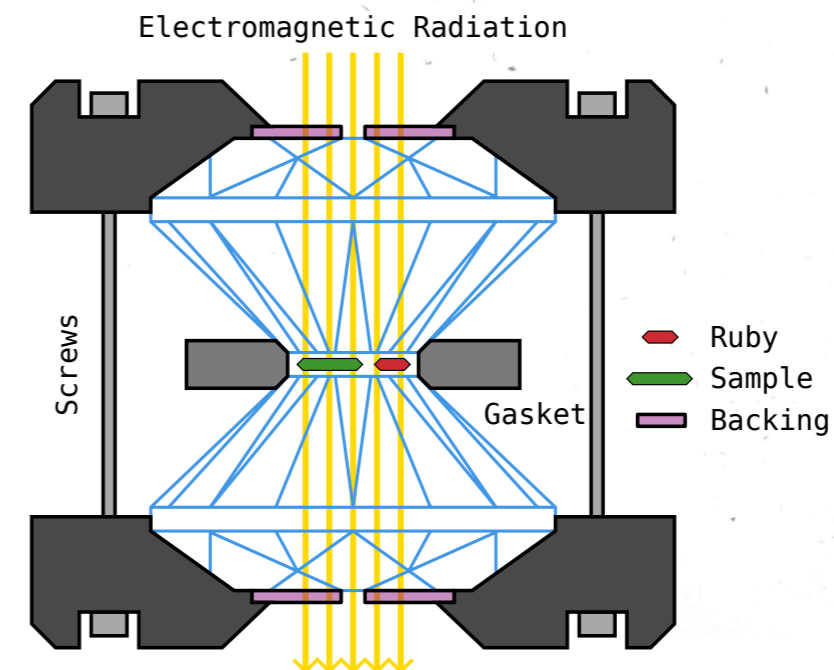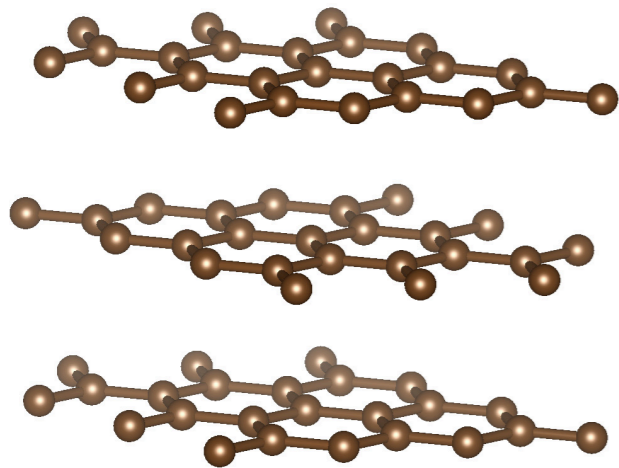

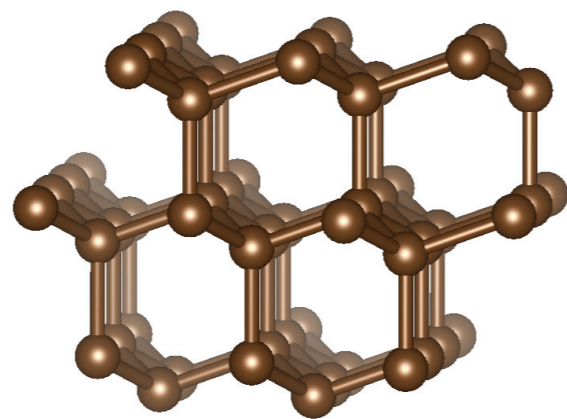## FIGURE 1

Diamond anvil cell
(image from Ref. [1]).

The prototype of a structural transition at high pressure is the transition graphite – diamond in carbon (Fig. 2). Under the influence of high pressure (and high temperature also helps), the neighboring graphene layers in graphite form bonds and connect. After the formation of strong bonds also in the di-

graphite   diamond

FIGURE 2

Graphite (image from Ref. [2]) and diamond (image from Ref. [3]) (top) and their crystal structures (bottom).

rection perpendicular to the planes, the soft black graphite converts into a translucent and shiny diamond, representing the hardest material that occurs in Nature. The change in properties during this transition is indeed extreme (and the price also changes dramatically).

To stay with substances known from everyday life, ice is also a very interesting example of rich polymorphism. The well-known form we use to cool drinks and to ski on it, is the so-called hexagonal ice I_h. The name derives from the hexagons that are characteristic of its structure. But in addition to this form, there are at least 17 other forms that have a completely different structure (Fig. 3), and at least two disordered solid forms (so-called amorphous). Among them there is also ice V which has an exceptionally complicated and exotic structure, occuring at a pressure of 5000 atmospheric pressures and a temperature of -20 °C.

| I | II | III | IV | V |
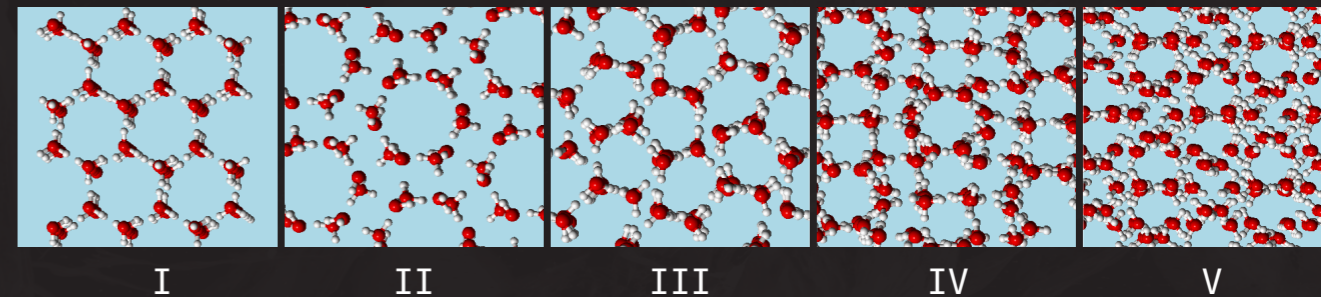
FIGURE 3

Examples of some important ice structures. Regular hexagonal ice I_h is the first (left). The red atom represents oxygen and the white one represent hydrogen.

Before moving on to other topics, we have to mention that perhaps the most spectacular example is the search for metallic hydrogen at extreme pressures (almost 5 million atmospheric pressures). Despite being the simplest element in the periodic table, it's a long, complicated and exciting story that has spanned nearly 100 years. In recent years, this story seems to be heading for a happy ending, but that would be a topic for a separate article.

03 Do such high pressures also occur in Nature?

Geophysics and Planetary Physics

If high pressures occurred only in the laboratory, the whole issue would be more of an academic problem. However, Nature does not avoid high pressures. If we were to imagine a journey to the center of the Earth, as dreamed of by Jules Verne, we would get under enormous pressure. The pressure in the center of the Earth, in its metallic core, is about 3.6 million atmospheric pressures. Even before reaching the metallic core, we would encounter vari-

ous (strongly compressed) minerals along the way, which change their form at a certain depth, where the pressure exceeds a certain value. This creates an interface on which seismic waves are reflected and refracted, and this allows us to „see" such structural changes in the depth of our planet.
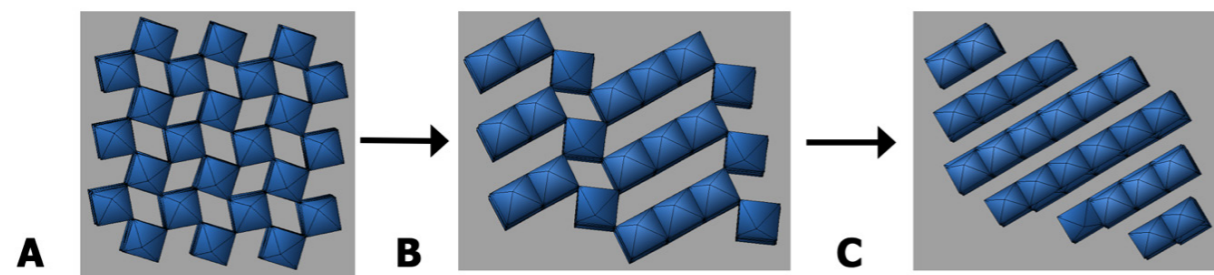
FIGURE 4

Transition from perovskite (A) to post-perovskite (C) via an intermediate structure (B) [6].

A well-known example is the so-called D'' layer at a depth of approx. 2700 km below the Earth's surface, where the structure of the mineral MgSiO3 changes from perovskite to the so-called post-perovskite. This phase transition was experimentally discovered by two groups in 2004 [4,5] and naturally explained the seismic anomaly observed at the mentioned depth. However, this discovery also brings us to the theory, because this transition was explained shortly after [6] (Fig. 4) using a method co-developed by the author of this article.

04 Why does a crystal actually adopt a given structure? Can we predict it?

The goal of science is to understand phenomena and develop a theory that can make predictions. The theory in this case is thermodynamics, which tells us that the problem of determining the structure of a crystal at a given pressure is actually the problem of finding an arrangement of atoms in space that gives the lowest possible value of a certain quantity that can be calculated. In mathematics, this type of problem is well known and is referred to as

the so-called optimization problem. It is also known that its solution is often very complicated. Even about 30 years ago, this problem was still considered practically unsolvable for crystals. The situation was concisely characterized by the well-known statement of J. Maddox, who was in 1988 the editor of the prestigious journal Nature: „One of the con-

> If we could theoretically predict the structure of a material before we prepare it in the laboratory, we could "design materials in computer".

tinuing scandals in the physical sciences is that it remains in general impossible to predict the structure of even the simplest crystalline solids from a knowledge of their chemical composition." [7] It was obvious that the importance of solving this fundamental problem is considerable. If we could theoretically predict the structure of a material before we prepare it in the laboratory, we could „design materials in computer", calculate their properties, and then try to produce the best ones. This represents the opposite of the traditional search for new properties by randomly examining a large number of materials. But as good as it sounds, in 1988 one still had to wait a few more years for this miracle.

05 Solving an intractable problem in 2006

If a problem is considered very difficult, few people want to solve it, because everyone knows that it „can't be done". However, in 2006, two papers appeared using different mathematical algorithms such as direct search [8] and evolutionary search [9], which convincingly showed that the problem is actually easier than hitherto believed (it doesn't

In 1911 Dutch physicist Kamerlingh Onnes discovered super-conductivity, i.e. lossless conduction of electric current (resistance disappears completely), for which he was awarded the Nobel Prize in Physics in 1913.

happen often, but it's always pleasant to see). Put simply, one just needs to randomly generate enough atomic arrangements, sort them and pick, in a sense, the best one. Of course, a problem could be the question how much is „enough". Fortunately, in this case, it is not an astronomical number, because usually several thousand to tens of thousands are enough. In evolutionary algorithms, one also accelerates the search by crossover of structures, which is inspired by biological evolution (we take a piece from one and a piece from another structure, and somehow „glue" them together). The methods work so well, that without exaggeration, they can be considered a revolution in the field.

06 Prediction of crystal structures using computers

Virtual journey to a new world

Of course, the fact that the problem seems relatively easy to us today is largely due to the high „brute force" of current computers (i.e. their high computing power). Finding the structure of common crystals is typically possible on a powerful PC within a few days. When deploying parallel supercomputers, even complicated structures can be found in a short time. It is even possible to optimize the proportions of elements in the compound (so-called stoichiometry). It may seem surprising, but this also depends on the pressure. Everyone knows that e.g. table salt, sodium chloride NaCl, is formed by combining sodium and chlorine in a ratio of 1:1. However, this only applies at low pressure. In 2013 it was shown that at high pressure, surprisingly, exotic compounds Na_3Cl, Na_2Cl, Na_3Cl_2, $NaCl_3$, and $NaCl_7$ [10] are stable.

