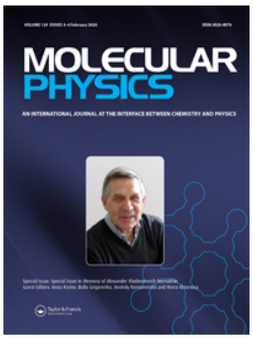

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EDITORIAL

Introduction to the Alexander Vladimirovich Nemukhin special issue

The life of Alexander (Sasha) Vladimirovich Nemukhin (1946–2023) was defined by his passion for science and his deep commitment to education [1,2]. His enthusiasm for quantum mechanics and quantum chemistry was infectious and unbounded. He devoted his life to advancing theoretical and computational chemistry through his research and teaching at the Lomonosov Moscow State University (MSU). The impact of his life's work extends beyond disciplinary and national borders.

Alexander Vladimirovich Nemukhin was born on June 9, 1946, in Moscow. He passed away on July 18, 2023, leaving behind a rich scientific legacy and generations of grateful students, collaborators, and friends.

After graduating from secondary school with distinction in 1964, Alexander Vladimirovich became a student in the Chemistry Department of MSU, where his journey into theoretical chemistry began. He graduated in 1969 with a Specialist Degree (the equivalent of an M.Sc. today) and joined MSU's Chemistry Department as a junior researcher.

His first research experience was under the supervision of Professor Vladimir Mikhailovich Tatevskii and, later, Nikolai Fedorovich Stepanov, in the Laboratory of Molecular Structure. These were the early years of quantum chemistry, when computing capabilities were very limited—one of his early scientific publications dealt with calculations of a model system with two electrons. Yet, anticipating the progress in computers that was to come, Alexander Vladimirovich began exploring the application of quantum mechanical methods to molecular spectroscopy and reactivity, including such challenges as calculations of excited states and spectra of molecules in rare-gas matrices. At that time, he combined self-consistent field and semi-empirical methods.

His Ph.D., awarded in 1975, focused on non-empirical potential energy curves of diatomic molecules. Already at this stage, his work demonstrated a characteristic blend of mathematical sophistication and chemical insight.

In 1980, Alexander Vladimirovich began a transformative period at the University of Oslo with Jan Almlöf, one of the pioneers of modern quantum chemistry. There, he became involved in the development of multiconfigurational methods, particularly the complete active space self-consistent field (CASSCF) approach. Upon returning to Moscow, he continued to advance these methods, applying them to a variety of problems. According to Trygve Helgaker, Alexander Vladimirovich brought to Moscow from Oslo the printout of the MOLCAS program and had it typed out on punch cards in order to run it on local computers. Later, he visited Almlöf's group at the University of Minnesota, where he gained access to their state-of-the-art supercomputing facilities. I vividly remember the seminar he gave upon his return to Moscow, in which he reported on his work and explained his vision—that advanced *ab initio* methods will eventually be able to tackle real chemical problems, once the necessary computer infrastructure is in place. This work culminated in his Doctor of Science (Habilitation) dissertation, *Multiconfigurational Approaches in the Theory of Electronic Structure of Molecules,* in 1989.

Building institutions: from molecular structure to biophysics

Alexander Vladimirovich channeled his enthusiasm for quantum chemistry into effective leadership, reshaping the organisational landscape of theoretical chemistry at MSU. In 1993, he took charge of the Laboratory of Chemical Cybernetics and modernised its research priorities to align with modern computational chemistry [3]. The story of this laboratory would not be complete without mentioning Dr. Bella Grigorenko, who joined the lab in 1994 and became a lifelong friend and true scientific comrade-in-arms. She led many scientific developments and taught dozens of students the nuts and bolts of quantum chemistry.

The 1990s were turbulent years in Russia. The collapse of seven decades of communist rule left science trapped under the ruins of decaying institutions. Many scientists left academia to pursue business endeavors, others immigrated, and some gave up science altogether. Not Alexander Vladimirovich. He found new ways to support his students and staff, and he learned how to navigate

the emerging grant system and how to leverage international collaborations. Thanks to his resourcefulness and resilience, the Chemical Cybernetics Laboratory became a thriving oasis in the Chemistry Department.

For three decades, Alexander Vladimirovich directed this laboratory, where he fostered an environment that combined rigorous theoretical work with the development of innovative applications. In 2020, the laboratory merged with the Laboratory of Molecular Structure and Quantum Mechanics to form the Laboratory of Quantum Chemistry and Molecular Modeling, which he continued to lead until his untimely death. Since 2006, he also led the Laboratory of Computer Modeling of Biomolecular Systems and Nanomaterials at the Emanuel Institute of Biochemical Physics of the Russian Academy of Sciences.

