CURRICULUM VITAE

1. Family name: KALUGIN
First name: Oleg
Middle name: Nikolaevich

2. Present position

Dean of the School of Chemistry,
Professor, Department of Inorganic Chemistry,
V.N. Karazin Kharkiv National University
Svoboda sq., 4, Kharkiv - 22, 61022, UKRAINE
Tel/Fax: +38 (057) 7075556
E-mail: onkalugin@gmail.com, chemdean@karazin.ua

3. Personal data

Title: Doctor
Date and place of birth: June 13, 1961; Velikiy Burluk, Kharkiv region, UKRAINE
Nationality: Ukrainian
Marital status: married, one child

4. Education

Period (from/to)	Name of institution	Position	Main subjects studied
09/1977-07/1982	Kharkiv State University	student	chemistry, physics, mathematics, English
09/1982-09/1986	Kharkiv State University	post graduate	physical chemistry, computers and programming, English

5. Qualification

Master degree (in Chemistry)	Kharkiv State University, 1982
PhD (Candidate of Science)	Kharkiv State University, 1987

6. Employment

Period (from/to)	Position	Employer and place of work
12/2006 - till now	Dean of the School of Chemistry	Kharkiv National University (KhNatUni)
12/2013 - till now	Professor	Department of Inorganic Chemistry, KhNatUni
12/1990 - 12/2013	Docent (Associate Professor)	Department of Inorganic Chemistry, KhNatUni
09/1988 - 12/1990	Senior teacher	Department of Inorganic Chemistry, KhStUni
10/1987 - 08/1988	Senior researcher	Institute of Chemistry, KhStUni
10/1986 - 09/1987	Junior researcher	Institute of Chemistry, KhStUni
11/1997 - 12/1997	DAAD Visiting Postdoctoral Fellow	Department of Theoretical Physics, Rostock University, Rostock, GERMANY
02/1998 - 02/1999	Visiting Postdoctoral Fellow within the Royal Society / NATO Programme	Division of Molecular & Life Sciences, University Abertay Dundee, Dundee, Scotland,UK
03/2009 - 04/2009	Visiting Scientist	Department of Chemistry, University of Washington, Seattle, USA
04/2012 - 04/2012	Visiting Professor, Erasmus Mundus Master of Science in "Advanced spectroscopy in chemistry"	LASIR, University of Science and Technology Lille1 Villeneuve d'Ascq, France
04/2013 - 05/2013	Visiting Professor	Division of Environment and Forensic Sciences School of Contemporary Sciences, University Abertay Dundee, Dundee, Scotland,UK
07/2013 - 07/2013	Visiting Scientist	Department of Chemistry University of Rochester Rochester, NY, USA
06/2013 - 06/2013 09/2013 - 09/2013	Invited Professor	LASIR, University of Science and Technology Lille1 Villeneuve d'Ascq, France
03/2015 - 03/2015	Invited Professor	LASIR, University of Lille1, Science and Technology Villeneuve d'Ascq, France
04/2016 - 04/2016	Visiting Professor (ERASMUS+)	University of Nice, Nice, France

02/2016 - 03/2016	Visiting Professor	University of Southern California, Los Angeles, USA
04/2016 - 04/2016	Visiting Professor (ERASMUS+)	LASIR, University of Science and Technology Lille1 Villeneuve d'Ascq, France
04/2017 - 04/2017	Visiting Professor (ERASMUS+)	LASIR, University of Science and Technology Lille1 Villeneuve d'Ascq, France
11/2017 - 12/2017	Visiting Professor (ERASMUS+)	University of Nice Nice, France
12/2017 - 12/2017	Visiting Professor (ERASMUS+)	LASIR, University of Science and Technology Lille1 Villeneuve d'Ascq, France
12/2018 - 12/2018	Visiting Professor (ERASMUS+)	LASIR, University of Lille Villeneuve d'Ascq, France
03/2019 - 03/2019	Visiting Professor (ERASMUS+)	Université Côte d'Azur Nice, France
04/2019 – 04/2019	Visiting Professor (ERASMUS+)	LASIR, University of Lille Villeneuve d'Ascq, France

