How to Cite: Ågren, H.S., Valiev, R.R., & Irgibaeva, I.S. (2023). Special Issue Foreword from Guest Editors. *Eurasian Journal of Chemistry, 111(3), 4-6.* https://doi.org/10.31489/2959-0663/3-23-0

PREFACE

Preface

Received: 04 August 2023 | Published online: 04 August 2023

https://doi.org/10.31489/2959-0663/3-23-0

Hans S. Ågren[1], Rashid R. Valiev[2, 3], Irina S. Irgibaeva[4]

[1]*Uppsala University, Sweden;*
[2]*University of Helsinki, Finland;*
[3]*National Research Tomsk State University, Russia;*
[4]*L.N. Gumilyov Eurasian National University, Astana, Kazakhstan*

Special Issue Foreword from Guest Editors

The editors, guest editors and advisory board members of «*Eurasian Journal of Chemistry*» decided to dedicate this Special Issue entitled «***Quantum Chemistry and Quantum Nanotechnologies of Materials***» to the anniversaries of our colleagues working in this field:

– 90th anniversary of Professor **Muldakhmetov Zainulla Muldakhmetovich** (Academician of the National Academy of Sciences of the Republic of Kazakhstan, Doctor of Chemical Sciences, Professor, Institute of Organic Synthesis and Coal Chemistry of the Republic of Kazakhstan, Karaganda, Kazakhstan);
– 80th anniversary of Professor **Minaev Boris Filippovich** (Doctor of Chemistry, Professor, Bohdan Khmelnytsky National University of Cherkasy, Cherkasy, Ukraine; Uppsala University, Uppsala, Sweden);
– 70th anniversary of Professor **Beznosyuk Sergey Alexandrovich** (Doctor of Physics and Mathematics, Professor, Altai State University, Barnaul, Russia).

In the frame of this Special Issue colleagues from Sweden, Finland, Ukraine, Kazakhstan, Russia, USA, Latvia and Nigeria share their research with readers of the «*Eurasian Journal of Chemistry*».

The contribution of Professor **Zainulla Muldakhmetovich Muldakhmetov** to the first appearance and development of quantum chemical research in Kazakhstan is outlined in the essay by Prof. **Gazaliyev Arstan M.** and **Ivanova Nina M.** (*Institute of Organic Synthesis and Coal Chemistry of the Republic of Kazakhstan*). The essay briefly describes the creation of a scientific school of quantum chemistry in Kazakhstan with the direct participation of Professor Z.M. Muldakhmetov.

An essay dedicated to the 80th anniversary and 55 years of scientific activity of Professor Boris Filippovich Minaev is presented by Prof. **Irgibaeva Irina S.** (*L.N. Gumilyov Eurasian National University, Astana, Kazakhstan)* and **Minaeva Valentina A.** (*Bohdan Khmelnytsky National University, Cherkasy, Ukraine).* The paper reflects Minaev's great contribution to scientific research and informs about his achievements in physical organic chemistry and molecular electronics.

Professor **Sergey Alexandrovich Beznosyuk** as the founder and leader of a new direction of quantum field chemistry in subatomic quantum nanotechnologies of materials is presented in the essay by Assoc. Prof. **Zhukovsky Mark S.** (*Altai State Technical University of the name of I.I. Polzunov, Barnaul, Russia*) and **Maslova Olga A.** (*Altai State University, Barnaul, Russia*). The contribution of Professor S.A. Beznosyuk to the establishment and development of two scientific schools, namely quantum field chemistry of the condensed state at the Buketov Karaganda University and subatomic quantum nanotechnology of materials at Altai State University is shown.

An article by Prof. **Minaev Boris F.** from *Uppsala University (Sweden)* dedicates to the 90th anniversary of Zainulla M. Muldakhmetov and considers chemistry as a science about spin and electric charge of

microparticles which provide driving forces of atomic interactions and molecular structure transformations. The tria(trichlorophenyl)methyl-carbazole (TTM-Cz) radical covalently coupled with anthracene were studied in this paper in order to explain how the doublet excitation delocalized to the linked anthracene during a picosecond lifetime can be evolved into the high-multiplicity (quartet) spin state of the mixed radical-triplet type at low excitation energy in the visible region.

