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## TO THE 100-th ANNIVERSARY OF KIRILL BORISOVICH TOLPYGO'S BIRTHDAY (May 3, 1916–May 13, 1994)



May 3, 2016 marks the 100-th anniversary of the birth of Kirill Borisovich Tolpygo, a prominent theoretical physicist, Corresponding Member of the National Academy of Sciences of Ukraine, who is recognized for his fundamental contributions to solid state physics and biophysics: theory of interatomic interactions and crystal lattice dynamics; band theory of semiconductors and dielectrics; theory of excitonic and impurity states in crystals; crystal optics; theory of kinetic phenomena in solids; theory of defects and defect formation; theory of molecular mechanisms of mutations; and theory of chemical energy conversion into mechanical energy at the muscle contraction and other conformation changes of biopolymers. K.B. Tolpygo was an eminent scientist, teacher, and science promoter recognized for mentoring and advising several generations of physicists and founding new schools of theoretical physics and biophysics in Ukraine. K.B. Tolpygo received a habilita-

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tion degree of Doctor of Sciences in Theoretical and Mathematical Physics in 1962. He became Professor of Physics in 1963 and in 1965 was elected Corresponding Member of the Academy of Sciences of the UkrSSR.

Kirill Borisovich, known as simply KB to his colleagues and friends, was born in Kiev in a distinguished family with pedigree of intellectuals and intelligentsia. His father, Boris Nikolaevich Tolpygo, was a well-known lawyer in Kiev, a graduate of the Saint Petersburg University and a veteran of the World War I. Tolpygo's ancestors lived in Ukrainian and Belarusian lands for many centuries. KB's mother, Tatyana Borisovna graduated from Bestuzhev's Higher Courses for Women and later worked as a librarian. She was a daughter of the prominent mathematician, Boris Yakovlevich Bukreev, a Professor at the Chair of Pure Mathematics at the Kiev University. Her grandfather was another Professor at the Kiev University, A.A. Kozlov, a well-known philosopher in the 19-th century and the publisher of the first Russian philosophical journal.

The life of KB, as many of his generation, was profoundly affected by the turmoil of that time. In 1923, his father was arrested for the publication of a few articles abroad about political persecutions in Soviet Ukraine and sentenced in 1924 to ten years of hard labor, along with other Kiev professors and intellectuals in the trial of the so-called Kiev Regional Center of Action. After many years of imprisonment and exile, he was allowed to return to Kiev only in 1956. Kirill Borisovich was raised in Bukreev's family. KB graduated from a 7-year school, then from a technical school and the worker's faculty (*rabfak*) of Kiev University. In 1934, he entered the Faculty of Physics and Mathematics of the Kiev University, which he graduated from with honors in 1939. In spring of 1939, he entered the graduate school at the Institute of Physics of the Academy of Science of UkrSSR to study theoretical physics. However, later in 1939, he was drafted into the Red Army, where he served till 1945. KB's first scientific paper was published in 1940, when he was already in the army. KB was a veteran of the World War II. A commander of a 45-mm antitank cannon, he was heavily wounded by a shell fragment during the counter-offensive at Yelnya.

Upon the demobilization, KB returned to Kiev and, in April 1945, re-enrolled in the graduate school at the Institute of Physics, whose operations had just resumed after the evacuation. Prof. Solomon Isaakovich Pekar, a well-known theorist, became his scientific advisor. From that time, they developed a personal friendship with deep mutual respect and scientific collaboration that connected them for the rest of their lives. Although they did not have a single joint publication, the scientific interests of S.I. Pekar had strongly influenced the initial direction of Tolpygo's research. This was the beginning of the scientific carrier of KB that from that time went on uninterrupted for almost 50 years.

From 1948 till 1960, KB worked at the Institute of Physics. In 1949, he got his PhD degree for a brilliant dissertation and, in 1950, became a Senior Scientist at the Institute of Physics. From 1946 till 1959, he also taught physics and theoretical physics at the Chair of Theoretical Physics of the Kiev University. In 1959, KB transitioned to the University and, from 1960 to 1966, was Head of the Chair of Theoretical Physics. From the moment of establishment of the Institute of Semiconductors of the Academy of Sciences of UkrSSR in 1960 and till 1966, he was also a Senior Scientist in the theoretical department of this institute. During all this period, KB maintained a tight collaboration with experimentalists in the Institute of Physics and the Institute of Semiconductors. KB's style was to present results of his theoretical work in a form allowing for a direct comparison with experiment. Especially close was his interaction with Academician V.E. Lashkarev and his group of experimentalists.