7. Subjects read at the Kharkiv National University

- Inorganic and General Chemistry
- Mathematical methods and their application in Chemistry
- Statistical Mechanics of Fluids
- Interparticle interactions and particle dynamics in solutions
- Molecular Dynamics simulations of disordered condensed matter
- Molecular Modelling
- Physical Research Methods
- Chemistry of Technological Solutions

8. Research interests

- Molecular modelling of structure, thermodynamic and dynamic properties of molecular and ionic liquids and non-aqueous electrolyte solutions by using (*i*) molecular dynamics simulation, and (*ii*) *ab initio* quantum chemical calculations
- Experimental and theoretical study of inter-ion, ion-molecular and intermolecular interactions and particle dynamics in molecular and ion-molecular systems in bulk phase and inside carbon nanomaterials for development of the Li-ion batteries and EDLSC
- Molecular design and optimization of photoinduced process for photovoltaic solar cells
- Atomistic simulations of coating of silver nanoparticles in liquid media

9. Computational and programming experience

Well experienced in operation systems: Windows and LINUX.
Experienced in usage of programming languages: Fortran, C and C++ and object-oriented methods.
Have coded a lot of programs for scientific calculations, including molecular dynamics simulations, non-linear optimisation and NDIS & QENS data analysis.
Experienced in using and installing computer software for carrying out computer modelling by using molecular and Brownian dynamics simulations (*DL_POLY* (UK), *GROMACS*, *MDNAES* (own) and *ab initio* quantum chemical calculations (*GAMESS* and *Gaussian*).
Fluent in using and installing modern desktop office software.

10. Research funding

- Physical-chemical bases of direct using of electrolyte solutions; Ministry of Education of Ukraine; Dates: 01/1994-12/1995; (Principal Investigator).
- Molecular dynamics and spectroscopy of ion-molecule systems; Fundamental Researches Fund of Ukraine; Dates: 01/1994-12/1995; (Grant Value Holder).
- Prediction of transport properties of unsymmetrical electrolytes in non-aqueous solvents in wide temperature range; International Science Foundation of J. Soros; Dates: 01/1994-12/1995 (Grant Value Holder and Principal Investigator).
- Non-Coulombic interparticle interactions in solvents with low and moderate dielectric constant; Ministry of Education of Ukraine; Dates: 01/1996-12/1997; (Principal Investigator).
- Dynamics of ion solvation and interparticle interactions in the solutions of symmetrical and unsymmetrical electrolyte solutions in non-aqueous solvents; Ministry of Education of Ukraine;
- Dates: 01/1998-12/1999; (Principal Investigator).

