

CURRICULUM VITAE

Family name: IVANOV

First name: Volodymyr (Vladimir)

Present position:

Professor,
Materials Chemistry department
V. N. Karazin Kharkiv National University

Address

Svobody sq. 4, Kharkiv-22, 61022, UKRAINE

Phone: +38(057)707-51-29

Email: vivanov@karazin.ua

Personal data

Title: Professor

Date and place of birth: November 24, 1959

Citizenship: Ukraine



Education

Period(from/to)	Name of institution	Position	Main subject studied
09/1977-07/1982	A. M. Gorky Kharkov State University	student	Chemistry

Qualification

Master degree (in Chemistry) Kharkiv State University, 1982

PhD (Candidate of Science) Kharkiv State University, 1992

DrSc (Doctor of Science) V. N. Karazin Kharkiv National University, 2010

Employment

Period (from/to)	Position	Employer and place of work
2010 – present time	Professor	Materials Chemistry Department V.N.Karazin Kharkiv National University
2002 – 2010	Docent (Associate Professor)	Materials Chemistry Department V.N.Karazin Kharkiv National University
2007	Visiting researcher	Chemistry department, University of Pisa, Pisa, ITALY
1998 – 2002	Visiting researcher	Computational Chemistry Laboratory, University of Arizona, Tucson, USA.
1992 – 2002	Senior Researcher	Institute of Chemistry Kharkiv National University
1986 – 1992	Junior Researcher	Institute of Chemistry Kharkiv National University
1983 – 1986	Junior Researcher.	Institute for Single Crystals, (Ukrainian Academy of Sciences, Kharkiv)
1982 – 1983	Chemical Engineer	Institute for Single Crystals, (Ukrainian Academy of Sciences, Kharkiv)

Lecturer. Subjects read at the V. N. Karazin Kharkiv National University

- Molecular modeling;
- Contemporary computational methods in chemistry;
- Chemoinformatic and informational technology in chemistry;
- Statistical and chemometric methods on chemistry;
- Computer aided drug design;
- Chemical information and chemometric;
- Applied quantum chemistry;
- UV-Vis Molecular Spectroscopy;
- Quantum mechanic and quantum chemistry;
- Numerical methods;
- Programming.

Research interests

- Electron Correlation phenomena and Coupled Cluster theory;
- Quantity Structure – Activity Relationships (QSAR);
- Theoretical Interpretation of Molecular Spectrum;
- Linear and Nonlinear optical (Frequency-Depended) molecular properties;

Computational and programming experience

- Quantum Chemistry Software developer under Windows and Linux
- Programming languages: FORTRAN, Python, JavaScript
- Nonlinear (up to non-smooth) optimization.
- Quantum Chemistry Calculations (packages: GAMESS, Gaussian, Dalton, Columbus, Orca)

10. Research funding

- Organic modifiers, ion-molecular systems for new materials in analytical and electrochemical use. Ministry of Education and Science of Ukraine. 2018 – 2020; (Principal Investigator).

PhD thesis defended under V. V. Ivanov supervision

1. Lyakh D. I. The Coupled Cluster Theory in ab initio calculations of potential energy surfaces for small molecules; Kharkiv, Ukraine, 2009.
2. Klimenko T. A. The Coupled Cluster theory of excited and perturbed electronic states; Kharkiv, Ukraine, 2011.
3. Zakharov A. B. Optical and non-linear optical properties of π -conjugated oligomers in local coupled-cluster theory; Kharkiv, Ukraine, 2016.
4. Berdnyk M. I. L_1 -regularization method for the description of the physical and chemical properties of molecules; Kharkiv, Ukraine, 2021.

More than a hundred articles have been published in Soviet, Ukrainian and International Science Journals.

List of selected publications.

1. A. B. Zakharov, D. K. Tsarenko, **V. V. Ivanov** *Topological characteristics of iterated line graphs in the QSAR problem: a multigraph in the description of properties of unsaturated hydrocarbons*. Struct. Chem. **32** (2021) 1629–1639.