For illustration we now mention one of the recent fascinating predictions. In 1911 Dutch physicist Kamerlingh Onnes discovered superconductivity, i.e. lossless conduction of electric current (resistance disappears completely), for which he was awarded the Nobel Prize in Physics in 1913. However, this remarkable phenomenon typically occurs at very low temperatures, and for more than 100 years it has been the dream of physicists to find a material that would be superconducting at room temperature. The aforementioned calculation methods are ideal for this goal. In 2017,

the material LaH_{10} was theoretically predicted (independently by two groups [11,12]), to be superconducting at a temperature above 270 K, i.e. around 0 °C. It is not for free, because it requires a huge pressure higher than 2 million atmospheric pressures. The structure is shown in Fig. 5 and we leave the assessment of its aesthetic qualities to the reader. The material was successfully prepared exactly as predicted, and two groups [13,14] in 2019 independently showed that at the predicted pressure it is indeed superconducting at a temperature higher than 260 K, i.e. -13 °C. This prediction and its confirmation can be considered as a triumph of theoretical prediction of crystal structures. It is still far from practical use, but we already know that superconductivity at room temperature is possible.
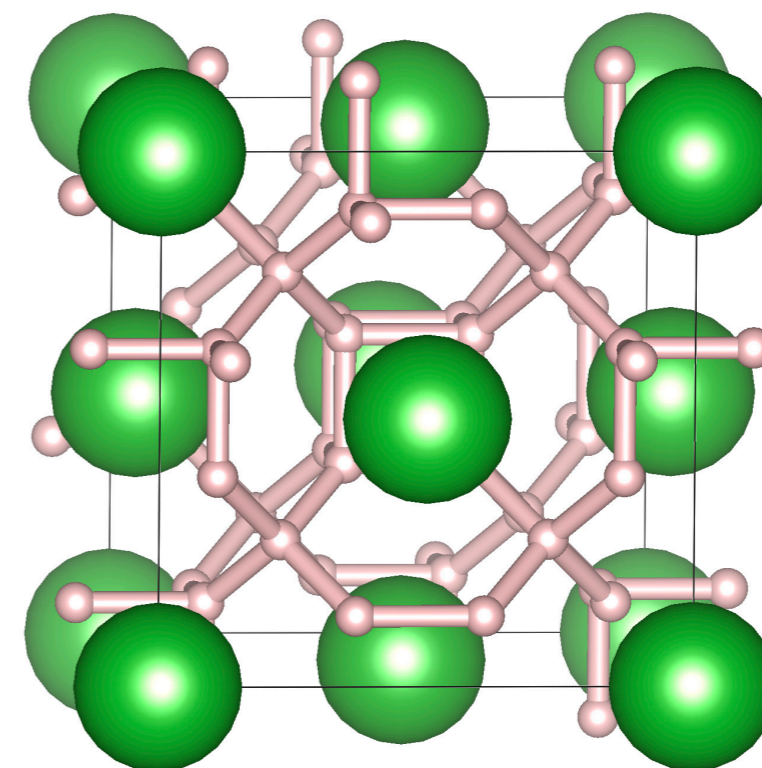
FIGURE 5

Structure of the high-temperature superconductor LaH_{10} [11,12].

07 Return from the "New World"

Finally, we cannot avoid the natural question – what happens when we release high pressure? Will the structure come back? After all, diamond should not exist at all at atmospheric pressure. Its very existence is in a sense a mistake of Nature (it

is called a metastable state). Diamond is a stable state at high pressure, but when it is released, carbon should return to its stable state at low pressure, which is graphite. Can this actually happen? Should we be afraid that expensive diamonds will one day turn into ordinary graphite? And what about high-pressure forms of other materials? Will they survive the return from the „new world" to the ordinary one?

Prof. Martoňák is mainly devoted to the investigation of the properties of matter in extreme conditions using computer simulations.

We can reassure diamond owners. As hard as diamonds are to make, they are hard to destroy. The bonds between carbon atoms are very strong and at room temperature it is practically impossible to break them. Strictly speaking, the diamond is protected by a high energy barrier, and this barrier is „good" for us. Due to it, it will not fall apart even after thousands of years. However, this does not apply to all new forms of matter that arise at high pressure. Some immediately return to their original form after pressure is released, or even change to a form different from the initial one. But diamonds are also special in this regard, and probably that's why they are believed to be forever (just don't heat them up too much, because it's still just carbon that can burn).

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Using ML/AI for chemistry applications – potential drugs for COVID-19

MARIÁN GALL

Bonds Lenght
Atomic Charge
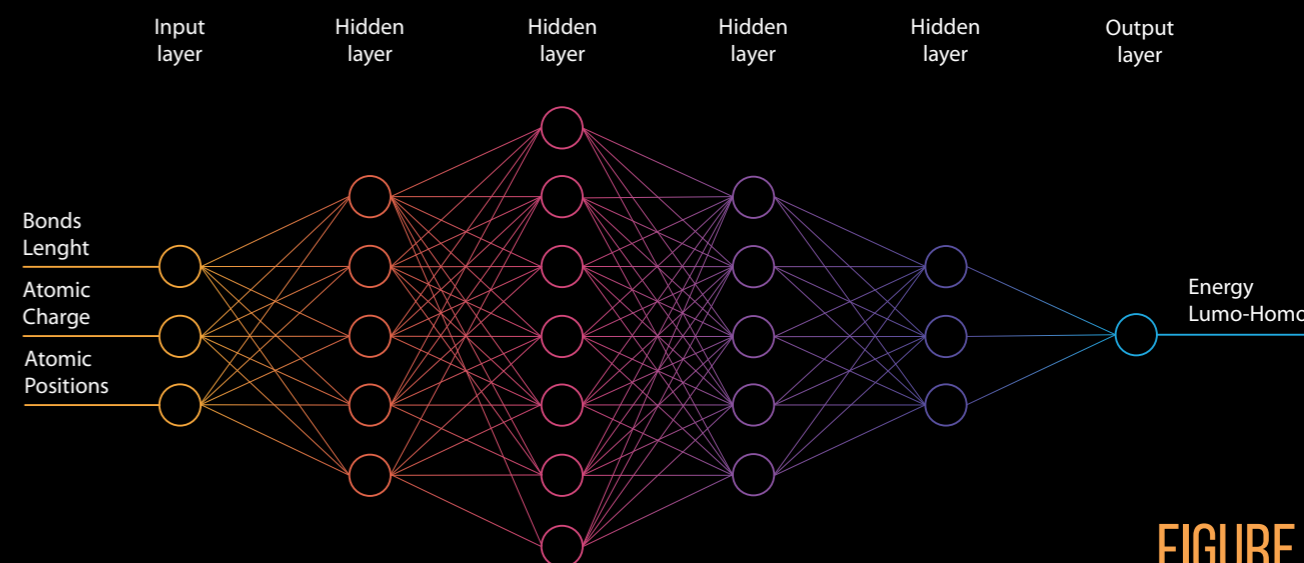Atomic Positions

Energy Lumo-Homo

FIGURE 1

A scheme of an illustrative neural network, in which the input is the structure of a chemical substance, such as the position of atoms, etc., and the output is the investigated property of the given structure, such as internal energy and so on.

Ing. Marián Gall, PhD. works at the Institute of Informatization, Automation and Mathematics FCHFT STU in Bratislava.

Neural networks and machine learning in general are the most widely used methods of artificial intelligence. Over the last few years, they have led to great progress in image and audio recognition, automatic text generation, and other areas. Practical applications of these new possibilities of computer technology include, to name a few, diagnosing diseases from computer tomography images in the health sector, product quality control in manufacture, or in the nowadays popular automated vehicle control systems. The areas of their use are wide-spread and, especially in recent years, they have become part of virtually every sphere of human activity.
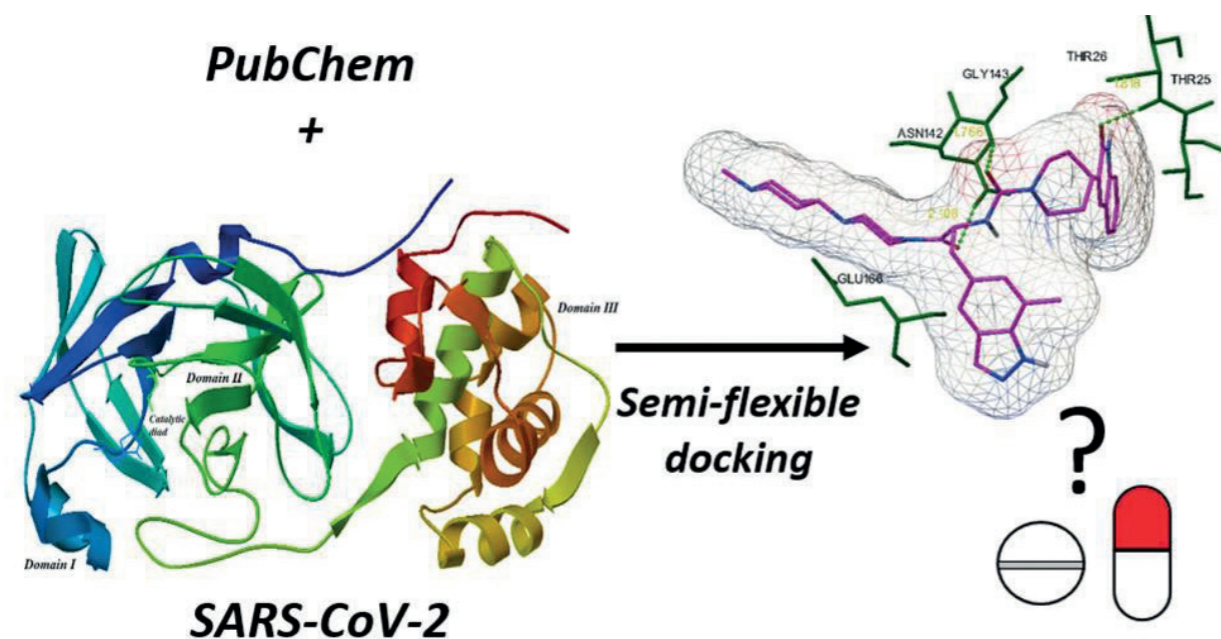
The basis of the universality of neural networks is that they mimic functioning of the brain. They not only model the way the brain performs its functions, but also how it learns. Neural networks consist of neurons that are interconnected in various ways, thus creating a network. There is usually a layer of neurons receiving input data at the entrance to the network, and a layer of neurons representing output data at the end of the network. There are other also layers of neurons between these layers that are interconnected in various ways,

see Fig. 1. The „learning" or „training" of the network, aside from its structure, forms the second important aspect of the properly functioning neural network. During this process the neural network learns which inputs should correspond to the respective outputs. This process is characterized by changes in the strength of the connections between neurons (weights in individual connections). From a mathematical point of view, neural networks represent so-called universal approximator – they can simulate any continuous automaton with any accuracy. Thus, neural networks can predict results in a completely different manner than regular computer simulations.

Neural networks have also been widely used in chemical and biochemical research and are currently one of the most common cheminformatics methods for identifying quantitative relationships between structure and properties of chemical substances. They are actively used to predict physical and chemical properties, biological activity of chemical compounds, and for the controlled design of chemical compounds and materials with predetermined properties which includes the development of new drugs, see Fig. 2.

The application of neural networks in chemistry is complicated by the fact that the description of molecules using atoms and their coordinates in space, which is commonly used in chemistry, is unsuitable as input for neural networks. Any translation or rotation of the structure in space would represent a completely different data input to the neural network. Therefore, so-called descriptors are used to describe molecules and chemical structures. These are various mathematical operations and algorithms that are used to convert the atom coordinates into a form that is unique for
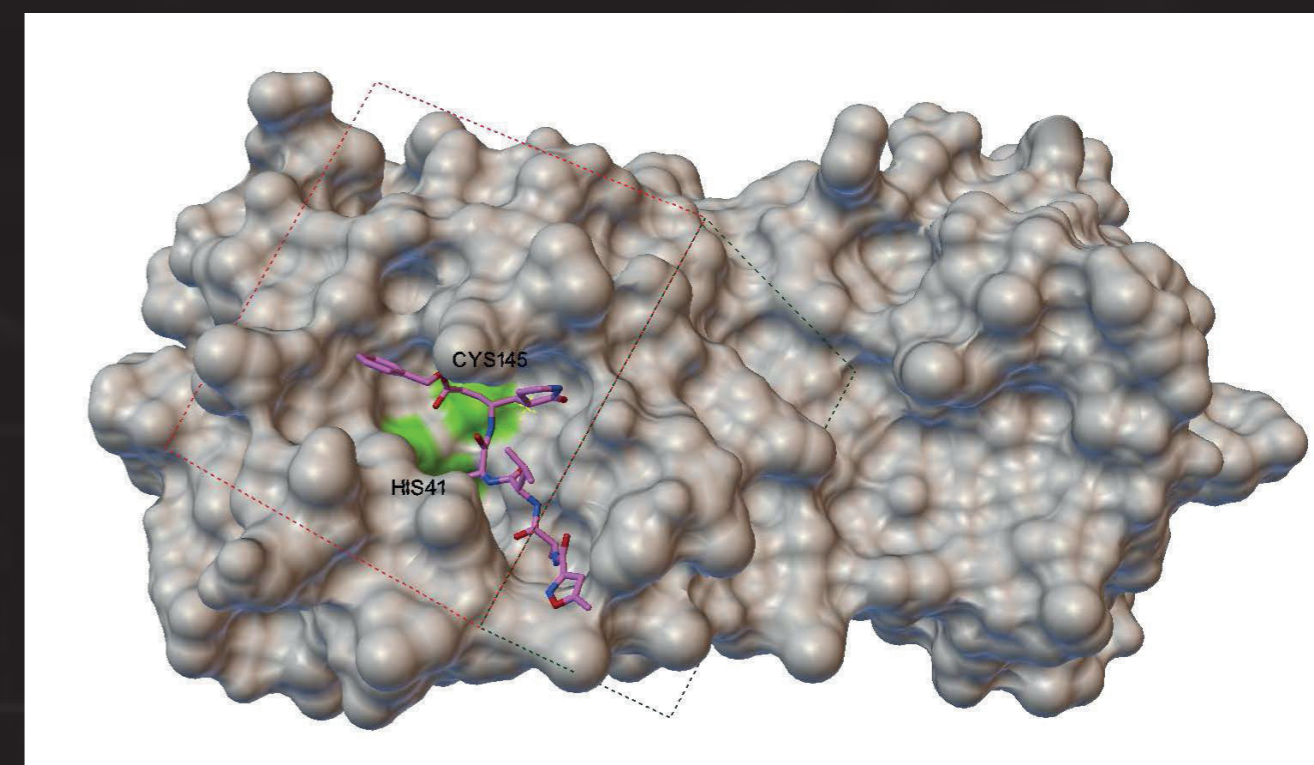
FIGURE 2

A scheme illustrating a search for suitable drug candidate; we know the structure of the protein produced by the virus with its active site and we have a database of structures of thousands of substances (PubChem). Using the docking score, we can determine the suitability of a given drug candidate.

the given structure (the so-called fingerprint) and translationally and rotationally invariant (remains unchanged upon translation and rotation of the given structure).