In January 1966, KB accepted the invitation of Academician A.A. Galkin to move from his beloved Kiev to Donetsk to a newly established Physical-Technical Institute of the Academy of Sciences of UkrSSR (DonPTI). Here, he created a Department of Theoretical Physics and was its Head from 1966 till 1988. The department now bears his name. From 1988 and till 1994, KB was a Principal Scientist at DonPTI. In 1966 KB, became also a Professor of physics at the Donetsk University, where he established and headed initially the Chair of Theoretical Physics. In 1967, he established also the Chair of Biophysics at the Faculty of Physics of the Donetsk University.

After the classical work of Max Born, the prominent contributions of K.B. Tolpygo to the theory of crystal lattice dynamics were the most influential in this area of physics. At the end of the 1940s – beginning of the 1950s, KB created a new quantummechanical theory of crystals, which considered the deformation and the polarization of ions and atoms at their vibrations and interactions with external fields, and the effects of retardation in their interactions. For the first time, he introduced additional variables into the theory of lattice dynamics – components of the electric dipole and higher moments of atomic shells. This theory is known as the Tolpygo model. In 1950, KB studied the interaction of light waves with long-wavelength optical vibrations of ionic crystals with account for the deformation of ions and the retardation and predicted, for the first time, the existence of coupled states of photons and phonons in crystals. These mixed states were later studied experimentally and termed polaritons. Presently, the research of pumped polaritons of various types: phonon polaritions, exciton polaritons, surface polaritions, cavity polaritons, etc., is a very active field of modern studies of light-matter interactions.

Tolpygo's theory has allowed for considering the optical, electrical, and elastic properties of crystals on the common footing. KB predicted several new effects, which were later found experimentally. For instance, an additional mechanism of electron-phonon scattering caused by the electrostatic interaction of electrons with atomic shells polarized by lattice vibrations, the emission of acoustic and optic phonons by current carriers with supersonic velocities – the analog of the Cherenkov effect, and the induction of the electric polarization by a nonuniform deformation of crystals. The latter was later termed the flexoelectric effect. The direct and inverse flexoelectric effects are presently a subject of active studies in various crystalline solids, nanostructures, liquid crystals, polymers, and biopolymers.

ISSN 2071-0186. Ukr. J. Phys. 2016. Vol. 61, No. 5

460

KB extended his theory of deformable ions to homopolar crystals of the diamond-type, Si, Ge, etc., and cryocrystals of noble gases, whose atoms in the absence of vibrations have no dipole moment. He showed that the long-range and short-range forces, originating from Coulomb and exchange interactions as a result of the deformation of atomic shells at vibrations, appear in these crystals and play an important role in their lattice dynamics. Later, he extended his theory to heteropolar crystals like ZnS and CuCl with mixed ionic and covalent bonding. KB also researched an important concept of an "effective charge" of ions in crystals and developed an original treatment that justified the use of fractional charges in the theory of ionic crystals. KB further developed his theory of lattice dynamics to account for quadrupole and octupole deformations of ions and atoms, which are important at short-wavelength vibrations, and explained, in particular, the deviations of elastic moduli from the Cauchy relations. He obtained the elastic moduli and calculated the phonon spectra for many alkali-halide crystals, crystals of diamond, Si, Ge, ZnS, CuCl, Ne Ar, Kr, etc., all in a good agreement with the experimental data and inelastic neutron scattering.

In the theory of band and local states of electrons and excitons, K.B. Tolpygo developed an effective theory based on the Heitler–London method and the adiabatic (Born–Oppenheimer) approximation. In this theory, the motion of an excess electron or hole is divided into the "fast" motion near the lattice site and a "slow" motion from site to site. This allowed him to obtain, for the first time, a so-called polarization correction to the energy of a band electron and develop a method of calculating the band states, polaronic states, and impurity states, as well as states of excitons of arbitrary radius.

