

## ELENA F. SHEKA

(TO 80 ANNIVERSARY OF BIRTH)

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November 20, 2014 marked the 80th anniversary of Elena Feodorovna Sheka, Doctor of Physical and Mathematical Sciences, Professor, Head of the Laboratory for Computational Nanotechnology of the Department of Theoretical Physics and Mechanics of the Peoples' Friendship University of Russia, a renowned expert in the field of experimental and computational spectroscopy of molecular crystals and quantum chemical modeling of nanoscale systems.

Elena F. was born in 1934 in Kiev, in the family of employees: Father Feodor Mikhailovich Dubovtsev - employee of the general service department of the Central Committee of the Communist Party of Ukraine, Valentina Emelyanovna mother - a housewife. Father went missing in the first months of the Great Patriotic War; Elena Feodorovna with her mother survived the occupation of Ukraine in the countryside and in 1945 returned to Kiev. After graduating the school number 65 with a gold medal in 1952, Elena F. entered the Physics Department of Shevchenko' Kiev State University. In the third year, EF Sheka is allocated to the chair of optics, headed at the time by Prof. A.A. Shishlovskiy. Here, under the guidance of Prof. Shishlovskiy she performs a diploma work devoted to the study of the luminescence of impurity centers in alkali halide

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crystals. After graduation in 1957, Elena Feodorovna is left on the chair, where she began her career as a laboratory assistant, then a senior laboratory one. In 1958 Elena F. enrolled in the graduate school of the Institute of Physics, Academy of Sciences of the UkrSSR, where, under the leadership of Acad. A.F. Prikhot'ko is engaged in low-temperature spectroscopy of molecular crystals. The results obtained were the basis of her PhD thesis "Exciton spectra of naphthalene crystal" that was defended in Moscow, at Lebedev' Physical Institute, Academy of Sciences of the USSR in 1962. She works at the Institute of Physics, Academy of Sciences of the Ukrainian SSR as junior researcher and then senior one until 1966. In 1966 Elena F. moved to Chernogolovka, Moscow region and hold the senior researcher position of the Institute of Solid State Physics, Academy of Sciences of the USSR. Here, in the Laboratory of Optics and Spectroscopy, led by her husband - the winner of the Lenin Prize, Prof. Vladimir L'vovich Broude – she continues to study exciton states of molecular crystals and starts a new research line - the study of phonon spectra of molecular and liquid crystals using inelastic scattering of thermal neutrons. In 1972, in Lebedev' Physical Institute, Academy of Sciences of the USSR she defended her doctoral thesis "Exciton spectra of molecular crystals." Soon Elena F. - head of the Laboratory of Optics and Spectroscopy of the Institute of Solid State Physics, Academy of Sciences of the USSR. At the same time she began teaching activities: Elena Fedorovna - associate professor since 1978 and full professor since 1985 at the Department of Solid State Physics, Faculty of General and Applied Physics, Moscow Institute of Physics and Technology in Dolgoprudny, Moscow region. Since 1986 to the present time Elena F. – full professor of the Department of General Physics, and then the Department of Theoretical Physics and Mechanics of the People's Friendship University of Russia, Moscow and the head of the Laboratory of Computational Nanotechnology. Under her leadership, nine PhD and one doctoral theses were defended.

Elena F. Sheka - author of over 300 scientific papers and four books on excitonics of molecular crystals, phonon spectra of molecular crystals (inelastic neutron scattering experiment and calculation), the electron-phonon interaction and vibronic spectra of molecular crystals, phase transitions in molecular

solids with liquid-crystal behavior (vibrational spectroscopy and neutron diffraction), vibrational spectroscopy of nanoparticles, quantum-chemical modeling of nanoscale systems, applied quantum chemistry and computational nanotechnology.