2. A. B. Zakharov, **V. V. Ivanov**, L. Adamowicz. *Electronic Perturbation Effects in the presence of Electric Field for π -conjugated systems: An electron correlation Study*. International Journal of Quantum Chemistry. (2020) e26260.
3. A. V. Ivachtchenko, S. M. Kovalenko, D. V. Kravchenko, O. D. Mitkin, **V. V. Ivanov** and T. Langer. *Crystal structure, Hirshfeld analysis and a molecular docking study of a new inhibitor of the Hepatitis B virus (HBV): ethyl 5-methyl-1,1-dioxo- 2-{[5-(pentan-3-yl)-1,2,4-oxadiazol-3-yl]methyl}- 2H-1,2,6-thiadiazine-4-carboxylate*. Acta Cryst. **E76** (2020)12
4. A. B. Zakharov, A. V. Dyachenko, **V. V. Ivanov**, *Topological Characteristics of Iterated Line Graphs in QSAR Problem: Octane Numbers of Saturated Hydrocarbons*. Journal of Chemometrics. **33** (2019) e3169.
5. M. I. Berdnyk, A. B. Zakharov, **V. V. Ivanov**, *Application of L_1 -regularization approach in QSAR problem. Linear regression and artificial neural networks*. Methods and Objects of Chemical Analysis. **14** (2019) 79
6. A. V. Ivachtchenko, O. D. Mitkin, D. V. Kravchenko, S. M. Kovalenko, S. V. Shishkina, N. D. Bunyatyan, I. S. Konovalova, I. G. Dmitrieva, **V. V. Ivanov**, T. Langer. *Synthesis, X-ray crystal structure, Hirshfeld surface analysis, and molecular docking study of novel inhibitor of hepatitis B: methyl 4-fluoro-3-(morpholinosulfonyl)benzo[b]thiophene-2-carboxylate*. Heliyon. **5** (2019) e02738 (10 pages).
7. V. Khristenko, A.V. Panteleimonov, R.Yu. Iliashenko, A. O. Doroshenko, **V. V. Ivanov**, O. S. Tkachenko, E. V. Benvenuti, Yu. V. Kholin *Heterogeneous polarity and surface acidity of silica-organic materials with fixed 1-n-propyl-3-methylimidazolium chloride as probed by solvatochromic and fluorescent dyes*. Colloids and Surfaces A: Physicochemical and Engineering Aspects. **538** (2018) 280.
8. M. O. Onizhuk, A. V. Panteleimonov, Yu. V. Kholin, **V. V. Ivanov** *Dissociation constants of silanol groups of silic acids: Quantum Chemical Estimations*. Journal of Structural Chemistry. **59** (2018) 275.
9. **V. V. Ivanov**, M. I. Berdnyk, L. Adamowicz, *L_1 – regularisation of the Coupled Cluster solutions*. Molecular Physics. **115** (2017) 2892.
10. M. O. Onizhuk, **V. V. Ivanov**, A. V. Panteleimonov, Yu.V. Kholin *Alternative Methods for Constructing of Linear Regressions*. Methods and objects of chemical analysis. **12** (2017) 105.
11. B. Zakharov, **V. V. Ivanov**, L. Adamowicz. *Optical Parameters of π -Conjugated Oligomer Chains from the Semiempirical Local Coupled-Cluster Theory*. in book: "Practical Aspects of Computational Chemistry IV" J. Leszczynski, M. K. Shukla (Eds.). Springer Science + Business Media, New York, 2016. Chapter 3, P. 57-102.
12. A. B. Zakharov, **V. V. Ivanov**, L. Adamowicz. *π -Electron Calculations Using the Local Linear-Response Coupled-Cluster Singles and Doubles Theory*. Journal of Physical Chemistry. C **119** (2015) 28737.
13. A. B. Zakharov, **V. V. Ivanov**, L. Adamowicz, *Molecular Nonlinear Optical Parameters of π -Conjugated Non-Alternant Hydrocarbons Obtained in Semiempirical Local Coupled-Cluster Theory*. Journal of Physical Chemistry. C **118** (2014) 8111.
14. **V. V. Ivanov**, A. B. Zakharov, L. Adamowicz, *Molecular dipole static polarisabilities and hyperpolarisabilities of conjugated oligomer chains calculated with the local π -electron coupled cluster theory*. Molecular Physics. **111**, (2013) 3779.
15. **V. V. Ivanov**, T. A. Klimenko, D. I. Lyakh, L. Adamowicz. *Multireference State-Specific Coupled Cluster Theory with a Complete Active Space Reference*. in book: "Practical Aspects of Computational Chemistry I: An Overview of the Last Two Decades and Current Trends" Eds. J. Leszczynski, M. K. Shukla and H. de Rode. Springer, 2012. Chapter 3, P. 69-101.

16. **V. V. Ivanov**, D. I. Lyakh, L. Adamowicz. *State-specific multireference theory of molecular electronic excited states*. Annual Reports on the Progress of Chemistry, Sect. C. **107** (2011) 169.
17. **V. V. Ivanov**, D. I. Lyakh, L. Adamowicz. *Electronic Excited States in the State-Specific Multireference Coupled Cluster Theory with a Complete-Active-Space Reference*. in book: "Recent Progress in Coupled Cluster Methods: Theory and Applications" Series: Challenges and Advances in Computational Chemistry and Physics, *V. 11*, Carsky, Petr; Paldus, Josef; Pittner, Jiri (Eds.). Springer, 2010, P.219-249.
18. T. A. Klimenko, **V. V. Ivanov**, D. I. Lyakh, L. Adamowicz. *A calculation of spectroscopic parameters for hydrogen fluoride with multi-reference state-specific coupled-cluster method*. Chemical Physics Letters. **493** (2010) 173.
19. **V. V. Ivanov**, D. I. Lyakh., L. Adamowicz. *Multireference state-specific coupled cluster methods. State-of-the-art and perspectives*. Physical Chemistry Chemical Physics. **11** (2009) 2355.
20. D. I. Lyakh, **V. V. Ivanov**, L. Adamowicz. *A generalization of the state-specific complete-active-space coupled-cluster method for calculating electronic excited states*. Journal of Chemical Physics. **128** (2008) 074101 (15 pages).
21. D. I. Lyakh, **V. V. Ivanov**, L. Adamowicz. *State-specific multireference complete-active-space coupled-cluster approach versus other quantum chemical methods: dissociation of the N₂ molecule*. Molecular Physics. **105** (2007) 1335.
22. **V. V. Ivanov**, L. Adamowicz, D. I. Lyakh. *Excited states in the Multireference State-Specific Coupled Cluster theory with the complete active space reference*. Journal of Chemical Physics. **124** (2006) 184302 (9 pages).
23. **V. V. Ivanov**, D. I. Lyakh, L. Adamowicz. *New indices for describing the Multi-configurational nature of the Coupled Cluster wave function*. Molecular Physics. **103** (2005) 2131.
24. D. I. Lyakh, **V. V. Ivanov**, L. Adamowicz. *Automated Generation of Coupled Cluster Diagrams. Implementation in the Multireference State-Specific Coupled Cluster Approach with the CAS Reference*. Journal of Chemical Physics. **122** (2005) 024108 (13 pages).



E-mail: vivanov@karazin.ua

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