

## Curriculum Vitae

Professor Boris F. Minaev

Head of Chemistry and Nanomaterials Department  
At Bogdan Khmel'nitskij National University in Cherkasy, Ukraine,  
The Honored Worker of Science and Technology of Ukraine.

**Birth day:** 21.09.1943; City Yekateriburg, Russia.

**Education and carrier:** 1962-1967 - student of Physical Faculty of Tomsk State University (Russia, Siberia)

14.07.1967: Master degree in Physics (Tomsk State University, Russia).

1967-1971 – PhD student at Spectroscopy Department of the Tomsk State University.

1971-1972 – Junior Scientific worker at Molecular Spectroscopy Laboratory of Siberian Physics-Technical Institute at the Tomsk State University.

1972-1974 - Junior Scientific worker at Chemical Faculty of the Tomsk State University.

31.01.1974 PhD defense in Physics and Mathematics at the Tomsk State University.

15/05/1974 PhD approval.

05.05.1974 – Assistant professor at Theoretical Physics Department in Karaganda State University (KarSU).

1975-1976: Senior Scientific worker at Chemical Faculty of KarSU.

1976-1984: Head of Physical Chemistry Department at Chemical Faculty of KarSU.

17.04.1984 - Defence of Dr. Sci. Dissertation in Chemistry at Moscow Institute of Chemical Physics of the USSR Academy of Sciences: “Theoretical analysis and progontication of spin-orbit coupling effects in molecular spectroscopy and in chemical kinetics”

21.09.1984: Approval of Dr. Sci. Degree by the USSR Attestation Committee.

1984-1989 – Head of Quantum Chemistry Department at Chemical Faculty of KarSU.

23.01.1986: Professor in Quantum Chemistry approval by the USSR Attestation Committee.

6.02.1989-12.10.2007: Head of the General Chemistry Department at Cherkasy State University of Technology, Cherkasy, Ukraine.

12.10.2007-nowadays: Head of Organic Chemistry Department at Cherkasy State University by B. Khmel'nitskij, Cherkasy, Ukraine.

**Scientific Awards:** 22.08.2012: The Honored Worker of Science and Technology of Ukraine.

1999: Life achievements award from American Biographic Institute for “The Singlet Oxygen Emission Theory”.

### **Leader and Coordinator of international research projects:**

NATO project in terms of the REHE program (Relativistic effects in heavy elements) 1998-1999 together with prof. Pekka Pyyko “Spin-orbit coupling effects in chemical reactions”. Head of Organizing Committee of the international conference in Torun (Poland) in January 1999.

Swedish-Ukrainian “Visby” project together with prof. Hans Agren (KTH): “Organic Light Emitting Diodes Theory” (2008-2011).

CRDF (USA-Ukrainian) project together with prof. Tom Slanger (SRI International, USA): “Spin-forbidden transitions of molecular oxygen and new emission bands from the upper atmosphere” (2006-2007).

Romanian-Ukrainian project: Organic-Inorganic Materials for Solar Cells (with prof. Mihai Girtu, Ovidius University in Konstanca) 2007-2009.

**Leader and Coordinator of national research projects:** a number of projects in organic synthesis and electronic structure calculations (2007-2015) governed by Ministry of Education and Science in Ukraine.

**Participatation in the project evaluation as an expert:** Expertise of 4 projects of the Swedish Research Council in 2008-2009, evaluation of Austrian, Romanian, Dutch national projects 2013-2015.

Expertise of 19 projects governed by Ministry of Education and Science in Ukraine during 2007-2015.

**Hirsch index:** 29(without self-citation – 24).

**Total number of publications – 546. (In journals with impact factor – 302).**

**Scientific interests:** Spin-forbidden transitions in molecular spectroscopy and in chemical reactions. Spin-catalysis concept and its implementation in heterogeneous and homogeneous catalytic reactions. Enzymatic reactions of molecular oxygen. Glucoseoxidase and electronic mechanism of its half-reaction. Hydrocarbons oxidation.

Spin-forbidden transitions of molecular oxygen and new emission bands from the upper atmosphere. Zero-field splitting in the triplet excited state of organic molecules and in metallo-complexes. Hyper-fine splitting in EPR and g-factor calculations by MC SCF and DFT methods.