These institutional contributions were as important as his scientific ones. They created a home for computational chemistry in Moscow, a place where students could receive top-notch training, and where international collaborations could be nurtured.

Scientific trajectory

Alexander Vladimirovich Nemukhin's scientific contributions spanned several domains of quantum chemistry. His early work dealt with the electronic structure of small molecules, often with application to spectroscopy.

In the 1990s, he turned his attention to molecules embedded in rare-gas matrices in close collaboration with experimental colleagues at MSU and abroad. During this time, he pursued a semi-empirical approach called diatomics-in-molecules (DIM).

By the early 2000s, Alexander Vladimirovich's research entered a new and highly fruitful field: systems of biological interest. Inspired by his collaborations with Drs. Igor Topol and Stan Burt from the National Cancer Institute (USA), this was a truly radical change of direction, which involved expanding the methodological toolkit to include tools for molecular modeling, most notably quantum mechanics/molecular mechanics (QM/MM). Alexander Vladimirovich, together with Bella Grigorenko, led the development of this field in Russia. By applying QM/MM methods to enzymatic catalysis and photobiology, his group's studies on hydrolases, ATPases, GTPases, and cyclases revealed the atomistic details of catalytic mechanisms. In parallel, Alexander Vladimirovich began exploration of photobiology, such as photochemical processes in fluorescent proteins, phytochromes, and light-harvesting complexes. To me, this area looked too complex and messy to be a subject of theoretical investigation. When Alexander Vladimirovich invited me to collaborate on green fluorescent protein (GFP), I joked that I am only interested in having proteins on my plate, not in my research portfolio. Yet, his enthusiasm for living systems was contagious and irresistible—soon I was a part of Team Biomolecules.

Conceptual contributions and international collaborations

Beyond his applied and methodological research, Alexander Vladimirovich engaged with fundamental questions of chemical bonding. In collaboration with Frank Weinhold (University of Wisconsin–Madison), he became an early advocate for the use of natural bond orbitals (NBO) and natural resonance theory (NRT) in Russian chemical pedagogy. By this time, Pauling's concept of resonance had already been rehabilitated from ideological condemnation, yet it still carried some baggage—after all, those who had led the condemnation campaign were still around. And the Party did not appreciate even implicit reminders of its past mistakes [4,5]. Alexander Vladimirovich helped reintroduce resonance as a legitimate and powerful interpretive tool. His efforts linked modern *ab initio* quantum chemistry with the intuitive representations of chemical structure that had long guided students and practitioners.

This intellectual bridge-building mirrored his broader role as a bridge between Russian and international science. He was instrumental in fostering collaborations that transcended political boundaries, from exchange programs with the University of Wisconsin in the late 1980s and early 1990s to numerous joint research projects—including many with my group at USC—in later decades.

Publications, service, and recognition

Over the course of his career, Alexander Vladimirovich published more than 350 papers in peer-reviewed journals, works that have had a sustained impact on multiple areas of chemistry [6].

Alexander Vladimirovich served the scientific community in numerous ways: as head of a dissertation council at MSU for almost twenty years, as an expert for the Russian Science Foundation and the Russian Foundation for Basic Research, and as an editor and reviewer for numerous Russian and international journals. His stature was recognised by the title of Distinguished Professor of Moscow State University, one of the institution's highest honors, and by the medal commemorating the 850th anniversary of the city of Moscow.

Teacher and mentor

If his scientific contributions were substantial, his role as an educator was even more profound. For decades, Alexander Vladimirovich taught core courses in quantum mechanics and quantum chemistry in both the chemistry and biology faculties of MSU. His lectures—*Quantum Mechanics for Chemists* and *Quantum Chemistry and Molecular Structure*—were renowned for their clarity, rigor, and accessibility. He had the rare gift of making even the most abstract formalism meaningful to students by illustrating its direct chemical significance.

In 2022, he published his lecture notes, condensing his decades of teaching experience into a concise volume. His ambition, cut short by his passing, was to expand this into a full textbook that would present molecular physics and quantum mechanics through the prism of chemical intuition.

His mentorship extended far beyond the classroom. For many years, he mentored students enrolled in two elite tracks in the Department of Chemistry: the 11th Group, which was dedicated to physical/theoretical chemistry, and the 13th Group, which was dedicated to computational chemistry [7,8]. It was in this capacity that I first met him in 1984 (more on this below).

Alexander Vladimirovich supervised dozens of M.Sc. and Ph.D. students as well as postgraduate researchers, many of whom now hold academic positions in Russia, Europe, Israel, and the United States. Among them are Ksenia Bravaya (Boston University), Anastasia Bochenkova (MSU), Maria Khrenova (MSU), Sofia Lushchekina (Weizmann Institute of Science), and Alexey Akimov (University at Buffalo), and myself. Others, including Evgeny Epifanovsky (IonQ, USA), Vitaly Vanovsky (Google, USA), Ilya Kaliman (Flowmill, USA), and Alexander Rogov (Gazprom, Russia), have pursued successful careers in technology and industry.

