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IN MEMORIAM: ALEXANDER IVANOVSKII, INNOVATIVE RESEARCHER AND SCIENCE MANAGER IN COMPUTATIONAL MATERIALS SCIENCE OF ADVANCED INORGANIC MATERIALS

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The paper is written to pay a tribute to Prof. Alexander Leonidovich Ivanovskii, Head of the Quantum Chemistry and Spectroscopy Laboratory at the Institute of Solid State Chemistry, Ural Branch of the Russian Academy of Sciences (RAS), and is devoted to recalling the most significant landmarks in his scientific career. A broad-minded man of great erudition, A. L. Ivanovskii made invaluable contributions in the field of computational materials science — a new field of research covering computational modeling for properties of existing substances and for compounds yet to be synthesized, including nanostructured materials. Under his leadership, a group of young, talented researchers have grown to become specialists in the electronic structure simulation and computational modeling to predict the properties of solids, which formed a unique school of thought in the field of quantum chemistry and spectroscopy research in the Urals.

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A well-bred intellectual, a man of noble principles and genuine culture, always pursuing an initiative, living positively with venture and verve — these are the attributes by which a leading scientist Alexander Leonidovich Ivanovskii will always be commemorated by his colleagues and friends.

A. L. Ivanovskii passed away on February 28, 2014, in his 62nd year of life, thus ending a remarkable career filled with scientific accomplishments: Doctor of Chemistry, Professor, Honored Scientist of the Russian Federation, National Prize Winner in Science and Engineering, and a remarkably creative leader of the Laboratory of Quantum Chemistry and Spectroscopy at the Institute of Solid State Chemistry, Ural Branch of the Russian Academy of Sciences. The scientific activity after Alexander Ivanovskii and his school of thought cover a broad spectrum of issues [1-20]: advanced solid solutions, alloys and intermetallic compounds, superconductors and superconducting magnets, antiperovskite-structured compounds, MAX phases, refractory interstitial phases, nanomaterials, just to mention a few. A. L. Ivanovskii has authored and co-authored more than 860 papers published in national

Fig. 1. Alexander Leonidovich Ivanovskii

and international science journals; he is the author of 14 monographs and more than 20 reviews on the scientific issues related to computational materials research in inorganic chemistry. The scientific accomplishments earned him wide respect in the scientific community, of which over six thousands of citations to his works is a convincing proof.

Over fifteen years, Alexander Ivanovskii gave lectures on the structure of matter to students at the Ural Federal University. Many of the students trained by Alexander can now be found in laboratories actively involved in quantum chemical modeling research.

Alexander Leonidovich Ivanovskii was born in Sverdlovsk on February 2, 1953. In 1976, he graduated from the Physical Engineering Department of the Ural Polytechnical Institute (currently, Ural Federal University named after B.N. Yeltsyn), and early upon graduation, he joined a group of researchers headed by Prof. V. A. Gubanov and by Academician-to-be, Prof. G. P. Shveikin at the Lab of Physical Methods of Investigations of Solids at the Chemistry Institute, Ural Branch of RAS. Starting from those days and over his entire career to the end of his days, one of the most significant directions of his research was devoted to refractory compounds and interstitial phases. In 1980, Alexander Ivanovskii received his Candidate of Science degree; and in 1988, at the age of 35, he earned his Doctor of Science degree, having defended his thesis titled "Electronic Structure and Chemical Bond in Refractory Compounds of $d-$Elements of IVA, VA Subgroups". In 1994, he was elected a corresponding-member of the Natural Science Academy and was appointed Head of the Quantum Chemistry and Spectroscopy Laboratory at the Institute of Solid State Chemistry, Russian Academy of Sciences. In 1995, Alexander Ivanovskii received the Russian Federation State Prize for a series of works "Quantum-Chemical and Radio-Frequency Spectroscopy Methods for Solid Chemistry Applications".

Contemporary solid state research is striking in its variety, bringing to the forefront such systems and objects as micro and nano-porous solids, low-dimensional crystals, nanosized and nano-structured objects. Nanomaterials came to be one of the topics most favored by Prof. Ivanovskii: a giant leap was made by him and his team in understanding the field of nanostructure design for both existing materials as well as newly synthesized substances, in studying their stability and investigating their physical and chemical properties, using a great diversity of computational techniques. The breadth of his research interests encompassed a great number of nanostructures: diversified forms of carbon allotropy (diamond-like modifications, nanotubes, fullerenes, graphene and its analogs) and various inorganic nanomaterials, such as nanofibers, nanotubes and fullerene-like particles of boron nitrides, carbides, borides, silicides, oxides, halogenides and chalcogenides. Prof. Ivanovskii had an in-depth and critical view of these science developments in the world, which was reflected in the number of his reviews published in international journals and monographs, with some of the publications having pioneered in this field of materials research on the national scale. The following results deserve special notice.