K.B. Tolpygo also proposed and justified a quasimolecular model of valence crystals, which allowed him to research comprehensively and treat, on the equal footing, excitations of electrons, holes, and excitons, lattice dynamics, and states of the multiply charged impurity centers. According to this model, any electron pair of the bond between the neighboring atoms is treated as a quasimolecule in a selfconsistent field created by all other bonds. By considering excited states of such quasimolecules, KB proved the existence of metastable Frenkel excitons and explained, by their formation, a mysterious ab-

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sorption bands lying at energies above the direct interband transition threshold. In the Tolpygo quasimolecular model, the electron and hole bands result from the translation-invariant superposition of states with the excess or deficit of an electron in one of the bonds. KB showed that this approach leads to a larger number of electron-like and hole-like bands than in a single-electron band theory. He applied this to explaining the existence of long-wavelength tails in the spectra of x-ray emission from crystals. Using his quasimolecular theory, K.B. Tolpygo studied the states of substitution impurities and multiply charged centers, built a theory of defect formation at the intrinsic light absorption, and treated many other phenomena.

In 1951–1952, K.B. Tolpygo gave, for the first time, a systematic description of all thermoelectric, galvanomagnetic, and thermomagnetic phenomena in semiconductors at the elastic scattering of current carriers with a power-law dependence of the meanfree paths of carriers on their energy. For a long time, this work remained foundational in this area and was included in the textbooks on the theory of semiconductors almost in its entirety.

In 1954–1957, Tolpygo (with É.I. Rashba) performed the first Soviet research in the theory of p-n junctions. He built a nonlinear theory of current transport through p-n junctions and obtained the main laws governing their current-voltage characteristics at the forward and reverse biasing and strong currents and a general expression for the junction capacitance as a function of the bias. For the first time, he created the theory of bipolar diffusion of current carriers, theory of current increase at the reverse biasing due to the generation of carriers in the region of volume charge, *etc.* Historically, these were the very first publications in the USSR on the bipolar transport in semiconductor devices. These important results were soon reproduced by American scientists.

In the last 20 years of his life, KB actively worked on problems of biophysics: molecular theory of mutations; theory of hydrogen bond and its role in conformation changes of biopolymers; microscopic theory of muscle contraction, and other problems. The selection of topics of KB's work during these years is extremely broad. He developed non-empirical methods for the band theory, theory of Mott excitons, theory of acceptor-donor complexes and their luminescence, theory of deep donors and acceptors, theory of F-centers, theory of self-localization of electrons in crystals of noble gases, plasma theory of ball lightning, theory of high-frequency dielectric permeability of BaTiO<sub>3</sub>, microscopic theory of light propagation in crystals, and theory of a new quasiparticle – protonic exciton.

During almost fifty years of his life, KB taught general and theoretical physics and devoted his time to training, mentoring, and advising several generations of physicists in Kiev and Donetsk. KB was a brilliant lecturer, an academic of great intellect, broad education and erudition, excellent memory, and quick mental reaction. His lectures had a very special style – all derivations were comprehensive and made to completeness, difficult problems were never swept under the rug in order to create an impression of simplicity and easiness, and the intensity and the amount of material covered were challenging over the limits of possible.

Remembering K.B. Tolpygo as a scientist and a teacher, it is important to see him also as a person and a citizen. KB was a Sakharov-type intellectual, who may not necessarily hold the key to the bright future, but will always fight against the ugliness of the dreary present. He had a nonconformist civic position and opposed the authoritarian and totalitarian methods of managing science and education. At the end of the 1940s and the beginning of the 1950s, he publicly – in lectures and publications – defended the principles of quantum mechanics and relativistic physics, when they came under the attack of official ideologists and obscurantists. In 1968, K.B. Tolpygo joined a group of 139 scientists, writers, artists, and other professionals in signing a famous "Kiev Letter of 139" against political persecutions in Ukraine,

in particular, against the prosecution of V. Chernovol and others. KB was one of the first to recognize the importance of the imminent ecological problems, especially crucial to Donbass. He started to lecture and write on ecology, preservation of the environment, and problems of sustainability. Being a person of democratic persuasions, with independent mind and comprehensive knowledge of history, KB was convinced that the independent development of Ukraine has no alternative.

The remarkable human qualities of KB, his intelligence, genuineness and sincerity, compassion and empathy, honesty and integrity, care about his disciples, and passion for science made him a center of attraction to young scientists and an example to follow. Around him, there was no place for pettiness, squabbling, and scheming. KB's charisma was so powerful that just his only presence lifted the audience to higher levels of civility. This is how he is remembered by all who knew him.

K.B. Tolpygo created his own scientific school, which produced many actively working theorists. Forty of his pupils obtained PhD degrees and successfully defended their dissertations made under his guidance. Twelve of them went on to obtain the habilitation degrees of Doctor of Sciences and Professor. Many of his disciples were working or continue to work in the leading scientific institutions in Ukraine and all over the world.

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