Phosphorescence of organic molecules and of metallo-complexes. Catalysis. The UV-visible, IR and Raman spectra of new organic species. Tetraoxa[8]circulenes, sulfloweres, Pt(II)acetylides. Ir(III) complexes with phenylpyridins and other ligands, Fe(II) bisimine pyridine catalysts of ethylene polymerization.

Polymerization of olefins and of large aromatic species. Spectroscopy of polymers. Quantum chemistry calculations of all types of spectroscopy.

30 papers from Minaev's list:

1. **Boris F. Minaev**. Ab initio study of the ground state properties of molecular oxygen. *Spectrochimica Acta*. Part A, 60 (2004) 1027–1041.
2. Mircea Grigoras, Ana Maria Catargiu, Teofilia Ivan, Loredana Vacareanu, **Boris Minaev**, Evgeniy Stromylo. Tuning optical and electronic properties of poly(4,4'-triphenylamine vinylene)s by post-modification reactions. *Dyes and Pigments* 113 (2015) 227-238.
3. E. V. Stromylo, G. V. Baryshnikov, **B. F. Minaev**, and M. Grigoras. Quantum-Chemical Investigation of the Structure and Electronic Absorption Spectra of Symmetric Triphenylamine Oligomers Conjugated to Vinylene, Imine, Azine, and Ethynylene Groups. *Optics and Spectroscopy*, 2015, Vol. 118, No. 5, pp. 703–710.
4. **B. F. Minaev**. Intensities of Spin-Forbidden Transitions in Molecular Oxygen and Selective Heavy-Atom Effects. *International Journal of Quantum Chemistry*, vol. 17, **367-374** (1980).
5. **B. F. Minaev**. Problem of the Stark effect in spectra of phosphorescent-microwave double resonance. *Optics and Spectroscopy*, Volume 50, Issue 2, 1981, pp.209-210.
6. **B. F. Minaev**. The singlet oxygen absorption to the upper state of the Schumann-Runge system. *Phys. Chem. Chem. Phys.*, 1999, 1, 3403-3413.
7. **Boris F. Minaev**, N. Arul Murugan, and Hans Agren. Dioxygen Spectra and Bioactivation *International Journal of Quantum Chemistry*, 2013, 113, 1847–1867.
8. **Boris F. Minaev**, Valentina A. Minaeva, Yuriy V. Evtuhov. Quantum-Chemical Study of the Singlet Oxygen Emission. *International Journal of Quantum Chemistry*, Vol 109, 500–515 (2009).
9. **Boris F. Minaev**, G.I. Kobzev. Response calculations of electronic and vibrational transitions in molecular oxygen induced by interaction with noble gases. *Spectrochimica Acta*, Part A. 59 (2003) 3387-341010.
10. **Boris Minaev**, Xin Li, Zhijun Ning, He Tian and Hans Ågren. **Organometallic Materials for Electroluminescent and Photovoltaic Devices**. In: Organic Light Emitting Diode – Material, Process and Devices. InTech, Rieka, 2011, pp. 62-100.
11. Ågren, H.; Vahtras, O., **Minaev, B.** Response theory and calculations of spin-orbit coupling phenomena in molecules. *Advances Quantum Chemistry*, (1996). Vol. 27, pp. 71-162.
12. Li, X.; **Minaev, B.**; Ågren, H. & Tian, H. (2011). Theoretical study of phosphorescence of iridium complexes with fluorine-substituted phenylpyridine ligands. *Eur. J. Inorg. Chem.* DOI: 10.1002/ejic.201100084.
13. Lindgren, M.; **Minaev, B.**; Glimsdal, E.; Vestberg, R.; Westlund, R. & Malmstrom, E. (2007). Electronic states and phosphorescence of dendron functionalized platinum(II) acetylides. *Journal of Luminescence*, Vol. 124, pp. 302-310.
14. **Minaev, B.F.** & Terpugova, A.F. (1969). Spin-orbit interaction in charge-transfer complexes. *Journal of Soviet Physics*, No. 10, pp. 30-36.
15. **Minaev, B.F.** (1978). Spin-orbit interaction in molecules and mechanism of the external magnetic field on luminescence. *Optics and Spectroscopy*, Vol. 44, No. 2, pp. 256-260.
16. **Minaev, B.F.** (1972). Spin-orbit interaction in doublet states of molecules. *Optics and Spectroscopy*, Vol. 32, No. 1, pp. 22-27.
17. **Minaev, B.**; Minaeva, V.; & Ågren, H. (2009). Theoretical Study of the Cyclometalated Iridium(III) Complexes Used as Chromophores for Organic Light-Emitting Diodes. *J. Phys. Chem. A*. Vol. 113, pp. 726-735.

