VITALIY V. KOVAL

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EDUCATION

Ph.D., Physical Chemistry, Southern Federal University, 2012
Dissertation: *Quantum Chemical Study of Metal Complexes with Redox-Active Phenoxybenzoquinonimine Ligands*
Dissertation Advisor: Andrey G. Starikov, D.Sc.

Postgraduate study, Mathematical and software support for computers, complexes and computer networks, Rostov State University, 1999-2003
Theme: The object-oriented implementation of the multipurpose program transformation system

M.Sc. in Mathematics, Applied Mathematics and Computer Science, Rostov State University, 1999
Dissertation: *Development of implementation methods and creation of an instrumental environment prototype for program transformations*
Dissertation Advisor: Alexander A. Bukatov, Ph.D.

B.Sc. in Mathematics, Applied Mathematics and Computer Science, Rostov State University, 1997
Final qualifying work: *Client program implementation of a remote access special protocol irlshp*
Advisor: Alexander A. Bukatov, Ph.D.

TRAINING & CERTIFICATION

High performance computing and artificial intelligence, *Program of additional vocational education training*, Lobachevsky State University, Nizhny Novgorod, Russia, 2022

Big Data in Medicine, *Program of additional vocational education training*, Autonomous noncommercial organization of additional vocational training “Softline Education”, Moscow, Russia, 2020

Introduction to Gaussian: Theory and Practice, *Workshop*, Gaussian Inc., Ulm, Germany, 2019

Quantum informatics, *Training course*, International Summer Supercomputing Academy of Moscow State University, Moscow, Russia, 2018

Advanced administration of SUSE Linux Enterprise Server 12, *Training course*, Autonomous noncommercial organization of additional vocational training “Softline Education”, Rostov-on-Don, Russia, 2017

Supercomputer technologies for solving natural science problems, *Program of additional education training*, Southern Federal University, Rostov-on-Don, Russia, 2011

TEACHING EXPERIENCE

Scientific consultant of the students and the postgraduate students: 2018-2023, Southern Federal University

Lector: 2015-2016, Southern Federal University
Courses: Prediction of structure and properties of dynamic materials

WORKING & RESEARCH EXPERIENCE

Senior researcher: 2014-present, Institute of Physical and Organic Chemistry, Southern Federal University
Junior researcher: 2003-2014, Institute of Physical and Organic Chemistry, Rostov State University (Southern Federal University since 2006)

System administrator: 2006-2012, CJSC “Empils Foh”
Programmer: 1997-2002, Rostov State University

There are more than 25 papers and more than 40 other publications in English and Russian.
H-index of Scopus is 8.
H-index of Web of Science is 8.

There was participation in the projects with the support of the Russian Foundation for Basic Research, the Russian Science Foundation, the Ministry of Science and Higher Education of the Russian Federation and the Russian Government as researcher and executive manager.

There was active taking part in the creation of the several high performance computing clusters which were in top-50 of supercomputers of CIS.

CURRENT SCIENTIFIC INTERESTS

Quantum chemical simulations, computer modeling of new materials, topology of potential energy surfaces, bifurcations of chemical reaction pathways, high performance computing systems.

MAIN PUBLICATIONS

1. Vitaliy V. Koval, Anastasia S. Kozlenko, Boris S. Lukyanov. DFT study of the stabilization preconditions of the indoline spiropyrans with a cationic substituent // *Mendeleev Communications*. **2023**. Vol. 33. № 5. P. 666–670.
2. Iliya V. Getmanskii, Vitaliy V. Koval, Nikolay V. Tkachenko, Stanislav A. Zaitsev, Alexander I. Boldyrev, and Ruslan M. Minyaev. Ultralight supertetrahedral aluminum: Stability at various temperatures // *MRS Bulletin*. **2023**. Vol. 48. P. 1–7.
3. Vitaliy V. Koval, Anastasia S. Kozlenko, Vladimir I. Minkin, Islam M. El-Sewify, Boris S. Lukyanov. DFT modeling of indoline spiropyrans with a cationic substituent in the gas phase // *Mendeleev Communications*. **2022**. Vol. 32. № 4. P. 467–470.
4. Iliya V. Getmanskii, Vitaliy V. Koval, Alexander I. Boldyrev, Ruslan M. Minyaev, Vladimir I. Minkin. Molecular Dynamics Study of a New Metastable Allotropic Crystalline Form of Gallium - Supertetrahedral Gallium // *J. Comput. Chem.* **2019**. Vol. 40. № 20. P. 1861–1865.
5. I.V. Getmanskii, V.V. Koval, R.M. Minyaev, A.I. Boldyrev, V.I. Minkin. Supertetrahedral Aluminum – A New Allotropic Ultralight Crystalline Form of Aluminum // *J. Phys. Chem. C.* **2017**. Vol. 121. № 40. P. 22187– 22190.
6. I.V. Getmanskii, R.M. Minyaev, D.V. Steglenko, V.V. Koval, S.A. Zaitsev, V.I. Minkin. From Two- to Three-Dimensional Structures of a Supertetrahedral Boran Using Density Functional Calculations // *Angewandte Chemie - International Edition.* **2017**. Vol. 56. № 34. P. 10118–10122.
7. V.V. Koval, R.M. Minyaev, V.I. Minkin. Geometric and Electronic Structures of Silicon Fluorides $SiF_n^{(n-4)-}$ (n=4-6) and Potential Energy Surfaces for Dissociation Reactions $SiF_5^- \rightarrow SiF_4 + F^-$ and $SiF_6^{2-} \rightarrow SiF_5^- + F^-$ // *Int. J. Quantum Chem.* **2016**. Vol. 116. № 18. P. 1358–1361.
8. R.M. Minyaev, I.A. Popov, V.V. Koval, A.I. Boldyrev, V.I. Minkin. Supertetrahedral $B_{80}H_{20}$, $C_{80}H_{20}$, and $Al_{80}H_{20}$ analogs of dodecahedrane and their substituted molecules // *Struct. Chem.* **2015**. Vol. 26. P. 223–229.
9. V.V. Koval, R.M. Minyaev, V.I. Minkin. Peculiar structure of the potential energy surfaces of typical electrocyclic reactions in the areas of the symmetry-forbidden reaction paths // *Comp. Theor. Chem.* **2014**. Vol. 1030. P. 44–52.
10. R.M. Minyaev, W. Quapp, B. Schmidt, I.V. Getmanskii, V.V. Koval. Unusual reaction paths of S_N2 nucleophile substitution reactions $CH_4+H^- \rightarrow CH_4+H^-$ and $CH_4+F^- \rightarrow CH_3F+H^-$: Quantum chemical calculations // *Chem. Phys.* **2013**. Vol. 425. P. 170–176.

MAIN PRESENTATIONS

1. Vitaliy V. Koval, Ruslan M. Minyaev. Noncovalent interactions in the New Nonclassical Compounds based on boron tetrahedrons. Paper presented at the 1st International Conference on Noncovalent Interactions (ICNI-2019), 2-6 September **2019**, Lisbon, Portugal.
2. Vitaliy V. Koval, Ruslan M. Minyaev. The Nature of Chemical Bonds in the New Nonclassical Compounds and Materials. Paper presented at the Global conference on Nanotechnology and Material Science (GNMS-2019), 8-10 April **2019**, Valencia, Spain.

RELEVANT SKILLS

Extensive knowledge of chemical program packages Gaussian 16 and Vasp.
Fluent in English.
Programming ability in C++ and Python.
Abilities of system administration in Linux.