If we want to employ neural networks for prediction of physical and chemical properties, we need to have a large database (tens to thousands) of substance structures, on which the neural network will learn to predict the given property. This database is most commonly created using one of the quantum-chemical calculation methods. These methods provide precise tools for describing the properties of molecules and their reactions. The rapid development of HPC (High Performance Computing) has paved the way for chemists to employ the computational chemistry methods in their daily work, e.g., for understanding and predicting the molecular properties and reactions of the substances of the specific compounds, studying the properties of materials at the atomic level, and modelling reactions and processes taking place in biological systems. Unfortunately, these methods are often very computationally time-consuming (depending on the required accuracy), yet they are sufficient to create a database for neural network training. Neural networks are less computationally expensive than quantum chemistry methods while achieving comparable results.

In our project [1], we have tried to replace the computationally expensive "docking" of molecules into the cavity of the target protein by methods of machine learning and neural networks.

We have selected SARS-CoV-2 3CL^{pro}, which plays a key role in the replication of the SARS-CoV-2 virus, (PDB ID: 6WQF) as the target protein, see Fig. 3.

My colleagues Lukáš Bučinský and Marek Štekláč, from the Institute of Physical Chemistry and Chemical Physics of the FCHPT STU, have prepared a database containing approximately 10,000 substances for which they had calculated the docking score. The docking score, simply speaking, expresses the energy with which the given substance bonds to the relevant active site of the protein, thus inhibiting its catalytic ability. The lower (more negative) value of the docking score loosely corresponds to the stronger bonding of the given structure to the protein and therefore such substances represent suitable potential drug candidates.

Together with other colleagues, namely Ján Matúška from the Institute of Physical Chemistry and Chemical Physics FCHPT STU and Michal Pitoňák from the Department of Physical and Theoretical Chemistry, Faculty of Natural Sciences, Comenius University in Bratislava, we have applied three different machine learning approaches to provided database of substances: a neural network implemented by a widely available library TensorFlow in Python, SchNetPack neural network,

FIGURE 3

The investigated target protein SARS-CoV-2 3CL^{pro} (PDB ID: 6WQF) with an active site where an unknown substance is bound.

GRAPH 1

Correlation of the docking scores predicted by the neural network of the test sample of compounds on the values calculated by computational chemistry methods. Ideally, all the blue points would be on the black dashed line.
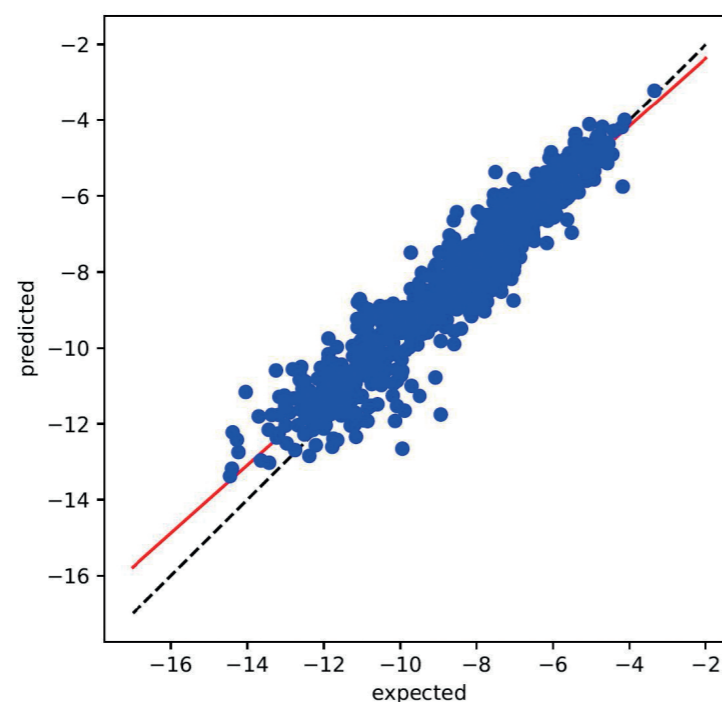

and XGBoost (gradient boosted decision trees) method, to predict the docking score. The success of the prediction ability of these methods on the test data sample can be seen in graph 1.

Followingly, we have applied the machine models trained in this way to the „in vivo" ZINC database containing 38,392 unique chemical substances and predicted their docking scores, see graph 2.

In this project, we have successfully demonstrated that it is possible to select suitable chemical structures, which can be further investigated as potential drug candidates for the viral disease COVID-19, from a database of thousands of substances relatively quickly and with sufficient accuracy.

A computing cluster at the Institute of Experimental Physics in Košice was used to train machine learning models [2].

As part of the European project PRACE, in which we are involved in the Computing Center of the Centre of Operations of the SAS, we also organize every year a two-month summer school for students from all over Europe called "Summer of HPC" (SoHPC). In addition to working on interesting projects, selected students gain their first experience with high-performance calculations on our computing systems. Even though this program has been online for the past two years due to the pandemic situation related
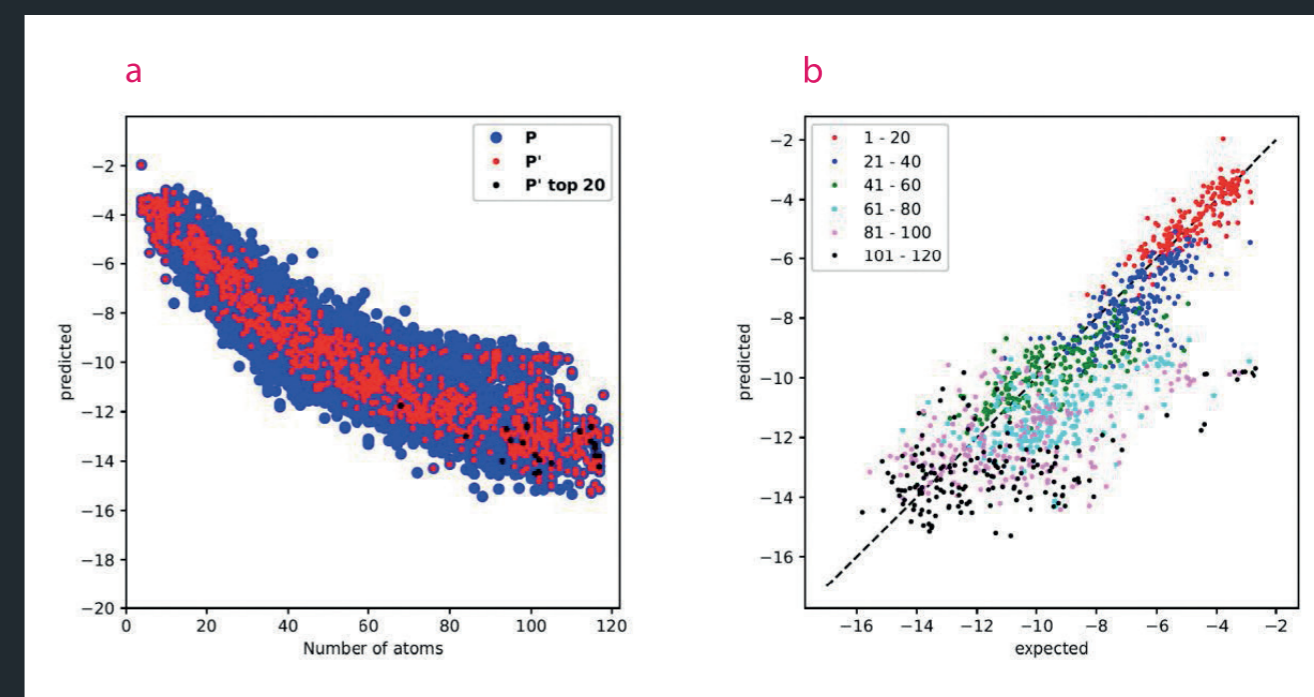
to COVID-19, we have been receiving very positive references from students. In the SoHPC 2021, Scott Le Roux, a student of applied mathematics at Trinity College, University of Dublin, joined this project and thanks to the acquired experience and inspiring collaboration decided to continue his studies and was accepted for a PhD position at the prestigious Oxford University:

"I wanted to let you know that I have accepted an offer to study in Oxford next year on the Autonomous Intelligent Machines and Systems PhD program. I would like to thank you for all your help with reference letters and supervision last summer which led me to pursuing this path. It definitely played a big role in developing my knowledge and skills and understanding where my interests lay."

Scott Le Roux

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GRAPH 2

(a) The prediction of the docking scores by the neural network on the production set of 38,392 compounds expressed as a function of the number of atoms (blue). The red points show structures for which the docking scores were also verified by computational chemistry methods. (b) The accuracy of the prediction with respect to the number of atoms shown in different colours.
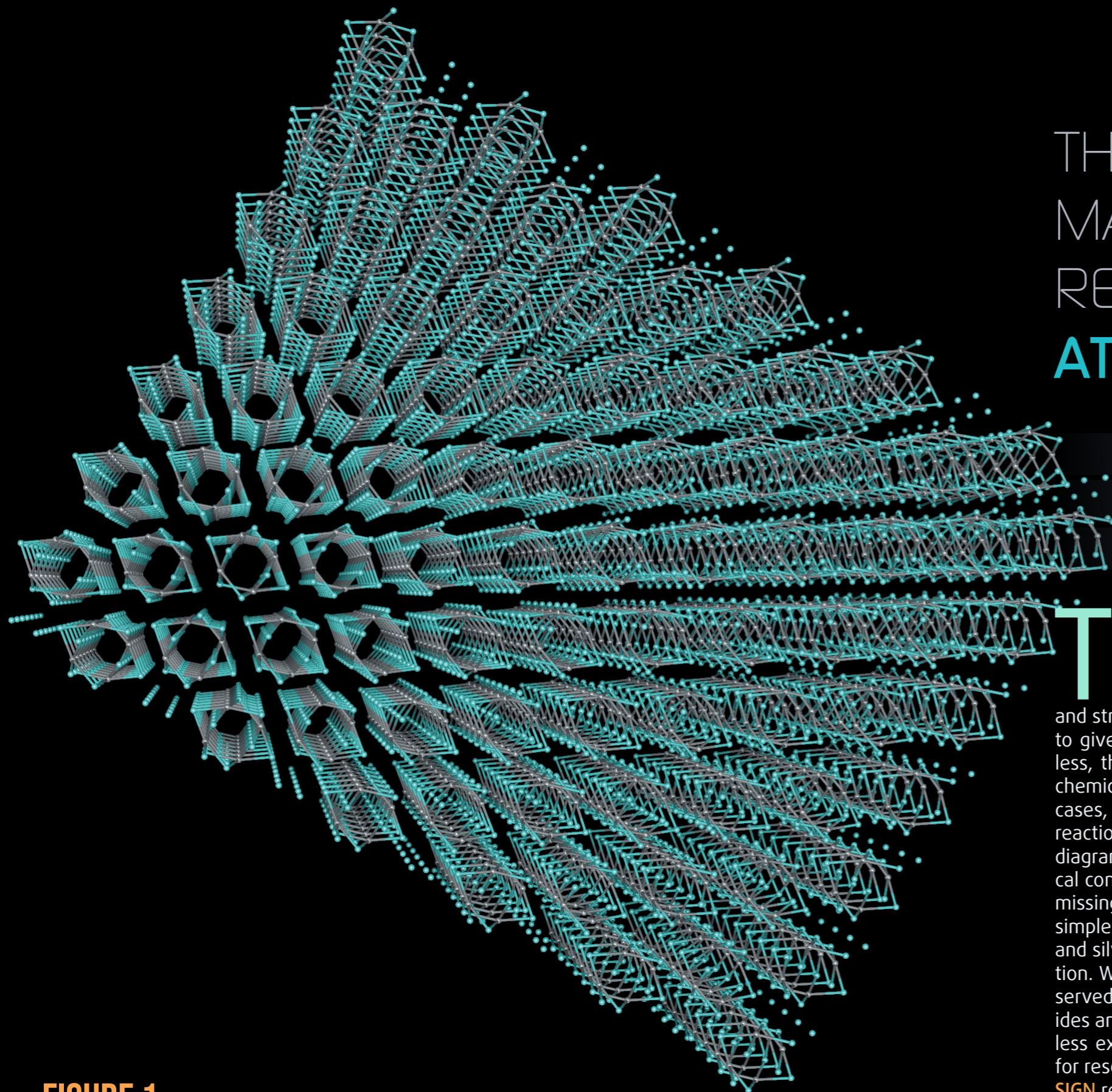
THE COMPUTATIONAL MATERIALS DESIGN RESEARCH GROUP at
ATRI MTF STU in TRNAVA