A. L. Ivanovskii became interested in nano-objects in the 1990's, when a surge of interest was generated by the experimental evidence for a new class of nanostructured titanium carbides, observed in gaseous phase as ultrasmall cubic 27-atom clusters. Nanosized titanium carbide clusters were found to transform into nonstoichiometric dodecahedral clusters, referred to as metalocarbohedrenes Ti_8C_{12} (or metcars for short). Combining his many years' experience of studying the chemical bonding of binary carbide systems with the then-available software and hardware capabilities made these nanoclusters an apt research endeavor. Along with his research group, he issued several fundamental publications related to the stability and reactivity of nano-systems. Furthermore, this direction of research evolved towards the computational design and study of structures, both theoretical and experimentally observed, and towards studying compounds plotted on a metal-carbon phase diagram: endohedral complexes of carbon and boron-nitrogen nanotubes with metcars, endofullerenes with d- and f-element atoms, and nanopeapods based thereon [1,2,3].

While studying metalocarbohedrenes, which, in fact, were regarded as heteroatomic analogs to ultra-small carbon fullerenes, Alexander Ivanovskii could not but get involved in studying other, then-new low-dimensional nanostructures, such as fullerenes and carbon nanotubes. He wrote a review and was the first Russian author to have written a monograph on the state-of-the-art production, characterization and modeling of carbon nanostructures [4]. Alexander Ivanovskii's enthusiasm and research interest was stimulating his team in pursuing the modeling of these low-dimensional objects and structurally related nanotubes based on hexagonal boron nitride and magnesium boride. Later, that triggered explosive growth of inventive research projects looking for new compounds as candidates for making hollow nanostructures. Under Ivanovskii's leadership, atomistic models were proposed and, for the first time in Russia and even in the world, quantum chemical computations were performed for the properties of inorganic nanotubes based on the oxides of titanium, vanadium, magnesium, on poly(titanic) acids, aluminum hydroxides, sulfides and selenides of molybdenum, niobium and zirconium. These computational results, along with the analysis of experimental data worldwide, were summarized by his team in a series of unique reviews and books, which were the first publications on this kind of research in the national scientific literature [5,6,7]. Along with inorganic nanotubular systems, hollow polyhedral nanoparticles — layered chalcogenides and halogenides-based inorganic fullerenes — were also of special interest to A. L. Ivanovskii. Their structure must have differed significantly from the carbon fullerene structure. Under Ivanovskii's leadership, the laboratory researchers were the first in the world to have performed quantum chemical computations of electronic and magnetic properties for some of these structures [8].

FIG. 2. Young scientists in the group of quantum chemistry in 1980: in the first row from left to right (sitting): Andrei Postnikov (now – Professor, Université de Lorraine Laboratoire de Chimie et Physique-Approche Multi-Echelles des Milieux Complexes, Metz, France;) and Alexander Ivanovskii (from 1994 to 2014 – Head of Laboratory of Quantum Chemistry and Spectroscopy, Institute of Solid State Chemistry, Ekaterinburg); in the second row from left to right: Alexander Lichtenstein (now – Professor, Institute of Theoretical Physics University of Hamburg; Germany, Max-Born-Preis, 2014), Sergei Freidman (now – Head of Software Department, Vidisco Ltd, Israel) and Michail Ryzhkov (now – Leading researcher, Institute of Solid State Chemistry, Ekaterinburg)

It is worth noting that early into this research, the experience gained by Ivanovskii and his laboratory had already drawn great attention from scientists abroad, involving both theoretical and applied aspects of materials science. That opened up an opportunity to establish fruitful and enduring collaboration between the Quantum Chemistry and Spectroscopy Laboratory and the Theoretical Chemistry Group headed by Prof. G. Seifert at TU Dresden, Germany, and the Materials Synthesis Group headed by Prof. R. Tenne, Weizmann Institute of Science, Israel. Numerous collaborative projects performed by Ivanovskii's lab jointly with these two research groups resulted not only in atomistic models being developed for carbon fibers, nano-diamonds, nanotubes and nanoparticles of layered chalcogenides, exo- and endohedral molecular complexes of carbon nanotubes, but also in the mechanisms underlying their formation having been verifiably established, in the correlation to have been proposed between their structure and thermodynamic stability, strength characteristics, electronic and magnetic properties.