- Theoretical basis of purposeful usage of non-aqueous electrolyte solutions in electrochemical devices and processes; Ministry of Education of Ukraine; Dates: 01/2000 – 12/2002; (Principal Investigator).
- Structure, dynamics and interparticle interactions in liquid non-aqueous ion-molecular systems. Ministry of Education and Science of Ukraine; Dates: 01/2003 – 12/2005; (Principal Investigator).
- Dynamic structure and conductance of ion-molecular systems in bulk phase and inside carbon nanomaterials. Ministry of Education and Science of Ukraine; Dates: 01/2006 – 12/2009; (Principal Investigator).
- Pico- and nanosized processes in ionic liquids and ion-molecular systems as a basis of contemporary functional materials. Ministry of Education and Science of Ukraine; Dates: 01/2009 – 12/2011; (Principal Investigator).
- Microscopic basis of the purposeful prediction of the functional properties of the molecular, ionic and ion-molecular liquids in the bulk phase and in Carbon Nanomaterials. Ministry of Education, Science, Youth and Sport of Ukraine; Dates: 01/2012 – 12/2014; (Principal Investigator).
- Modelling and creation of nanoconjugates for pharmaceutical application. Ministry of Education and Science of Ukraine; Dates: 01/2013 – 12/2016; (Principal Investigator).
- Conceptual basis of prognosis of the functional properties of ion-molecular systems and molecular complexes. Ministry of Education and Science of Ukraine; Dates: 01/2015 – 12/2017; (Principal Investigator).
- Organic modifiers, ion-molecular systems for new materials in analytical and electrochemical use. Ministry of Education and Science of Ukraine; Dates: 01/2018 – 12/2020; (Principal Investigator).
- High-performance photovoltaic solar cells based on new dye-sensitizers. Molecular design and optimization of photoinduced process. Joint Ukraine-France R&D projects “DNIPRO” for the period of 2019–2020. Ministry of Education and Science of Ukraine & French Embassy in Ukraine; Dates: 01/2019 – 12/2020; (Grant Value Holder).
- Fundamental principles of management of physico-chemical and operational properties of micro- and nanostructures: theoretical forecasting and experimental study. Ministry of Education and Science of Ukraine; Dates: 01/2019 – till now; (Grant Value Co-holder).

11. PhD thesis defended under O.N. Kalugin’s supervision

1. Smortsova Ye. Yu. Dye sensitized solar cells efficiency improvement: optimization of the electrolyte using ionic liquids/molecular solvents mixture and study of the photodynamic properties of organic indolinic derivative dyes; Lille, France, 2018.
2. Koverga V.A. Local Structure Organization in Ionic Liquids and Molecular Solvents Mixtures: A Molecular Dynamics Simulation; Lille, France, 2017.
3. Chernozhuk T.V. Electrical conductivity, solvatation and interparticle interactions in lithium salts solutions in γ-butyrolaktone, propylene carbonate and a mixtures of propylene carbonate with 1,2-dimethoxyethane; Kharkiv, Ukraine, 2015.
4. Marekha B.A. Microscopic Structure and Dynamics in Mixtures of Imidazolium-Based Ionic Liquids with Polar Aprotic Solvents: NMR, Raman Spectroscopy and Molecular Modeling; Lille, France, 2014.
5. Lukinova O. V. Peculiarities of physical and chemical properties of highly concentrated solutions of R_4NX (R=Bu, Et, X=BF_4, Br) in acetonitrile; Kharkiv, Ukraine, 2013.
6. Voroshylova Iu. V. Physical and chemical properties and microstructure of binary mixtures based on imidazolium and pyridinium ionic liquids with acetonitrile and methanol. Kharkiv, Ukraine, 2013.
7. Agieienko V. N. Electrical conductivity, association and complexation in acetonitrile solutions of double charged metals perchlorates with participation of 3-hydroxyflavone.; Kharkiv, Ukraine, 2011.
8. V.V. Chaban. The Peculiarities of Microstructure and Dynamics of Non-Aqueous Solvents and Electrolyte Solutions Confined by Carbon Nanotubes; Kharkiv, Ukraine, 2009.
9. Kolesnik Ya.V. Microscopic structure and dynamics of electrolyte solutions in acetonitrile and methanol: molecular dynamics simulation; Kharkiv, Ukraine, 2004.
10. Gorobets M.A. Viscosity and dynamics of interparticle interactions of 1-1 and 2-1 electrolytes in aprotic solvents; Kharkiv, Ukraine, 2001.
11. Volobuev M.N. ; Computer simulations of dimethylsulphoxide and its electrolite solutions by using molecular dynamics method.; Kharkiv, Ukraine, Kharkiv, Ukraine, 2000.
12. Nerukh D.A. ; Interparticle interactions and dynamics of molecules in electrolyte solutions of n-hexanol and acetonitrile by vibrational spectroscopy.; Kharkiv, Ukraine, 1996.
13. Rebie Mohamed Naser Jalah; Solvation of 1-1 electrolytes in DMF at 25-70°C from the viscosimetry and radiometry data; Kharkiv, Ukraine, 1995.