PREDICTION
OF NEW INORGANIC
COMPOUNDS

Today's research in the field of materials, whether inorganic organic or biological, is focused on more complex and exotic materials. In principle, chemists can synthesize compounds with almost any stoichiometry and structural complexity, and materials scientists know how to give them the desired form, structure or size. Nevertheless, there remains an unexplored area in relatively simple chemical compounds which are awaiting discovery. In many cases, this problem concerns common chemical bonds and reactions and related large unmapped places on the phase diagrams of already known and extremely important chemical connections. As an example there is the large number of missing transition metals oxides and halides. Among them, simple binary oxides and halides of nickel, palladium, copper and silver are of particular importance and require our attention. While numerous phases and rich polymorphism are observed in oxides and haldies of early transition elements, oxides and halides of late transition elements represent a much less explored territory. This territory creates the foundation for research program of the COMPUTATIONAL MATERIALS DESIGN research group.

The COMPUTATIONAL MATERIALS DESIGN research group was established recently in 2018 in Trnava at the Advanced Technology Research Institute, which is part of the Faculty of Materials Science and Technology of the Slovak University of Technology in Bratislava. Its founder is Dr. hab. Mariana Derzsi and together with Dr. Kamil Tokár they lead a young team consisting of undergraduate, graduate and PhD students and postdocs.

Within our research activities we focus on the problems of solid-state physics and crystal chemistry. Primarily, we specialize in the **modelling of inorganic crystalline compounds on an atomic scale with computers** using quantum-mechanical methods based on the Density Functional Theory (DFT) and Evolutionary Algorithms (EA). The main subject of our research is the prediction of new inorganic compounds with interesting properties and exploring their potential as new functionalized materials. On the path to new functional materials, transition metals are highly attractive basic building blocks thanks to their open d-shell orbitals (valence shell), which provides rich possibilities to play with electronic degrees of

FIGURE 1

Nanotube structure,
AgF_2 material.

The Computational Materials Design Research Group at MFT STU in Trnava was founded by Dr. hab. Mariana Derzsi (left). Together with Dr. Kamil Tokár (right) they lead a young team consisting of undergraduate, graduate, PhD. students and postdocs.

freedom in their compounds. Mutual interplay between the electron and lattice degrees of freedom leads to a diversity of crystalline structures and their physical properties. Our target materials are inorganic crystalline solids containing transition metals in the form of oxides and halides, where we are interested in lesser known or as yet unknown phases. In the late transition metals group we focus on nickel, copper, palladium and silver, because there exist a few documented simple oxide and halide phases, all of which are extensively used technologically. This also represents our further motivation to search for new transition-metal oxides and halides.

Predicting a new inorganic compound using computers starts from modelling its molecular structure and, in the case of a crystalline substance, its crystal structure, which is the positional arrangement of atoms in a crystal. Knowledge of crystal structure is key to calculating a wide spectra of physico-chemical properties, including thermodynamic stability, or conditions (temperature and pressure) at which the investigated material compound can exist. Therefore, our primary task is prediction of the crystal structure in the researched material.

We use advanced techniques to predict the crystal structures of new phases in systems with the required chemical stoichiometry. These methods are based on EA in conjunction with the quantum-mechanical DFT technique. First-principle EA modelling of new crystal structures exploits the processes of selection, mutation, crossing of individuals

and natural selection known in biology and genetics. This approach significantly and effectively reduces the selection of generated model structures from an unimaginably large number of possible complex connections that can be generated by 'brute force' according to random selection rules. This contributes to a significant reduction in the necessary large number of evaluated structures from tens of thousands to thousands. To optimize EA generated models of crystal structures and to calculate their ground-state energies, which are taken as the basic criteria for the selection process, and consequently to simulate the physico-chemical properties of already predicted crystal structures we use DFT methods. Our candidate models for crystal structures contain usually tens to hundreds of atoms. In practice, the quantum-mechanical calculations of such multi-atom models represent extremely complicated task of describing multiple-electron systems (thousands of electrons), in which electrons can interact not only with the ions creating the crystal lattice, but also with each other. The DFT method offers a significant simplification of this problem. Schematically it is based on the effective reduction of the multi-electron interacting problem to a single-electron one, where the electron itself moves in a kind of substitute effective potential formed by other electrons and ions. The relevant equations of quantum mechanics are thus considerably simplified and can be solved more easily by numerical algorithms, which to some extent decrease the duration of the calculation to acceptable time scales. The basic principles of this approach were proposed by Kohn and Sham back in 1965. Walter Kohn was awarded the Nobel Prize for his contribution to the development of this method only in 1998. The DFT method and its improvements (DFT+U, hybrid DFT, meta-GGA) thus play a key role and have long been the gold standard in quantum-mechanical modelling of crystal structures. The connection of DFT methods with evolutionary algorithms today is the most effective way of predicting crystal structures, and has been in practice for less than two decades. The implementation of evolutionary algorithms requires access to large-scale computing resources that are available to us in Slovakia thanks to the National Supercomputer Centre. A key person helping us with the implementation and application of EA for the prediction of crystal structures is **Dr. Oto Kohulák**, who has been involved with our group since 2019. For the needs of our research activities, Oto has developed several computing tools that serve to automate the calculational procedures and EA data analyses. He currently works at the International School for Advanced Studies (SISSA) in Italy, whilst continuing his collaboration with our group.

Dr. Oto Kohulák in our group deals with the hardware and software problems regarding implementation and applications of evolutionary algorithms (EA) for prediction of the crystal structures. For our research needs he developed a computing tools for automation of DFT+EA calculations and their data analyses.

Silver

Ag
47

Silver

The most investigated transition element by us thus far is silver. We are intensively engaged in the modelling of its compounds with fluorine and chlorine. Silver in conjunction with these halogens has the potential to create materials with exceptional properties, which may make them the multifunctional materials of the future. Recent discoveries in the field have convinced us about their importance, for example: a compound with anomalously strong magnetic interactions ($Ag^{2+}SO_4$) [1], potentially the first silver material of the multiferroic type, or a new unique form of nanotube (the different $Ag^{2+}F_2$ phases) [2,3]; what defines the uniqueness of these compounds is above all the presence of the specific silver cation Ag^{2+}. However, its occurrence in common inorganic compounds is very rare. The extremely strong oxidizing properties of this type of cation are responsible for its rarity as evidenced by the ability of Ag^{2+} to oxidize the inert xenon to Xe^{2+} cation. Finding an equal partner for such an aggressive electron-hungry species is very difficult and, moreover, a dangerous task for experimental chemists. In this regard, computer modelling represents a highly desirable alternative to such risky chemical experiments. The simplest ligands, which have the potential to be suitable partners for Ag^{2+} cation are fluorine and chlorine thanks to their high electronegativity. Therefore, our research regarding silver is concentrated on its fluoride and chloride compounds.

Silver with fluorine
A candidate for a new high-temperature superconductor

Materials based on silver and fluorine have great potential to become the precursors of a new family of highly desired high-temperature superconductors. A superconductor is a material that conducts electric current without resistance (and heat loss) when the temperature drops below a critical level. For most known superconductors the critical temperature is extremely low and very close to absolute zero (-273.15 °C), therefore, they are not suitable for practical use. An exception to this are ceramic materials based on copper and oxygen (so called oxocuprates) with critical temperatures close to the temperature of liquid nitrogen

FIGURE 2

Fragment of the crystal structure of layered oxocuprate La_2CuO_4 compared with the crystal structure of AgF_2. Both contain isoelectronic chess-board like layers $[CuO_2]^{2-}$ or $[AgF_2]$. While in oxocuprates these layers are ideally flat, in AgF_2 they are puckered.
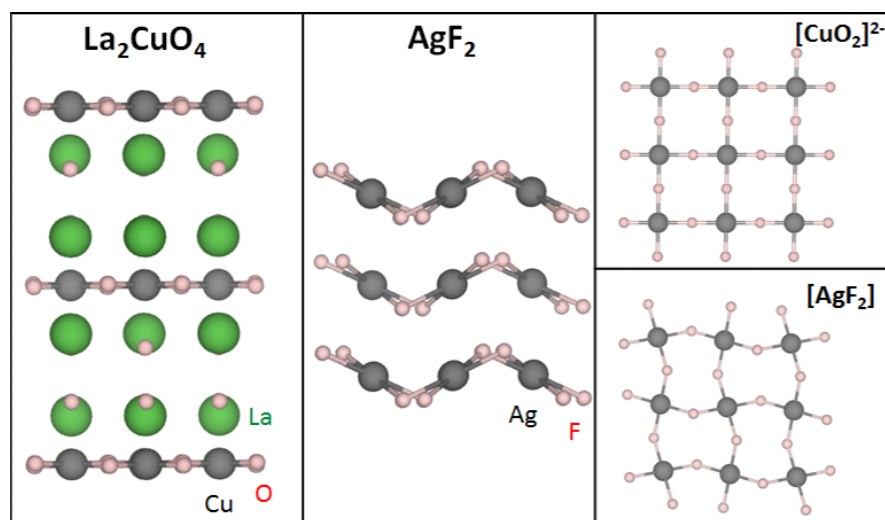
After [J. Gawraczyński, D. Kurzydłowski, W. Gadomski, Z. Mazej, T. Jaroń, A. Ozarowski, S. Hill, P. J. Leszczyński, K. Tokár, M. Derzsi, P. Barone, K. Wohlfeld, J. Lorenzana and W. Grochala, The silver route to cuprate analogs, PNAS, 116 (5) 1495-1500 (2019)].

La₂CuO₄   AgF₂   [CuO₂]²⁻   [AgF₂]
La   Ag   Cu   O   F

(-196 °C). Such temperatures are already technologically more accessible. In the world of known superconductors, such high critical temperatures are rare, so materials that exhibit them are called high-temperature superconductors.

Silver fluoride AgF₂, which we primarily study, shows many similarities with the oxocuprates and makes it an attractive candidate for the precursor of a new family of superconducting materials [4]. From the point of view of accessing superconductivity, the most important properties of oxocuprates are considered to be almost perfectly flat layers formed by copper and oxygen atoms, which together form a chess-board like motif in the structure with strong antiferromagnetic interactions between the copper atoms. More specifically, a so-called antiferromagnetic superexchange is mediated between coppers by an intermediate oxygen atom. In silver fluoride there exist analogous 'chess-board' layers with identical magnetic interactions (Ag²⁺ and F⁻ are isoelectronic with Cu²⁺ and O²⁻), but instead these sheets are puckered (Fig. 2). Whether and how these layers can be flattened is one of the key problems we have been working on for a long time with help of computer simulations. According to our previous DFT calculations, the flattening of these layers can lead to a significant strengthening of the magnetic interactions, which in turn implies a higher critical temperature at which AgF₂ could potentially be set in the superconducting state. We believe that the value of this critical temperature could be comparable or even higher than it is in the case of oxocuprates. In oxocuprates, the superconducting state can be induced either by some impurities (a small amount of another chemical element – doping)

and/or by changing the oxygen concentration in the material (by creating oxygen vacancies or adatoms). The purpose of these chemical modifications is to induce a small excess of electrons that the given chemical bonds can accept (we call this process electron doping), or, conversely, a slight lack of valence electrons shared by the bonds (hole doping). Besides the chemical route, such a situation can also be introduced via suitable modification of the external pressure and temperature (self-doping). Possible methods of AgF₂ doping represent the second main problem we are solving on the way to new superconducting materials based on silver and fluorine. In our simulations, we have

focused on several scenarios: (i) introduction of fluorine vacancies and adatoms (formation of $AgF_{2-\delta}$ or $AgF_{2+\delta}$), (ii) doping with electrons and holes without any chemical modification, (iii) substitution of silver atoms with another transition element (e.g. study of AgMF₄ ternary phases), (iv) exposure of AgF₂ to high external pressures, (v) the charge-transfer mechanism $Ag^{2+} \rightarrow Ag^{1+/3+}$.