As early as the beginning of 2000's, being completely immersed in his studies on carbon nanotubes and fullerenes, Alexander Ivanovskii was also making research efforts towards the design of new allotropes of carbon and boron nitride. He was very keen on sp^2- and sp-hybridized atom-based nanostructures, which could form layers. He was also eager to study the structures designed from sp^3-hybridized atoms, which tended to form "monolithic" diamond-like modifications. The former nanostructures, in his opinion, could demonstrate a set of nontrivial electronic properties that could be modified using chemi- or physisorption [9]. The latter family of compounds, however, showed promise as superhard refractory materials that could compete with transition metal carbides and nitrides [10]. Long before the graphene boom, following the world trends in the field of computational design, Alexander Ivanovskii and his colleagues had studied a great number of potential allotropic modifications of carbon and boron nitrides and carbonitrides, including layered graphene-like materials: graphynes, graphdiynes, nanotubes and fullerenes based thereon, icosahedral nanodiamonds and diamond nanofibers, having pioneered in the design of so-called interpenetrated fullerite structures.

Even with the strong competition in the field of computational materials science relating to carbon materials, Alexander Ivanovskii maintained warm relations with several researchers, which was, for example, reflected in collaborative projects with Prof. E.A. Belenkov from Chelyabinsk State University and with Prof. V.V. Porkropivny from the Institute for Problems in Materials Science, National Academy of Sciences, Ukraine [11, 12]. Ironically, despite being performed at a world class level of research excellence in this field, Alexander Ivanovskii's series of early papers had met some skepticism from his scientific opponents, who had labeled this kind of basic studies as "nano-centaurs research". However, the discovery of grapheme, and the technology boom that followed, gave an extra impetus to the research by Prof. Ivanovskii and his group in the field of modeling layered carbon and inorganic analogs of grapheme, graphene-based and graphene-like materials. [13,14]. In a wondrous fashion, the topic of his most recent review overlaps with the research objects of his earlier thesis for Candidate's degree and covers the problems of materials science and prospects of the intensely shaping research direction: the so-called MAX phases – a family of transition metal layered carbides [15].

It is noteworthy that A. L. Ivanovskii was one of the leading authorities in the world for studying the electronic structure, chemical bonding, stability and mechanical properties of binary and ternary refractory phases. This research allowed the prediction of homogeneity regions, which were caused by the presence of vacancies and 2, 3d- element impurities in a wide spectrum of refractory compounds. These results were published in a large number of scientific papers and monographs [16-18]. Scientific achievements gained by the group were welcomed in the scientific community and were held in great esteem by the Russian Government, which awarded A. L. Ivanovskii the State Prize in Science and Engineering in 1995, and with the title of Honored Scientist of the Russian Federation in 2007.

The obtained knowledge about binary transition metal carbides and nitrides had formed the basis for research into an advanced novel family of ternary layered MAX phases which exhibited a unique combination of properties, intrinsic to both ceramic and metal materials. Such nanolaminates of $M_{n+1}AX_n$ (n=1,2,3...) are composed of layers of transition d-element carbides or nitrides, M_{n+1}, sandwiched by layers of p-elements designated as : (Si, Ge, Al, S, Sn, etc.); and carbon or nitrogen (X_n). The phases exhibit totally reversible plasticity, excellent shockwave resistance, high thermal and electrical conductivity, corrosion resistance, and show promise for industrial application as refractory materials that call for further investigation into their properties. Theoretical studies of the electronic structure and properties of $M_{n+1}AX_n$ phases using *ab initio* techniques were initiated by A. L. Ivanovskii in the mid 1990's, and are still intensely ongoing. In particular, specifics for the electronic properties and chemical bonding in Ti_3SiC_2 were established for the first time, and non-stoichiometry and doping effects were studied in different sub-lattices [19,20]. A significant experimental contribution was made by A. L. Ivanovskii into the studies of MAX phases, predicting new nanolaminates and modeling the properties using the state-of-the-art *ab initio* quantum chemistry methods. The superconducting transition, experimentally detected in a number of MAX phases, set forth a series of theoretical studies exploring the fundamentals of this phenomenon in nanolaminates.