18. **Minaev, B.**; Ågren, H. & De Angelis, F. (2009a). Theoretical design of phosphorescence parameters for organic electro-luminescence devices based on iridium complexes. *Chemical Physics*, Vol. 358, pp. 245-257.
19. **Minaev, B.**; Jansson, E. & Lindgren, M. (2006). Application of density functional theory for studies of excited states and phosphorescence of platinum(II) acetylides. *J. Chem. Physics*, Vol. 125, pp. 094306-094313.
20. **Minaev, B.** & Ågren, H. (2005). Theoretical DFT study of phosphorescence from porphyrins. *Chem. Physics*, Vol. 315, pp. 215-239.
21. **Minaev, B.** & Ågren, H. (1999). Spin uncoupling in molecular hydrogen activation by platinum clusters. *J. Molecular Catalysis, A: Chemical*, Vol. 149, pp. 179-195.
22. **Minaev, B.**; Wang, Y.H.; Wang, C.K.; Luo, Y. & Ågren, H. (2005). Density functional study of vibronic structure of the first absorption Qx band in free-base porphyrin. *Spectrochimica Acta, A*. Vol. 65, pp. 308-323.
23. **Minaev, B.F.**; Jansson E.; Ågren, H. & Schrader, S. (2006). Theoretical study of phosphorescence in dye doped light emitting diodes. *J. Chem. Physics*, Vol. 125, No. 23, pp. 234704.
24. **Minaev, B.F.**; Minaeva, V.O.; Baryshnikov, G.V.; Girtu, M. & Ågren, H. (2009b). Theoretical study of vibration spectra of sensitizing dyes for photoelectrical converters based on ruthenium (II) and iridium (III) complexes *Rus. J. Appl. Chem.* Vol. 82, pp. 1211–1221.
25. Xin Li, **Boris Minaev**, Hans Ågren, and He Tian. Density Functional Theory Study of Photophysical Properties of Iridium(III) Complexes with Phenylisoquinoline and Phenylpyridine Ligands. *J. Phys. Chem. C* 2011, 115, 20724–20731.
26. **Boris Minaev**, Gleb Baryshnikov and Hans Ågren. Principles of phosphorescent organic light emitting devices. *Phys. Chem. Chem. Phys.*, 2014, 16, 1719—1758.
27. Dmytro Volyniuk, Vladyslav Cherpak, Pavlo Stakhira, **Boris Minaev**, Gleb Baryshnikov. Highly Efficient Blue Organic Light-Emitting Diodes Based on Intermolecular Triplet–Singlet Energy Transfer. *J. Phys. Chem. C* 2013, 117, 22538–22544.
28. V. Cherpak, P. Stakhira, **B. Minaev**, G. Baryshnikov, E. Stromylo, I. Helzhynskyy, M. Chapran. Efficient “Warm-White” OLEDs Based on the Phosphorescent bis-Cyclometalated iridium(III) Complex. *J. Phys. Chem. C* 2014, 118, 11271–11278.
29. Vladyslav Cherpak, Pavlo Stakhira, **Boris Minaev**, Gleb Baryshnikov, Evgeniy Stromylo. Mixing of Phosphorescent and Exciplex Emission in Efficient Organic Electroluminescent Devices. *DOI: 10.1021/am507050g. ACS Appl. Mater. Interfaces.* (2015).
30. Corneliu I. Oprea, **Boris F. Minaev**, Hans Ågren, Fania Cimpoesu. **Comparative computational IR, Raman and phosphorescence study of Ru- and Rh-based complexes.** *Molecular Physics*, 2013, Vol. 111, Nos. 9–11, 1526–1538.
31. **B F Minaev**, G V Baryshnikov, V A Minaeva. Electronic structure, aromaticity and spectra of hetero[8]circulenes. *Russian Chemical Reviews* 84 (5) 455 – 484 (2015)