We simulated the fluorine vacancies and adatoms by creating a model of the AgF₂ supercell, which contains 192 atoms (32 AgF₂ units). In this model, we gradually 'took out' and 'added' fluorine atoms. By removing fluorine atoms from the structure, we simulated the formation of $AgF_{2-\delta}$, which is an equivalent to electron doping of AgF₂. By supplying extra-fluorine atoms, we simulated the for-

FIGURE 3

A sample of AgF_2 stored in a protective case so that it could not react with air.

Credit: Laboratory of Technology of Novel Functional Materials, CeNT, University of Warsaw.

FIGURE 4

A fragment of an AgF_2 crystal with a simulated vacancy (left; removal of a fluorine atom) and a simulated adatom (right; addition of an extra fluorine atom). $AgF_{2-\delta}$ is formed by vacancy and $AgF_{2+\delta}$ is formed by adding the adatom

Legend: large balls – silver atoms, small balls – fluorine atoms.

vakancia

adatom

In this way, we can focus on the purely physical essence of the problem without involving chemistry (and the additional complications associated with it). Such strategy was considered in a 24-atom model (supercell with 8 AgF2 units). The model contains a total of 200 electrons. By adding or removing one electron, we simulated doping with electrons/holes with a concentration of 1/8 (a value typical in the case of oxocuprates).

mation of $AgF_{2+\delta}$ and thus hole doping. We took into account the doping concentrations δ = (1/8, 1/16 and 1/32), while the usual value of δ at which superconductivity state is achieved in oxocuprates is close to 1/8. Our simulations suggest that neither electron nor hole doping leads to the desired metallization of the AgF2 compound. The new electronic states that arise as result of doping become highly localized. In addition, the introduced defects (adatoms and vacancies) tend to cluster and lead to phase separation (structure breakdown). These results indicate that the method of chemical doping of AgF2 will be extremely difficult, if not impossible [5].

Whether chemical doping of AgF2 will be possible or not, we can simulate solely electron and hole doping even without knowing the chemical identity of the doped element. Instead of adding or removing a chemical element, we can simply add or remove electrons from our modelled system. In other words, we can define the total number of electrons in the crystal.

In this part of the study, we discovered that doping with both electrons and holes leads to another undesirable effect, namely the formation of polarons. A polaron is a quasiparticle that arises from the bound state of an electron (or hole) and a cloud of phonons (represented by collective vibrations in the crystal lattice). It is manifested by a deformation of the crystal lattice, which moves along with the electron (hole). The formation of polarons in AgF2 is undesirable because it is associated with charge localization and additional layer deformation, which is exactly the opposite effect of what we want to achieve. Polarons are absent only in the special hypothetical case, when the AgF2 layers are ideally flat (unlike in the natural material where they are puckered). The doping of flat AgF2 layers can thus lead to the desired metallization while, according to our calculations, the application of an AgF2 monolayer on a suitable substrate appears to be the ideal solution. Such a solution makes it possible to circumvent the problem of polaron formation even in the case of hole doping. These results underline the above-mentioned requirement of flat layers in AgF2 material as in oxocuprates [6].

One seemingly intuitive approach to flatten out puckered layers is to apply an external pressure to the structure. In the past, we spent a lot of effort studying AgF2 under high pressure. But this led us to a surprising result that was contrary to what we expected. Instead of flattening the crumpled layers, atoms rearranged into a tubular shaped substructures. Based on the theoretical model predicted by us, the crystal structure of the high-pressure form of AgF2 was successfully resolved from the crystallographic data obtained by X-ray diffraction. This way we unexpectedly discovered a new type of nanotube formed purely by silver and fluorine atoms (Fig. 1) [2,3]. We originally discovered a new crystal structure, that consisted of AgF2 nanotubes stacked side by side to form a hexagonal motif. Considering the exceptionality of the discovery, we then focused on the next theoretical study of the properties of one ‚freestanding' AgF2 nanotube. We found that, although we obtained this material under high pressure conditions, both forms (crystalline and free-standing AgF2 nanotube) behave as stable even at low pressures, i.e. under normal ‚laboratory conditions' [7,8].

Returning to the original plan to flatten and metallize the puckered AgF2 layers, we focused on the effects of substitution. We asked ourselves whether it would be possible to
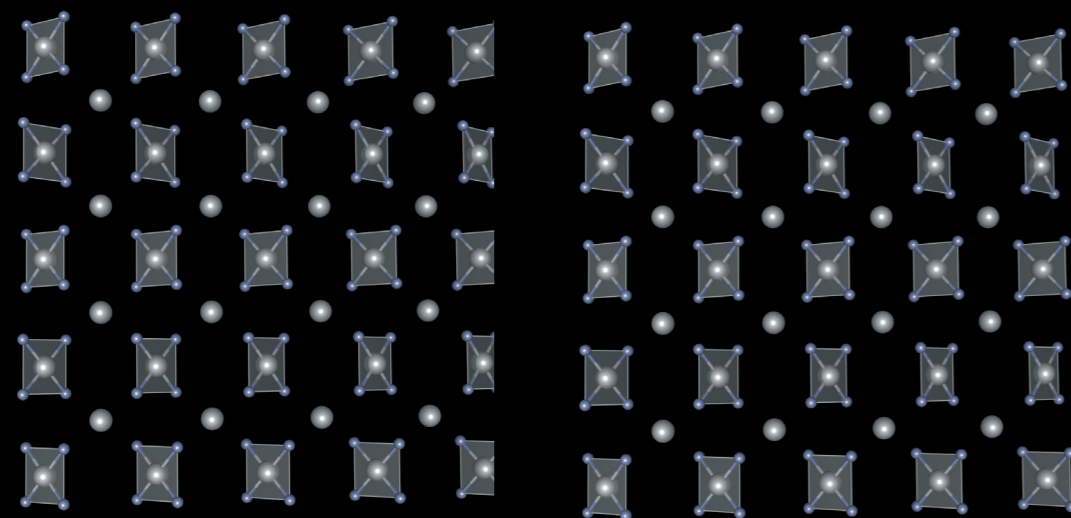
We have unexpectedly discovered a new type of nanotube based on silver and fluorine. Originally a new crystal structure consisted of AgF_2 nanotubes stacked side-by-side to form a hexagonal motif.

FIGURE 5

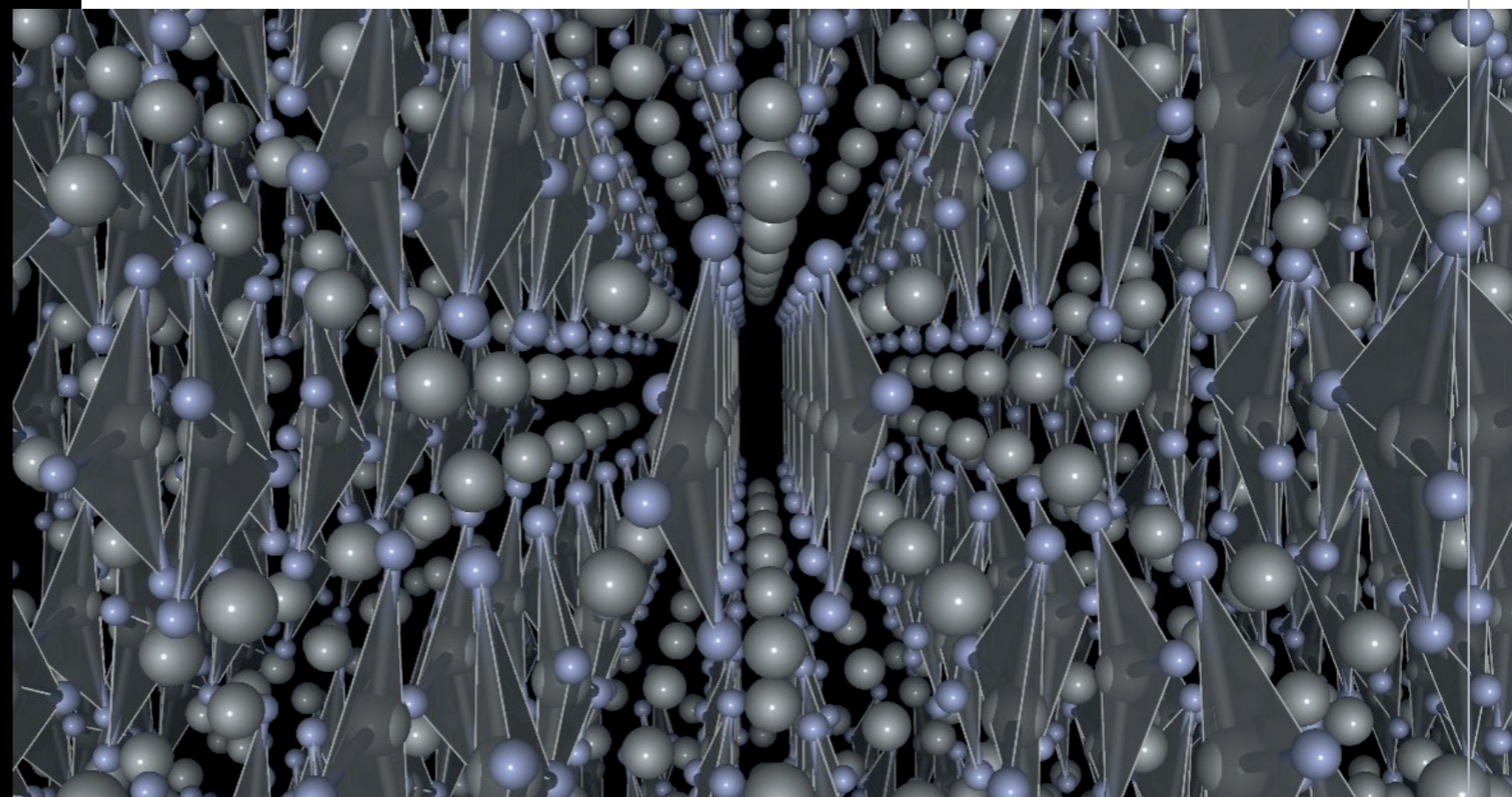Two polymorphs of crystalline silver fluoride AgF_2. On the left: a polymorph with an unbroken network of chemical Ag-F bonds (layered polymorph α). On the right: a polymorph with a broken network of chemical Ag-F bonds (polymorph β, CO AgF_2 phase $Ag^{1+}Ag^{3+}F_4$).

Legend: large balls – silver atoms, small balls – fluorine atoms.

The superconducting state in the oxocuprates often coexists or intermingles with another state characterized by electron charge rearrangement. As a result of this rearrangement, various so-called charge-ordering (CO) phases may be stabilized. It is not completely clear whether these phases compete with the superconducting state or instead support it. However, the scientific community is increasingly convinced that there exists a link between CO and superconductivity in oxocuprates. For this reason, we are interested in the potential of AgF_2 crystal to form CO phases and how the various charge-ordering mechanisms works in its system. One CO AgF_2 phase

replace half of the Ag^{II} silver cations with another M^{II} cation in the AgF_2 layers with the possibility of a partial transfer of electrons from M to Ag ion. By replacing the silver atoms with elements of another transition metal we moved towards the study of ternary compounds with $AgMF_4$ stoichiometry. To achieve this goal, it is necessary to carefully select such M^{II} cations whose electronic configuration would allow the formation of square coordination by ligands, so that the chessboard character of the layer may be preserved, the nature of the magnetic interactions in the layers would not change and that the given cations would be able to resist oxidation by the Ag^{2+} silver cation. For example, the Co^{2+}, Ni^{2+} and Cu^{2+} cations have such potential. Our further calculations indicated that, in order to achieve stabilization of the new ternal compounds $AgMF_4$ with M = (Co, Ni, Cu) elements, it is necessary to apply high pressure once more. Under low pressures (under normal conditions) these ternary compounds appear to be metastable with respect to their prototype binary precursors of AgF and MF_2 [9].

FIGURE 6

A fragment of the computer model of the Ag_3F_4 crystal, the formation of which we predicted under both low and high pressures up to 20,000 million pascals (~200,000 atmospheres).

Legend: large balls – silver atoms, small balls – fluorine atoms.

($Ag^{1+}Ag^{3+}F_4$) was indicated earlier. It was not possible to characterize this phase in more detail from the experimental data and therefore we focused on it in our computer simulations. We described its proposed crystal structure and compared its physical properties with those of the dominant layered AgF_2 phase [10]. Subsequently, in our latest study, we explained why the CO phase in AgF_2 has thus far been allusive and elucidated the nature of the CO mechanism in AgF_2 [11,12].