In 2011, an original method was proposed for the synthesis of a new family of MAX phase-based graphene-like (quasi-two-dimensional) nanocarbides and nanonitrides of d-metals, which were named MXenes. These materials possessed a nontrivial combination of properties, and showed promise for various technology applications. Under the leadership of A. L. Ivanovskii, modeling new 2D nanostructures was carried out, their stability factors were determined, and directional modifications were proposed for their electronic, cohesion, mechanical and magnetic properties [21,22]. Models were developed and systematic studies were performed for structural and electronic properties and for relative stability of 2D graphene-like carbide structures of $Ti_{n+1}Al_{0.5}C_n$ and $Ti_{n+1}C_n$ (n = 1 and 2), which could be obtained from the corresponding MAX phases. The possibility of obtaining new 2D graphene-like carbides and nitrides, which had electronic and magnetic properties, such as semiconductors, nonmagnetic and magnetic materials controllable by altering the type and degree of atomic coverage of the 2D carbides and nitrides with various ad-atoms and molecules was shown. Structural, cohesion and electronic characteristics for graphene-like carbide nanotubes were predicted.

One of the most significant directions of A. L. Ivanovskii's research was the theoretical modeling of properties for tungsten carbides and nitrides and for multicomponent phases based upon those materials. His interest in this was piqued by the unique physical and chemical properties of tungsten carbide (WC), which is characterized with a small thermal expansion coefficient and improved hardness over a wide temperature range and which is now widely used as a basic component for making wear-resistant, hard alloys and high-strength coatings. Besides, from the theoretical point of view, tungsten carbides and nitrides could be considered as “transitional” phases between the series of new crystalline carbides and nitrides of platinum-group elements (Ru, Rh, Pd, Os, Ir, Pt) and the “classical” carbides and nitrides of d-metals of IV and V groups [23]. Alexander Ivanovskii was the first in Russia to have published a review on computational materials science exploring these materials [18]. Under his direct guidance, a series of studies were carried out to predict the electronic structure, chemical bonding, phase stability and mechanical properties of binary carbides and nitrides of tungsten (WC, W_2C, WN, W_2N) and ternary solid solutions and individual phases.

In particular, the energy stability and a number of physical and chemical characteristics were established for all known polymorphous modifications of tungsten sub-carbide W_2C (α, β, γ, ε), which differ one from another in the type of carbon atom distribution over octahedral interstices of the crystal lattice and which, when added as doping elements, cause an effect on the performances of carbide-metal WC/M composites and coatings. Structural and electronic properties were determined, and the role played by carbon vacancies was established for the synthesized solid solutions — tungsten aluminocarbides $W_{1-x}Al_xC_z$, which were formed by nonstandard substitution, when *d*-element (W) is replaced by a *p*-element (Al) in the nodes of the metallic sublattice of the hexagonal tungsten carbide WC. As a result, introducing aluminum into tungsten carbide reduced the carbide density considerably, while maintaining its strength properties. Other remarkable results of his research include the prediction of electronic and magnetic properties of the so-called η-phases (M_3W_3C, M_6W_6C), which appear in composite materials in the region between the WC grains and transition metals or their alloys, and which cause a significant impact on the functional (e.g., mechanical) properties of tungsten-containing materials [24,25].

Predicting new doped and non-stoichiometric semiconducting phase-based magnetic materials was another direction of his research that Alexander Ivanovskii eagerly pursued, thus developing quantum chemical materials science for spintronics applications. Along with the traditional approach, which comprised doping nonmagnetic semiconductors with atoms of magnetic 3*d*- and 4*f*-metals, Alexander Ivanovskii was engaged in developing a new research direction, which is referred to as d^0-magnetism and involves inducing the magnetic state of a system by doping the system with the atoms of *sp*-elements (B, C, N) in the anion sub-lattice or by vacancy-induced spin polarization of the states near the Fermi level. Alexander Ivanovskii was the first Russian author to have published such an in-depth review of science literature on this issue [26]. Under his direct guidance, a number of research projects were performed devoted to the theoretical prediction of d^0-magnetism for a wide range of crystalline systems and nano-objects. In particular, a vacancy-induced mechanism was predicted for non-stoichiometric oxide of BeO_{1-x},; it was demonstrated that doping wide-band oxides (such as MgO, La_2O_3, $SrTiO_3$ and related perovskites) with *sp*-elements allows a magnetic semimetal state to be realized in some cases, resulting in a material with 100% spin polarization of current carriers – which, without a doubt, is of great practical significance for various applications. Modeling the magnetic properties of nanotubes was also carried out for carbon-, BN-, AlN- and MgO- nanotubes doped with nonmagnetic *sp*-impurities.