12. Key publications

1. **O.N. Kalugin**, et al. *IR and NMR Studies of Hydrogen Bond in 1-Hexanol - Bu_4NI Solutions on the Temperature Range 28-145°C and in CCl_4 Medium.* J. Chem. Soc. Faraday Trans. II. 90 (1994) 297.

2. **O.N. Kalugin**, et al. *Dynamics of acetonitrile molecules in its electrolyte solutions from Raman spectra*. J. Inorg. Chem. (Russ.) **41** (1996) 261.
3. **O.N. Kalugin**, A.V. Lebed and I.N. Vyunnik. *Properties of 1-1 Electrolytes Solutions in Ethylene Glycol at Temperatures from 5 to 175°C. II. Limiting ion conductances and Ion-Molecular Interactions*. J. Chem. Soc. Faraday Trans. II. **94** (1998) 2103.
4. **O.N. Kalugin**, M.N. Volobuev and Ya.V. Kolesnik. *MDNAES: the program set for computer modelling of ion molecular systems by using molecular dynamics method*. Kharkiv University Bulletin, Chemical Series. **454** (1999)58.
5. L. Bianchi, A.K. Adya, **O.N. Kalugin** and C.J. Wormald. *The structure of liquid methanol: A molecular dynamic study using six-site model.* J. Phys: Condens. Matter, **11** (1999) 9151.
6. **O.N. Kalugin** and A.K. Adya. *Microscopic structure of nickel(II) co-ordination shell in $NiCl_2$-methanol solution: neutron diffraction and ab initio studies*. Phys. Chem. Chem. Phys. **2** (2000) 11.
7. L. Bianchi, **O.N. Kalugin**, A.K. Adya and C.J. Wormald. *The structure of liquid methanol: A molecular dynamics study using three-site models*. Molec. Simul. **25**(5) (2000) 321.
8. A.K. Adya and **O.N. Kalugin**. *Microscopic structure of Cl^- co-ordination shell in $NiCl_2$- methanol solution: neutron diffraction study*. J. Chem. Phys. **113** (2000) 4740.
9. **O.N. Kalugin**, M.N. Volobuev, A.V. Ishchenko and A.K. Adya. *Structure and dynamics of Na^+ and Cl^- solvation shells in liquid DMSO: molecular dynamics simulations*. J. Mol. Liq., **91** (2001) 312.
10. A.K. Adya, **O.N. Kalugin,** M.N. Volobuev, Ya.V. Kolesnik. *Microscopic structure of liquid dimethyl sulphoxide and its electrolyte solutions: molecular dynamics simulations.* Molec. Phys., **99** (2001) 835.
11. Ya.V. Kolesnik, **O.N. Kalugin,** M.N. Volobuev. *New algorithm of integration of motion equations for multiatomic molecules in molecular dynamics simulations.* Chem. Phys. (Russ.) **20** (2001) 14.
12. **O. N. Kalugin**, M. N. Volobuev, Ya. V. Kolesnik. *Molecular dynamics simulation of microscopic structure and dynamics of ion solvation in dimethyl sulphoxide: ion charge influence.* Chem. Phys. (Russ.). **21(**7) (2002) 16.
13. **O. N. Kalugin**, Ya. V. Kolesnik. *Structure peculiarities of salvation and association of $LiClO_4$ in methanol*. J. Phys. Chem. (Russ.), **77**(6) (2003) 1.
14. Ya. V. Kolesnik, **O. N. Kalugin**. *Collective charge movement in solutions of lithium tetrafluoroborate in acetonitrile*. Elektrochem. (Russ.) **39** (4) (2003) 485.