In addition to the AgF_2 compound, we also focused on the search for new binary phases of silver with fluorine in a wide range of pressures [13]. Among the other predicted interesting compounds, the silver tetrafluoride AgF_4 stands out. It is the only one among all known and predicted Ag-F phases to exhibit electrical conductivity (half-metal) and silver ions formally in the fourvalent (very exotic) state Ag^{4+}. The disadvantage of this fourvalent phase is that it stabilizes only under very high pressures far above 50 GPa. Among all Ag-F phases, both already known and predicted by us, ultimately AgF_2 remains the most important candidate for the precursor of a new high-temperature superconductor.
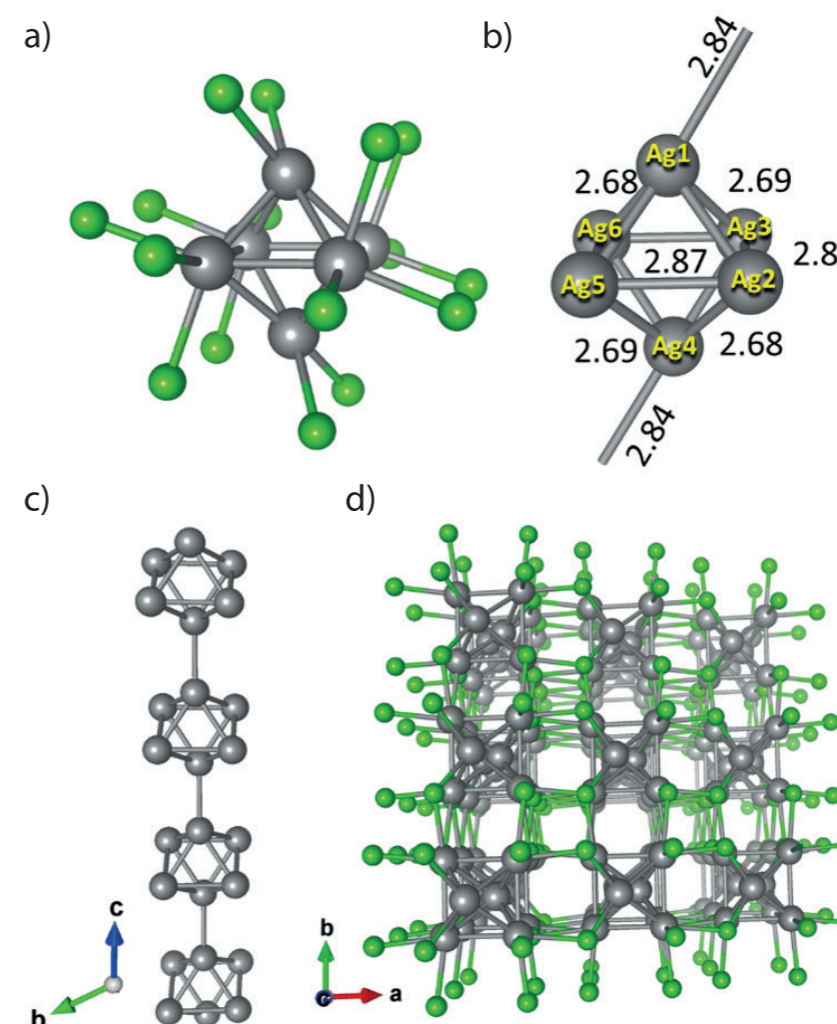
Silver with chlorine

As mentioned above, there is only one phase of silver with fluorine that has the required properties suitable for achieving the superconductivite state. Therefore, it is more than desirable to step beyond the known realm of fluorides. Chlorine is the second most electronegative chemical element after fluorine and, under suitable conditions, it should tolerate the presence of 'aggressive' silver cations such as Ag^{2+} or Ag^{3+}. That's why we decided to focus intensively on chlorine as an alternative to fluorine.

The only known phase of silver with chlorine is silver chloride AgCl. No silver chloride substance with Ag^{2+} or Ag^{3+} is known thus far. We know nothing about these materials. All we do know is that copper and gold, which together with silver belong to the common chemical group in the periodic table of elements, form such compounds. Silver chloride AgCl is a well-known crystalline solid that has been widely used for two centuries thanks to its photoactive properties and is still intensively researched as such. It can be prepared in variety of structural forms, morphologies and dimensionalities. Interestingly, no other crystalline phase of silver and chlorine is yet known. This is also surprising in view of the existing richness of stoichiometries in other transition metal chlorides, the most common of which are monochlorides together with di- to pentachlorides (MCl_n, n=1,2,3,4,5). Therefore, we decided to find an answer to the question of why we still have not found other phases of silver with chlorine. This requires extensive simulations of Ag_xCl_y models with varying content of silver and chlorine atoms from pure metallic silver (0% Cl) to molecular chlorine (100% Cl).

The first candidate we focused on was $AgCl_2$, as it represents a possible chloride variant of AgF_2, using our standard combination of EA+DFT methods. We concluded that the synthesis of $AgCl_2$ would require non-equilibrium thermodynamic approaches, while the desired layered structure, analogous to AgF_2, is not the most energetically favourable one [14]. At the same time, this initial study provided us very valuable information that significantly simplified our further effort in simulations. Our results showed that all stable structures of $AgCl_2$ can be derived from a simple cubic (fcc) lattice in which silver crystallizes with counterions in the interstitial sites. We have thus confirmed the common structural building principle observed across the

entire spectrum of known binary metal halides. In further simulations, we used this structural principle as a starting point for modelling a wide spectrum of Ag-Cl phases. Our investigated models are based on a basic cubic cell of silver into which Cl atoms are gradually added to the interstitial spaces. In this way, we could bypass much more demanding EA calculations for the part of the phase diagram consisting of subchlorides (with a predominant content/representation of chlorine atoms). Our ongoing study began to reveal the rich crystal chemistry possible in the binary Ag-Cl system including simple subchlorides, cluster compounds, ionic crystals and compounds with polychlorine anions. At the same time, it was revealed to what extent the silver chlorides with different Ag/Cl ratios follow the principle of close packing of atoms in the crystal lattice. This valuable information will serve us in the future to form the principles governing the crystal chemistry of silver chlorides. It is encouraging that the first experiments

a)   b)

c)   d)

FIGURE 7

The first predicted silver subchloride, Ag_6Cl_4. It consists of Ag6 clusters surrounded by chlorine atoms (a,b). Ag_6 clusters form infinite chains (c). A fragment of the crystal structure is shown in panel (d).

Taken with the permission of the authors from [M. Derzsi, M. Uhliar and K. Tokár. On the possible existence of the first $[Ag_6]^{4+}$ cation in a chloride environment. Chem. Commun. 57,10186-10189 (2021)].

Matej Uhliar worked in The Computational Materials Design Research Group in 2018-21. He devoted himself to computer DFT+EA modelling of silver chlorides as part of his Bachelor's and Master's theses and extracurricular activities.

MODELLING & EXPERIMENTATION

Together with Dr. Pavol Noga (left) and Prof. Martin Kusý (right), we are training a new generation of young materials researchers in a joint approach in the search for new functional materials, which combines computer modelling with experimental techniques.

of our partners from Poland, China and the USA, in the interpretation of which we took part, are beginning to confirm our predictions [15].

Another of the most remarkable results we achieved in the study of the binary Ag-Cl system was the prediction of silver subchloride Ag_6Cl_4 [16]. This yet experimentally unknown compound should possess exceptional properties. It contains very rare octahedral Ag_6 clusters with localized excess electrons. These Ag_6 clusters are arranged in the manner of infinite chains in which they interact with each other through argentophilic interactions. Argentophilic interactions describe attractive interactions between Ag^+ silver cations with formally closed d-shells.

In the case of silver, there exist additional mutual electrostatic interactions between the cations and, therefore, we would naturally expect them to repel each other rather than attract. Additionally, we discovered, that Ag_6Cl_4 behaves as a diamagnetic semiconductor with an unexpectedly wide energy band gap. This can be considered an unexpected finding since compounds, in which the presence of a metallic element predominates, behave in general as electrical conductors (their properties are close to metals). In inorganic chemistry such compounds are very rare. They are limited to only a small group of silver-containing suboxides (e.g. Ag5GeO4). No other inorganic material has

such a combination of physicochemical properties. This discovery has shown that silver can also achieve these properties in combination with halogen elements. We owe this discovery to Ing. Matej Uhliar, currently a PhD student at Faculty of Chemical and Food Technology STU in Bratislava, who devoted his work to computer modelling of new Ag-Cl phases as part of his Bachelor's [17] and Master's theses [18] and extracurricular activities [19, 20].

COMPUTER MODELLING & EXPERIMENTATION

Computer modelling on the atomic scale represents the most modern approach to the discovery of new materials. Therefore, the mission of our Computational Materials Design research group is not only to add to the research itself, but to also make sure that computer modelling becomes an integral part of the development of new materials at the Advanced Technologies Research Institute MTF STU. For this purpose, we are cooperating closely with the Department of Ion-Beam Technologies and the Institute of Materials MTF STU situated at our Institute and Faculty, respectively, where our colleagues are doing every effort to 'materialize' the materials predicted by us. Under the leadership of Ing. Pavol Noga, PhD., we are trying to synthesize the compounds theoretically predicted by us using the physical and physicochemical methods, such

as ion beam synthesis and reactive magnetron sputtering, also in combination with plasma supported ion implantation. The characterization of the experimentally synthesized materials is being carried out in cooperation with the Institute of Materials. The primary method for detecting the crystal structure is X-ray diffraction performed by prof. Martin Kusý. Together with appreciable collaboration with prof. Kusý and dr. Noga, we are training a new generation of young materials researchers in a joint approach to search for new functional materials that combines computer modelling and experimental techniques.

COMPUTING RESOURCES, COLLABORATIONS & OUTPUTS

Every single result we obtained and described in the above text represents the consumption of days, weeks and months of pure computing time. Our research would not be possible without a well-functioning and powerful supercomputing HPC infrastructure, as most of our simulation tasks would not be feasible. For parallelized DFT and EA calculations we use mainly the SIVVP infrastructure, particularly the Aurel supercomputer at SAV in Bratislava and the cluster located in Košice, as well as HPC infrastructures at international partner institutions. We closely collaborate with our international partners, in particular from the University of Warsaw, the Polish Academy of Sciences, the University of Buffalo, the Università di Roma "La Sa pienza", and the State University of New York at Buffalo. As part of these collaborations, we have hosted several foreign students, including master's, PhD students, and postdocs. The results we obtained during the study of the silver halides system thanks to the Slovak Supercomputer Infrastructure were the subject of six scientific publications [10, 11, 13, 14, 16], five contributions at international conferences [7, 8, 12, 19, 20], one Bachelor's thesis [17] and one diploma thesis [18].

Our research would not be possible without a well-functioning and powerful supercomputing HPC infrastructure, as most of our simulation tasks would not be feasible.

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Computer modelling on the atomics cale represents the state-of-the-art approach to the discovery of new materials.

MEMO98

MEMO 98 is an internationally recognized, independent organization specializing in media monitoring and research, especially during elections. MEMO 98 experts have participated in more than 120 election observation missions and some 150 projects and training sessions on media and elections in more than 60 countries (in the former Soviet Union as well as in the Balkans, Africa, Asia, South America, and the Middle East).

Slovak female politicians & journalists on social networks

Rasťo Kužel[1]
Ivan Godársky[1]
Michal Hollý[2]

[1] MEMO98
[2] Centre for Joint Activities of the SAS, v. v. i., Computing Centre of the SAS, National Competence Centre for HPC

The importance of social networks and their impact on society is great and growing. In addition to being a platform for connecting and keeping in touch between their users and their communities, they are also an important source of information. However, this information is difficult to verify and is often false – moreover, it is disseminated with the aim of influencing public opinion. Based on a report issued annually by Kepios Pte. Ltd., there were 4.91 million internet users in Slovakia in January 2022, representing about 90.0% of the total population. The same report states that there were 4.06 million social media users in Slovakia in the same period,

representing about 74.4% of the total population. Kepios also reports that the number of social media users in Slovakia will increase by 30,000 (+0.7%) between 2021 and 2022 [1].

Our project focused on monitoring Facebook, which is the most popular in Slovakia, specifically on the dissemination of information about female politicians and journalists, especially in connection with their professional activities. **The aim of our monitoring was also to evaluate the use of stereo-types and misinformation against women, whether in the context of anti-Western and anti-American sentiments or in the context of coordinated campaigns against prominent female politi-cians and journalists and to determine to what extent the attackers are linked to those who spread pro-Kremlin narratives.** The monitoring period was 12 months (3 May 2021 – 1 May 2022), and the criteria for selecting female politicians and journalists included the possession of a public Facebook account (public page or publicly accessible personal profile) and the number of followers (follow-ers). Out of the 11 subjects, we will focus on 2 Slovak female politicians (Zuzana Čaputová and Ve-ronika Remišová) and two female journalists (Monika Tódová and Zuzana Kovačič Hanzelová), and the comprehensive research will be available on the MEMO98 website [2].

In addition to being a platform for connecting and keeping in touch between their users and their communities, they are also an important source of information.