In the same context, another intriguing direction of modeling new magnetic materials is remarkable, which was initiated and supervised by Alexander Ivanovskii in the Quantum Chemistry and Spectroscopy Laboratory at the Institute of Solid State Chemistry, UB RAS. This research direction is called "fine tuning" the electronic and magnetic properties of layered semiconducting phases, for instance, having the structure of ZrCuSiAs or $ThCr_2Si_2$, and involves co-doping of the phases in various structural domains, when varying the type and content of each dopant is instrumental in making flexible adjustment in the electronic and magnetic properties of such compounds. His efforts in this direction resulted in the prediction of the first realization of a bipolar magnetic semiconductor (a material with external electric field "switchable" spin polarization carriers). This bipolar magnetic semiconductor was realized among crystalline systems and comprised a manganese and iron-doped layered semiconductor YZnAsO [27]. Further, experimental data on the magnetic properties of LaZnAsO and LaCuSeO phases, co-doped with the atoms of 3*d*− and alkali-earth metals, were also clarified [28]. There is hardly a common opinion on whether a theorist should avoid abstracting far off from the experimentally observed reality or if it is better to be daring enough to go ahead. However, to do justice to the Alexander Ivanovskii's nontrivial intuition, which was amplified by his phenomenal ability to find his bearing among the colossal volumes of science literature, he was surely well balanced in resolving this dilemma.

A. L. Ivanovskii made a significant contribution in the quantum chemistry research of new superconducting materials. Hence, of the vast variety of the research projects, two stand out — the pioneering research endeavors directed and contributed by Alexander Ivanovskii most appreciably. Firstly, a series of works was devoted to studying the properties of superconducting compound MgB_2 and its structural analogs [29-33]. Ivanovskii's laboratory has taken a leading position in the field of diboride research. Note that the article [30] on MgB_2 had once been the only non-empirical study available at the moment of discovery that had investigated the electronic structure and chemical bonding parameters of the compound. Under Ivanovskii's leadership, a large series of modeling works was performed dealing with the analysis of the effect caused by band occupation and crystalline parameters on the band structure, Fermi surface; and major criteria were established for superconductivity in diborides. Secondly, the basic research works on a large family of compounds related to the so-called Fe-As superconductors were devoted to studying their electronic, magnetic, spectroscopic and mechanical properties [34-38].

Analyzing the scientific activity of Alexander Ivanovskii, one cannot overestimate his outstanding qualities as a scientific manager. Throughout his carrier, he pursued collaborations with scientists from Ekaterinburg, Novosibirsk, Saint Petersburg, Moscow, and his contacts were sustaining and fruitful. To honor Ivanovskii's outstanding scientific accomplishments, the State Prize was awarded to him for the research work, which was performed in cooperation with scientists from the Institute of Solid State Chemistry and with a research group headed by Prof. S.P. Gabuda from the Institute of Inorganic Chemistry, Novosibirsk. Most appreciably, his remarkable organizing skills and managerial competence were manifested in his role as Scientific Secretary, Head of Laboratory and Deputy Director at the Institute of Solid State Chemistry. His graciousness to those around him, his democratic approach and most considerate attitude to people, when combined with his ardent zeal and excellence in understanding science mechanisms and research functionality, contributed to a great extent to the efficient work of the Institute and the laboratory that he was leading. His laboratory was a regular winner of scientific grants from the Russian Foundation for Basic Research and other science-oriented foundations (INTAS, CRDF). Alexander Ivanovskii's scientific and managerial competence was a significant contribution that had helped to establish strong links with scientific organizations in Germany, France, USA, and Spain.

In the memory of so many people, Alexander Ivanovskii made a long-lasting impression as a prominent scientist and decent man, truly dedicated to science, education and culture. Being genuinely talented, his creativity extended far beyond his occupational interests: he loved and understood music deeply, relished the beauties of art and literature. In 1982, he received a university degree in art history (from Ural State University after A.M. Gorky). A genuine Russian intellectual, a man of great culture and wisdom, living on drive and determination, with creative excitement and verve — these are his qualities by which he will always be remembered. He was a fascinating researcher, a valuable colleague and a good friend. It is so hard to think of him gone, and words, once written by a Russian poet Nikolay Nekrasov in his 'In Memory of Dobrolyubov' verse, are drumming in our memory as a refrain: "What a torch of reason ceased to burn, What heart has ceased to beat!"

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