This wide network of alumni reflects the breadth of his influence. More importantly, it reflects the kind of mentor he was: generous, supportive, and deeply invested in the personal as well as professional success of his students.

Personal memories

I first met Alexander Vladimirovich in 1984, when I entered the Chemistry Department at Moscow State University. Our first encounter took place shortly after I was admitted. I had intended to sign up for the special elite track with heavy emphasis on physics and mathematics, the celebrated 11th Group, which he co-curated with other scientists from Stepanov's lab. At the time, I actually had no idea what theoretical chemistry was—I chose the field on a dare, in response to an offhand remark by a friend that the program would be too rigorous for a girl, as even guys were struggling and dropping out in droves [9]. Still elated by my success on my entrance exams, I located the room for students to sign up for the 11th Group and entered my name.

But then an unexpected obstacle emerged. After admission, all students had to undergo a mandatory medical exam, aiming, in part, to identify conditions, such as color blindness (my future husband had gotten past it by memorising the test tables), that would be disqualifying for chemistry. I did not expect there to be a problem, but suddenly, I found my dreams shuttered—a small stress-induced rash on my neck was deemed a disqualifying dermatological condition. In tears, I rushed back to the 11th Group signup room. Luckily for me, Alexander Vladimirovich was there. After hearing my sob-punctuated story, he calmly said—not a problem, we will sign you up for the computational chemistry track (the 13th Group), which is exempt from the dermatological assessment. I did not quite know the difference between the two tracks, but I knew I wanted to be in the 11th Group, not the 13th! Don't worry, he said, we will get you there. We will sign you up for the 13th Group, which will get you a clearance from the medics, and then transfer you to the 11th Group the next day—no one will know. And that is indeed what happened.

Alexander Vladimirovich was one of the most inspiring teachers I had ever encountered, and it was his lectures that ignited my fascination with quantum mechanics. He had the unique ability to make quantum mechanics look and feel simple. As I progressed through my studies, I completed a couple of course projects under his supervision and then went on to do my diploma project with him (which was co-supervised by Dr. V.I. Pupyschev).

Upon graduation, I began Ph.D. research under his supervision, which was interrupted by my immigration to Israel. Alexander Vladimirovich had infinite patience for students, no matter how confused, unfocused, obnoxious, arrogant, or insecure. I know from experience—I was all of the above. He would listen with empathy and offer sympathy and advice. His encouragement played a decisive role in convincing me to pursue a career in science despite my being caught in the drama of my life, unfolding as part of the bigger, national drama—food shortages, fears of civil war, and the collapse of the social order. Alexander Vladimirovich had that rare gift of making students believe in themselves, and I remain deeply grateful for his guidance in those formative years.

In the late 1990s and early 2000s, our paths crossed again in research. By then, his interests had shifted toward biological systems, and he drew me into this new direction with his characteristic enthusiasm. Together with

Bella Grigorenko, we embarked on a highly productive collaboration on the quantum chemistry of photoactive proteins, such as GFP. Together, we published 25 papers (including two from my diploma work), the galley proofs of the last, dedicated to understanding mechanistic details of the covalent inhibition of the SARS-CoV-2 main protease, arriving just weeks before his sudden death. Our collaboration—extending over nearly two decades—produced impactful results and was a pure joy for me. What struck me most during these years was his inexhaustible energy: Alexander Vladimirovich never slowed down, never lost his enthusiasm for science, and always approached new problems with curiosity and optimism.

For me, as for many others, Alexander Vladimirovich was more than a teacher or collaborator—he was a mentor who shaped the course of my career. He was also a friend and a role model. He was always open to conversation and ready to hear and discuss opposing views—whether on science, art, or politics. One important lesson I learned from him is the importance of building consensus and bridges between people—and, above all, being kind. His absence will be deeply felt, but his example as a scientist, a teacher, and a human being will continue to inspire [10].

Conclusion

Alexander Vladimirovich Nemukhin's life and career embodied the best traditions of Russian science while also internationalising it by building bridges with the broader scientific community. From his early work in Prof. Stepanov's laboratory, through his leadership of the Laboratory of Chemical Cybernetics, to his pioneering studies of biomolecular modeling, he consistently advanced both the methods and the conceptual foundations of theoretical chemistry.

He will be remembered for his brilliance as a researcher, his passion as a teacher, his generosity as a mentor, and his humanity as a colleague and friend. This special issue is dedicated to his memory. Let the works collected here reflect not only the depth and breadth of his scientific influence but also the spirit of enthusiasm and curiosity that he embodied [10].

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