The CrowdTangle tool, which was used to collect the data, is a product of Meta (Facebook) devel-oped for the purpose of monitoring, creating statistical analyses, and evaluating the Facebook plat-form itself for optimizing or targeting products to social network users. Since CrowdTangle only monitors publicly accessible content and does not allow monitoring of private personal profiles or private groups, in our analysis, we focused on 11 public Facebook pages of selected entities and also on keyword searches within public pages and groups on Slovak Facebook.

To process the collected data, we developed a custom script in Python programming language to analyze it further. For computation, i.e. data processing together with visualization, we used the computational cluster at the Institute of Experimental Physics in Košice [3], which is managed by the Centre for Joint Activities of the Slovak Academy of Sciences, v. v. i. We used the open-source network mapping tool Gephi [4] to track the propagation of key-words within groups or pages.

The result is the so-called network map, which is an interactive schema that allows to search, clus-ter, and analyze the propagation of specific terms and web addresses. Thus, we were able to identi-fy the actors (Facebook groups, pages, accounts) that showed the highest number of interactions and shares of posts containing the keywords under study. In our case, the keywords were the names of the politicians and journalists under study.

Network graphs could also be used for identification:

- which accounts shared certain URLs most frequently;
- which URLs were most frequently shared between these accounts;
- which accounts shared content most frequently with each other (e.g. were grouped together).

On the network map, we can see nodes - circles and points that represent Facebook pages or groups, as well as their connections. Their size corresponds to the intensity of sharing (the larger the node, the higher the share rate of certain content) or to the en-gagement with the content (the larger the node, the higher the number of interactions with the respective post).

Edges are the lines that connect the nodes. In our case, edges are the connection between an entity and the URL it shared. The method used cannot determine whether the interactions were or-ganic or bot-generated.

ZUZANA ČAPUTOVÁ

Slovak President Zuzana Čaputová has become the target of attacks by several actors, ranging from political parties to disinformation portals with close ties to extremist parties. The most extensive media coverage, including on social net-works, was an incident on 1 March 2022, when at a public demonstration in Nitra organised by the SMER-SD party in connection with the May Day celebrations, the party's deputy chairman, Ľuboš Blaha, stirred up the crowd gathered there by chanting sexual insults against the president.

This incident was not a one-off event but rather the result of a long-term negative campaign by Blaha and other members of the SMER-SD party against the head of state. Both Blaha and Fico regu-larly insulted the president on their Facebook accounts (traitor, American agent, agent of a foreign power, or that she is controlled by the United States).

As in the past, a doctored photo of the president appeared on social media, accompanied by an anti-Semitic and anti-Amer-ican text in which a well-known extremist with close ties to the Republican Party mocked her for her physical appear-ance. From a list of pro-Kremlin actors compiled by Gerulata Technologies [5], she was targeted by the extra-parliamen-tary Slovak Renaissance Movement (SHO), which makes no secret of its sympathies for the fascist wartime Slovak state, its Eurosceptic orientation, and its demands for Slovakia's de-parture from Euro-Atlantic structures.

The monitoring also found that the president has been the target of attacks by the DAV DVA Facebook page and other media outlets known for spreading disinformation, including Inenoviny.sk, Information without Censorship, and others.

Zuzana Čaputová, nee. Strapáková is the fifth President of the Slovak Republic. On 6 May 2019, she received the European Personality of the Year award in Brussels.

Zdroj: TASR – Martin Baumann

IMAGE 1

Cutouts from the network map tracking the occurrence and spread of the keyword „Čaputová" on Slovak Facebook pages/groups (from May 3, 2021, to May 1, 2022) – clusters with a predominance of pro-Russian actors.

The size of the „node" (Page/group) corresponds to the number of interactions to posts in which the keyword (Čaputová) was used.

VERONIKA REMIŠOVÁ

Veronika Remišová, Deputy Prime Minister of the Slovak Republic and Minister of Investment, Regional Development, and Informatization presented herself as a strongly pro-European politician during the monitoring period with extremely active content on her own Facebook page. This profiling deepened and intensified after the Russian invasion of Ukraine – according to the results of the analysis War in Ukraine, conducted by MEMO 98, Veronika Remišová had the second highest number of posts (66) among Slovak parliamentary party presidents. Fifty-eight of them were about the war and its consequences, 46 of them were strongly supportive of Ukraine and the related domestic Slovak measures (the third highest number), while V. Remišová's posts were about the war and its consequences. Remišová did not publish a single post against Ukraine.

Such a strongly pro-European stance found its „echo" among pro-Russian actors – many of them focused on criticizing Veronika Remišová, especially Extra plus, I vote for Harabin, the Slovak-Russian Society, Eduard Chmelár, Slobodný vysielač, Nocomment.SK, and various websites of SHO and Róbert Švec. These groups have been linked to politicians Marián Kotleba and Ľuboš Blah. Other important actors in this direction were Hlavný denník, DAV DVA, Hlavné zprávy and Blog of Investigative Journalism.

Veronika Remišová, nee. Belošovičová is a Slovak politician, chairwoman of the political party FOR THE PEOPLE, Deputy Prime Minister of the Slovak Republic, and Minister of Investment, Regional Development and Informatization of the Slovak Republic.

IMAGE 2

A cutout from the network map tracking the occurrence and spread of the keyword „Remišová" on Slovak Facebook pages/groups (from 3 May 2021 to 1 May 2022) – clusters with a prevalence of pro-Russian actors.

The size of the „node" (page/group) illustrates the number of shares of posts in which the keyword (Remišová) was used.

Zdroj: bielavrana.sk

MONIKA TÓDOVÁ

Slovak women journalists have been the target of dehuman-izing, vulgar, and sexist attacks, especially from politicians who have been the subject of their investigative reporting. In particular, Denník N journalist Monika Tódová has repeat-edly been the target of sexist insults and attacks by politi-cians from the SMER-SD party. While covering topics related to corruption and the collusion of the previous government, she publicly admitted that she had received threats and hate messages, with her attackers wishing she would end up like Ján Kuciak, calling her Soroš's girlfriend or commenting on her physical appearance.

Monika Tódová, nee. Žemlová is a Slovak journalist, current editor of Denník N (since 2014), winner of the White Crow Award (2018), and several times winner of the Journalism Award (2008-2021).

Zdroj: SME – Marko Erd

In the monitored period, it became the target of attacks ma-inly by Ľuboš Blaha, Milan Uhrík, Eduard Chmelár, Martin Daň, and his portal Ginn and others.
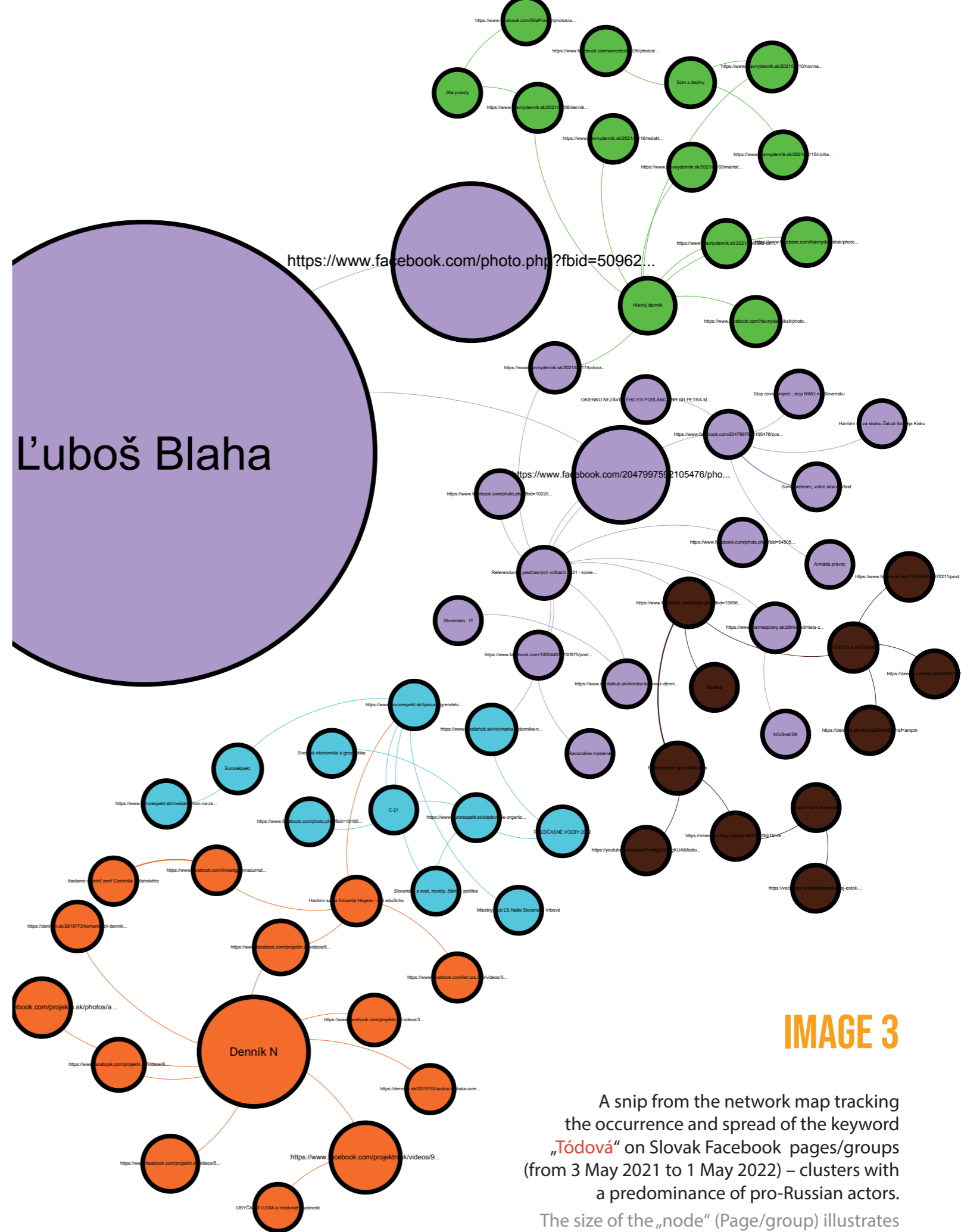

IMAGE 3

A snip from the network map tracking the occurrence and spread of the keyword „Tódová" on Slovak Facebook pages/groups (from 3 May 2021 to 1 May 2022) – clusters with a predominance of pro-Russian actors.

The size of the „node" (Page/group) illustrates the number of interactions for posts in which the keyword (Tódová) was used.

Zuzana Kovačič Hanzelová was born on 2 July 1988 in Bratislava. She studied journalism at the University of Constantine the Philosopher in Nitra. She mainly works on politics, poverty, and sexual harassment. She is a laureate of the Journalism Award (2021).
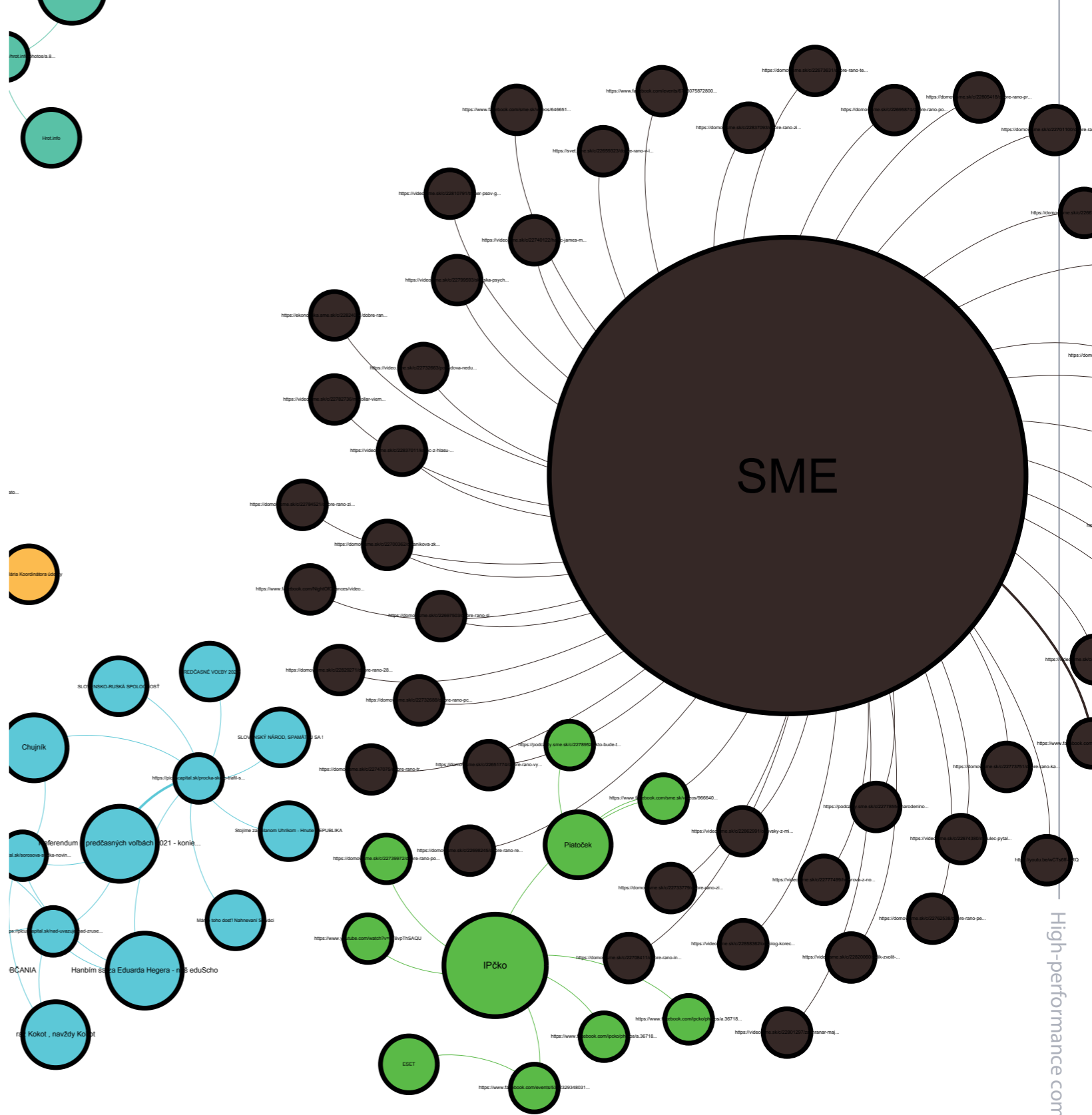
ZUZANA KOVAČIČ HANZELOVÁ