Among the most significant scientific results of Elena Feodorovna - the first direct evidence of Davydov' splitting of exciton absorption bands in molecular crystals (1961), the first direct calculation of the exciton bands of the anthracene crystal (1964), the first evidence of the Rashba effect (delocalization of the impurity states near the exciton band of crystal - 1961 in the absorption and 1984 in luminescence), the manifestation of two-particle vibronic states in the absorption spectra of molecular crystals (1966), the first direct measurement and calculation of dispersion and density of states of phonons of naphthalene and anthracene crystals (1978-1982); the discovery of metastable liquid crystalline phases in the solid molecular solids (1984), of technological polymorphism of silica nanoparticles (1992), and of the STM-tip stimulated graft oligomerization reaction on the surface of diamond-like films (1995); the prediction of magnetism of clean surfaces of silicon crystal (1997, confirmed experimentally in 1999) and of magnetic nature of the ground state of silicon fullerenes (2001); the development of parallel codes of quantum-chemical calculations for multiprocessor supercomputers as the basis of computational nanotechnology (2001); the revealing of peculiarities of the electronic structure of fullerenes (2004-2007) and carbon nanotubes (2007) caused by odd-electron nature of the systems; the classification of types of donor-acceptor complexes based on fullerenes (2004); the explanation of nanostructured magnetism of polymerized fullerenes (2005); the suggestion of a computational algorithm of fullerenes polyderivatives (2006) and chemically modified nanotubes (2007); the disclosure of the leading role of the donor-acceptor interaction in fullerene oligomerization (2007) and of clustering of fullerene molecules in dilute solutions as reasons for the amplification of spectral and nonlinear optical properties of solutions (2008); the explanation of the molecular nature of magnetism of nanostructured graphene (2009); the establishment of molecular theory graphene (2013); the development of the basic concepts of theoretical chemical physics of graphene.

A wide range of scientific contacts is inherent to the working style of Elena Feodorovna. Among the latter there are occasionally interrupted cooperation with the Frank Laboratory of Neutron Physics, JINR (Dubna) from 1976 to the present; cooperation with the Laue-Langevin Institute (France) in 1976-85; tight contacts with the Solid State Institute of the

Central Physical Institute of Hungary in 1976-85 years, the contract with the Institute of Physical and Chemical Research (RIKEN) in Japan, 1997-99; the collaboration with the Technical University of Delft (1999-2001). Led by EF Sheka, the Laboratory of Computational Nanotechnology was a collective member of nanoscience projects of the European Research Foundation in 1999-2000 and NWO project with the Technical University of Delft (Netherlands), 1999-2001; the cooperation with the Institute of Problems of Chemical Physics, from 2004 to the present time; the cooperation with the Ioffe Physical-Technical Institute RAS (St. Petersburg).

E.F. Sheka is a member of the Russian Nanotechnology Society, the American Chemical Society, and the European Society of Computational Methods in Science and Industry. She is the regional representative of Russia in the International Society of Theoretical Chemical Physics. The results obtained have also received recognition in the form of numerous grants.

E.F. Sheka was awarded by the medal "Honored Worker of Higher Professional Education", diplomas of the People's Friendship University of Russia.

E.F. Sheka - member of the editorial boards of several international journals, including "Molecular Crystals and Liquid Crystals" (CRC Press; Taylor & Francis Group.) and "Journal of Nanoparticle Research" (Springer), co-editor of "International Journal of Nanomaterials, Nanotechnology and Nanomedicine" (Peertechz Publ.). She took part in the work of more than 250 national and international conferences. Elena F. is the soul and motor of Moscow Workshop "Graphene: Molecules and Crystals" regularly operated over two years under the guidance of Prof. S.P. Gubin.

High scientific erudition, a fantastic working capacity, integrity and responsibility brought to EF Sheka a deserved prestige and wide recognition of the scientific community.

Friends, colleagues and students sincerely congratulate Elena Feodorovna Sheka with a glorious jubilee and wish her good health, good luck and success in research and teaching.

Editorial Board of RENSIT of the Department of Problems of Radioelectronics, Nanoscale Physics and Information Technology RANS heartily joins these wishes to its good acquainted and always wished author.

**Edition**