A review by Prof. **Beznosyuk Sergey A.** *(Altai State University, Barnaul, Russia)* analyzes the future development of quantum nanotechnology based on attosecond physics of the subatomic level of the condensed. Author considered in the paper the ways of realizing the main achievements of the second quantum revolution in subatomic nanotechnologies of materials, namely quantum entanglement, quantum contextuality and quantum dissipativity.

A review by Prof. **Kucherenko Michael G.** and Prof. **Chmereva Tatiana M**. (*Orenburg State University, Russia*) is focused on the quantum theory of electronic energy transfer in a layered nanostructure with molecular J-aggregates of polymethine dyes. The authors briefly analyze a series of works that laid the foundation for a general quantum description of the features of the exciton-plasmon and exciton-exciton interactions in hybrid organometallic nanosystems, as well as the kinetics of phototransformations of quasiparticles, taking into account the mesoscopic specifics inherent in such nanosystems.

Prof. ***Valiev Rashid R.*** and coauthors (*National Research Tomsk State University, Russia)* studied relationship between the electric polarizability and aromaticity of metallocene-containing macrocycles. Magnetically induced ring currents, polarizability and second hyperpolarizability for metallocene-containing macrocyclic molecules were evaluated by means of density functional theory (B3LYP/def2-TZVP) calculations. It was shown that the aromatic character and the number of conjugated electrons in the structure are the key factors leading to an increase in the polarizability of the studied molecules.

Prof. **Ibrayev Niyazbek Kh.** and Dr. **Seliverstova Evgeniya V.** from *Karaganda University of the name of academician E.A. Buketov, Kazakhstan* synthesized S,N-doped carbon quantum dots (CQD) based on citric acid and L-cysteine. The properties of the long-lived luminescence of CQDs solutions were studied. It was shown that the synthesized CQDs species are the singlet oxygen sensitizers, as evidenced by the observed luminescence of molecular oxygen upon excitation of solutions in the CQDs absorption band.

The article by Prof. **Semire Banjo** (*Ladoke Akintola University of Technology, Ogbomoso, Nigeria*) and coauthors is focused on the TD-DFT and DFT investigation of electron transporting efficiency of 2-cyano-2-pyran-4-ylidene-acetic acid and 2-cyanoprop-2-enoic acid as acceptors for thiophene-based π-linkers dye-sensitized solar cells. B3LYP/6-31G** level of theory was used by authors to study the molecular architecture of the donor-π-acceptor (D-π-A) type of dyes. The molecular and electronic properties, light harvesting efficiency, open circuit voltage (V_{OC}), injection force (ΔG^{inject}), regeneration force (ΔG^{regen}) and excitation state lifetime (τ_{esl}) were calculated.

Researchers from *National Research Tomsk State University, Russia* (Prof. **Cherepanov Victor N.** and **Sunchugashev Dmitry A.**) studied vibronic emission spectra of dithiophene and terthiophene molecules and their complexes with hydrogen sulfide and its dimmer at the TD-DFT / CAM-B3LYP / 6-31G(d) theory level. Clear vibronic structure was shown for the emission spectra of bithiophene and terthiophene molecules. As a result of calculations, it was found that the positions of peaks in the vibronic emission spectra of these compounds agreed well with the experimental data.

Prof. **Minaev Boris F.** (*Bohdan Khmelnytsky National University, Cherkasy, Ukraine*) and coauthors highlight IR absorption spectra of the recently synthesized series of benzoyl-containing thianthrene derivatives in the context of their structural identification. A good agreement between experimental data and DFT calculated by the author's IR spectra provides additional structural support to results of the X-ray diffraction analysis of all synthesized compounds. The paper also presents the Hirshfeld surfaces analysis of the 3-fluorobenzoylthianthrene (**T3F**), which was carried out to study intermolecular interactions in the T3F crystal.

Mechanisms of docking of superoxide ions in the catalytic cycle of manganese and iron superoxide dismutases was studied by Prof. **Beznosyuk Sergey A.** *(Altai State University, Barnaul, Russia)* and coauthors. At the level of a pure quantum-chemical calculation using an ORCA 5.0.3 program, a PBE functional and a def2-SVP and def2-TZVP basis sets, the possible mechanisms of superoxide ions binding to the active sites of enzymes, the electron transfer distances and their characteristics were established.