Another prominent journalist, Zuzana Kovačič Hanzelová, complained about receiving similar messages, which forced her to stop using her Facebook account on 17 December 2021 (she continues to use her Instagram account). In her farewell post, she pointed to several disturbing tendencies that were the main reasons for her decision, including trolling by pro-Kremlin actors.

The results of our monitoring indicate that during the monitoring period, various actors, ranging from the media, political parties, and personalities to cultural centers and civic initiatives, commented on Zuzana Kovačič Hanzel's Facebook page. At the same time, anti-system actors also got involved, although mostly in a rather fragmented way (Hlavný denník, Artur Bekmatov, Zdroj, hlavnespravy.sk, Kulturblog portal, Extra Plus, Slovanské Noviny, Anna Belousovová, the Office of the Coordinator of the Strike). Perhaps the only exception was the grouping of citizens and groups driven by disagreement with the current political establishment and its main protagonists. The map shows that this cluster also includes various pro-Kremlin entities, such as Picuscapital. sk, Slovak-Russian Society, I am a patriot, I vote for the Vlasť party, We stand for Milan Uhríko – REPUBLIKA Movement.

IMAGE 4

A snip from the network map tracking the occurrence and spread of the keyword „Kovačič Hanzelová" on Slovak Facebook pages/groups (from 3 May 2021 to 1 May 2022) – clusters with a prevalence of pro-Russian actors.

The size of the „node" (page/cluster) illustrates the number of shares of posts in which the keyword (Kovačič Hanzelová) was used.

FINDINGS

The fact that pro-Kremlin propaganda is operating in Slovakia was admitted by state institutions as early as 2016 when the Ministry of the Interior officially stated that „Slovakia, like other Central and Eastern European countries, has become the subject of information influence by the influence structures of the Russian Federation." The newly adopted Security Strategy 2021 further states that ‚harmful strategic propaganda, including disinformation activities, has the potential to polarize society,

subvert the political system, undermine the trust and will of citizens to defend the democratic and the rule of law state and call into question the importance of the Slovak Republic's membership of NATO and the EU.'

The identified actors spreading disinformation have been active on the Slovak internet and social networks for several years, spreading a nationalist, pro-Russian, and anti-immigration view of the world, opposing the EU/NATO/USA, and often supporting a right-wing, nationalist agenda. They have supported the far-right Kotleba party – the People's Party Our Slovakia (SNS), the Republika movement (formed from defectors from the SNS), as well as the Slovak Revival Movement.

However, their activities against female politicians and journalists have not yet been more systematically investigated. We used a list of pro-Kremlin actors compiled by Gerulata Technologies [5] and compared it with findings from our media monitoring. We found that of the 14 actors on this list who have a Facebook page and are identified in the three main threat categories, 13 actors in our findings were involved in

negative campaigns against the female politicians and journalists we studied.

The 13 identified actors of disinformation can be divided into two main categories – 7 political actors (politicians or parties, whether current or former) and six disinformation portals.

Of the seven politicians or parties, the most visible on Facebook was the deputy chair of the SMER-SD party, Ľuboš Blaha, who had a huge number of followers until 14 June, when Meta shut down his public page for repeatedly violating community standards. Among the active disseminators of pro-Kremlin propaganda on our list is also Tomáš Taraba, a non-attached MP who ran on the candi-date list of the fascist party Kotleba – People's Party Our Slovakia for the 2020 parliamentary elec-tions, Milan Uhrík from Republika (formerly Kotleba's People's Party Our Slovakia), Róbert Švec (chairman of the nationalist Slovak Revival Movement), university teacher and former politician Eduard Chmelár, and Štefan Harabin, former chairman of the Supreme Court of the Slovak Republic and Minister of Justice (in Robert Fico's government).

As for the other actors on the list, there are also Slobodný vysielac, DAV DVA, Hlavné zprávy, No-comment.sk, Blog of Investigative Journalism and Hlavný denník.

Tackling misinformation is extremely challenging and requires a comprehensive approach at multiple levels, from education and promoting critical thinking to monitoring and regulating content on the internet. Especially after the start of the Rus-

sian aggression in Ukraine, a number of countries, including Slovakia, started blocking disinformation sites. The National Security Office (NSA) has this power under Act No. 69/2018 Coll. on Cyber Security until 30 September 2022. Until recently, four sites were blocked – Main News, Army Magazine, Main Daily, and Infovojna.

At the same time, the NSA has submitted for comment an amendment to the aforementioned law on cyber security, which, if approved, would introduce better rules for blocking websites. The proposal for blocking would come from an authorized law enforcement entity (not the NSA itself) and would further be subject to court approval. It would take effect during the autumn of 2022.

Gerulata Technologies
Top Pro-Russian Sources in Slovakia

gerulata

Gerulata Node ID	Title	Type	Activity Category	Impact Category	Influence Category	Threat Category
3345509527	Ľuboš Blaha	Facebook Page	medium	catastrophic	extreme	catastrophic
9621918752	Slobodný vysielač	Facebook Page	high	high	extreme	catastrophic
2722275368	Veľvyslanectvo Ruska na Slovensku/ Посольство России в Словакии	Facebook Page	extreme	medium	extreme	extreme
8799273843	Extraplus (extraplus.sk)	Web	extreme	n/a	extreme	extreme
4952167164	Tomáš Taraba - predseda ŽIVOT NS	Facebook Page	medium	extreme	high	extreme
911785421	DAV DVA	Facebook Page	extreme	high	medium	extreme
9357350490	Hlavné Správy	Facebook Page	high	medium	high	extreme
3390562675	nocomment.sk	Facebook Page	medium	high	high	extreme
8515467263	Hlavný denník (hlavnydennik.sk)	Web	high	n/a	high	extreme
6955415866	Slovenské Hnutie Obrody	Facebook Page	medium	medium	extreme	high
8766189209	Milan Uhrík • Republika	Facebook Page	low	extreme	extreme	high
7558265631	Blog investigatívnej žurnalistiky	Facebook Page	extreme	medium	medium	high
6256802347	Hlavné správy (hlavnespravy.sk)	Web	extreme	n/a	medium	high
4587968579	Hlavný denník	Facebook Page	catastrophic	high	low	high
3559939781	Eduard Chmelár	Facebook Page	low	high	extreme	high
7492753507	Štefan Harabin	Facebook Page	low	high	extreme	high
2213788472	Róbert Švec • Slovenské Hnutie Obrody	Facebook Page	medium	medium	high	high
9140108057	MAGAZÍN 1 (magazin1.sk)	Web	medium	n/a	high	high

Source: https://www.gerulata.com/docs/gerulata_top_pro_russian_sources.pdf

REFERENCIE

[1] https://datareportal.com/reports/digital-2022-slovakia

[2] https://memo98.sk/

[3] The calculations were performed using the computing infrastructure of the SIVVP - Slovak Infrastructure for High-Performance Computing project, ITMS project 26230120002 and 26210120002, which was supported under the ERDF-funded Operational Programme Science and Research.

[4] Bastian M., Heymann S., Jacomy M. (2009). *Gephi: an open source software for exploring and manipulating networks.* International AAAI Conference on Weblogs and Social Media.

[5] https://blog.gerulata.com/russian-propaganda-network-in-slovakia/, https://www.gerulata.com/docs/gerulata_top_pro_russian_sources.pdf

HPC
Popularization

EuroCC
International
Collaboration

Twinning Slovakia
— Czech Republic

National competence centers for HPC from the Czech Republic and Slovakia organized two twinning events during the spring months.

We met with the representatives of the CESNET association (M. Ruda, D. Antoš) and IT4I (B. Jansík, T. Karásek) on April 19, 2022 at Smolenice castle in Slovakia with the goal of exchanging best practices in the field of providing cloud services to users from academia and also industry.

The second workshop was aimed at the so-called engineering applications, e. g. complex fluid dynamics, turbulence, heat transfer, acoustics and mechanics. The workshop was also attended by representatives from private companies. A short introduction of the National Competence Centre and the EuroCC project was therefore a part of the program as well as HPC capacities and services access in Slovakia and Europe. We debated successful collaborations with SMEs in the area of engineering applications with T. Karásek a T. Brzobohatý.

Twinning Slovakia
— Slovenia

Slovak National Competence Centre for HPC started a collaboration with the Slovenian Competence Centre in the area of education. The partnership started with an online workshop, where both competence centers introduced their activities, especially concerning trainings. They followed it up by organizing joint online courses for participants from both countries, which will continue in the fall of 2022. You can find more information at our website.

Short
News

EuroCC 2
– the Competence Centre Continues

The EuroCC 2 project, which oversees the activities of the Competence Centre for HPC, will start in January 2023. Its hosting institution in Slovakia will be the newly established National Supercomputing Centre. In the next three years the project will focus especially on the development of the competences and services in the area of high-performance computing and support for small and medium enterprises, academia and public sector through cooperation and solutions based on HPC technologies.

TREX CoE Quantum Monte Carlo
Summer School

TREX Centre of Excellence in HPC for Quantum Chemistry in cooperation with the SAS Institute of Physics and the National Competence center for HPC organized a workshop on Quantum Monte Carlo methods (QMC).

The workshop took place in-person in Slovakia at the manor house Mojmirovce and the participants had a chance to gain a complex theoretical overview as well as practical experiences with the Quantum Monte Carlo methods and their application to molecular (Quantum Package and CHAMP) and periodic systems (TurboRVB). The lectures were given by world-class experts from the TREX Center of Excellence.
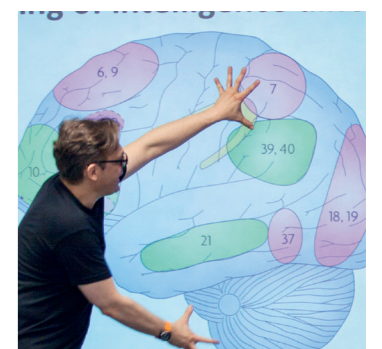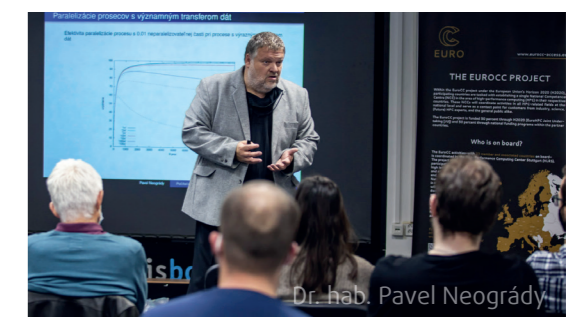
HPC Promotional Talks
– Come Learn More

During the last academic term NCC for HPC organized promotional talks on various subjects concerning high performance computing. You can view the recordings of various interesting talks on artificial intelligence and its deployment in our video archive. We plan to provide talks on the topic of quantum technologies from a number of Slovak experts during the next semester – follow our webpage and social media!

Dr. Andrej Lúčny

Prof. Ivan Štich

Dr. hab. Pavel Neogrády

Prof. Ivan Sekaj

Dr. Jozef Vivoda

Dr. Tomáš Hromádka

eurocc.nscc.sk

hpc focus

2022