Prof. **Irgibaeva Irina S.** (*L.N. Gumilyov Eurasian National University, Astana, Kazakhstan*) and coauthors presented quantum-chemical study of 5-(4'-dimethylaminobenzylidene)barbituric acid aggregation. The

unusual spectral behavior of 5-(4'-dimethylaminobenzylidene)barbituric acid was shown theoretically by DFT and TD DFT methods using the Gaussian 98 program. Zindo and *ab initio* calculations confirmed the appearance of a new band during aggregation and its shift to the red region with an increase in the number of molecules.

Quantum-chemical calculations of the magnetic properties (magnetically induced ring-current strength, magnetizability) of even- and odd-number cyclo[n]carbons (n = 10–34) is reported by Prof. **Valiev Rashid R.** and coauthors (*National Research Tomsk State University, Russia*). The total energy of the studied molecules as a function of the external magnetic field was found for the first time. The obtained dependences predict correctly the magnetic nature of cyclo[n]carbons.

Dr. ***Aldongarov Anuar A.*** and coauthors (*L.N. Gumilyov Eurasian National University, Astana, Kazakhstan*) presented theoretical study of charge mobility properties of complexes Si(DPP)$(CH_3)_2$ and Si(bzimpy)$(CH_3)_2$. Data on the calculation of reorganization energies, intermolecular transfer integrals, transfer rates and charge mobility for the optimized structures of pentacoordinated silicon complexes Si(DPP)$(CH_3)_2$ and Si(bzimpy)$(CH_3)_2$ were obtained using the B3LYP hybrid functional and the 6-31G* basis set with the help of Gaussian09 program.

Theoretical approach was used by Prof. **Abulyaissova Lyazzat K.** and coauthors (*Karaganda University of the name of academician E.A. Buketov, Kazakhstan*) to study the intramolecular interactions of two aminoglycoside antibiotics. Quantum chemical modeling and full geometry optimization of sisomicin and gentamicin were carried out by the authors using Gaussian16 program and DFT-based B3LYP method with a split-valence 6-311G(d) and Dunning's correlation consistent cc-pVDZ basis sets. Based on the obtained data, classical electrostatic nature of the weak H-bonds and conjugation effects stabilizing the molecules were suggested.

The team of authors led by Prof. **Nikolskiy Sergey N.** (*Karaganda University of the name of academician E.A. Buketov, Kazakhstan)*) reported the theoretical study of proton transfer dynamics in complexes of some substituted benzoic acids with 3,6-di-tert-butyl-2-hydroxyphenoxyl radical. The calculations were performed by the DFT method at the UB3LYP/6-31G+(d,p) level of theory in vacuum and toluene medium using Gaussian16 program. Geometric and kinetic parameters of complexes with o-, p-, and m-isomers of nitrobenzoic and chlorobenzoic acids were calculated.

In this Special Issue you will find authors from 8 countries, with 12 of the 17 papers involving researchers from outside the Kazakhstan. The Guest Editors of this Special Issue are really pleased with the result and hope what the compiled articles will provide a lot of new knowledge and a positive reader experience!

Information about Guest Editors*

Ågren, Hans S. — Doctor of Physical Sciences, Professor, Ångstrom Laboratory, Department of Physics and Astronomy, Uppsala University, P.O. Box 256, SE-752 37, Uppsala, Sweden; e-mail: hans.agren@physics.uu.se, hagren@kth.se; https://orcid.org/0000-0002-1763-9383

Valiev, Rashid Rinatovich — Doctor of Chemical Sciences, Senior Researcher, University of Helsinki, P.O. Box 4 (Yliopistonkatu 3), 00014, Helsinki, Finland; Assistant Professor, National Research Tomsk State University, 36 Lenin Avenue, 634050, Tomsk, Russia; e-mail: valievrashid@mail.ru; http://orcid.org/0000-0002-2088-2608

Irgibaeva, Irina Smailovna — Doctor of Chemical Sciences, Professor of Chemistry Department, L.N. Gumilyov Eurasian National University, Satpayev street, 2, 010000, Astana, Kazakhstan; e-mail: irgsm@mail.ru; https://orcid.org/0000-0003-2408-8935

*The editor's name is presented in the order: *Last Name, First and Middle Names*