15. **O.N. Kalugin**, A.K. Adya, M.N. Volobuev, Ya.V. Kolesnik. *Solvation of solvophilic and solvophobic ions in dimethyl sulphoxide: microscopic structure by molecular dynamics simulations*. Phys. Chem. Chem. Phys., **5 (**8) (2003) 1536.
16. **O. N. Kalugin,** N. A. Otroshko, I. N. V'yunnik. *Electroconduction, Association, and Ion–Molecular Interactions in Nickel Chloride Solutions in Methanol at 5–55°C.* Russ. J. Electrochem. **40** (7) (2004) 743.
17. **O. N. Kalugin,** V. G. Panchenko, and I. N. V'yunnik. *A Conductometric Study of Ionic Association and Interparticle Interactions in Solutions of 1-1 Electrolytes in Ethyl Acetate at 5–45 °C.* Russ. J. Phys. Chem., **79**(4) (2005) 629.
18. Ashok K Adya, **Oleg N Kalugin** and W Spencer Howells**.** Dynamics and structure of nickel chloride–methanol solutions: quasi-elastic neutron scattering and molecular dynamics simulations. J. Phys.: Condens. Matter **19** (2007) 415120 (22pp) doi:10.1088/0953-8984/19/41/415120.
19. **O. N. Kalugin**, Ya. V. Kolesnik, M.N. Volobuev. Microscopic structure and particle dynamics in ion-molecular systems on the basis of acetonitrile, dimethyl sulphoxide and methanol: Molecular Dynamics Simulations, pp. 408-524. In: Scientific heritage of N.A. Izmailov and topical problems of physical chemistry. Eds: V.I.Lebed, N.O. Mchedlov-Petrossyan, Yu.V. Kholin. Kharkov, 2007, 675p.
20. **O. N. Kalugin**, V. G. Panchenko, A. P. Dolgareva, A. G. Nikolaichuk, and I. N. V'yunnik. *Electrical Conductivity and Ionic Association of Lithium and Sodium Perchlorates in Tetrahydrofuran.* Russ. J. Phys. Chem. A **82** (2008) 1480.
21. Chaban V.V., **Kalugin O.N**. Structure and Dynamics in Methanol and its Lithium Ion Solution Confined by Carbon Nanotubes. J. Mol. Liq. (2008). doi:10.1016/j.molliq.2008.06.003
22. **Kalugin O.N.,** Chaban V.V., Loskutov V.V., Prezhdo O.V. *Uniform Diffusion of Acetonitrile inside Carbon Nanotubes Favors Supercapacitor Performance.* Nano Letters. (**2008)**. doi: 10.1021/nl072976g.
23. Bradley F. Habenicht, **Oleg N. Kalugin**, and Oleg V. Prezhdo. *Ab Initio Study of Phonon-Induced Dephasing of Electronic Excitations in Narrow Graphene Nanoribbons*. Nano Letters **8** (2008) 2510.
24. Chaban V.V., **Kalugin O.N.** *Structure and Dynamics in Methanol and its Lithium Ion Solution Confined by Carbon Nanotubes* // J. Mol. Liq. 145 (**2009**) 145–151.
25. Chaban V.V., **Kalugin O.N.** *Liquid dimethyl sulphoxide confined by carbon nanotubes* // J. Mol. Liq. **151** (2010) 113–116.
26. **Oleg N. Kalugin**, Vitaly V. Chaban and Oleg V. Prezhdo. In: Carbon Nanotubes - Synthesis, Characterization, Applications, Siva Yellampalli (Ed.), InTech (2011). ISBN: 978-953-307-497-9. Chapter 16, pp. 325-344.
27. V.V. Chaban, Iu.V. Voroshylova, **O.N. Kalugin**. *A new force field model for the simulation of transport properties of imidazolium-based ionic liquids* // Phys. Chem. Chem. Phys. **13** (17) (2011) 7910-7920.
28. V.V. Chaban, Iu. V. Voroshylova, **O. N. Kalugin**. *The Phenomenological Account for Electronic Polarization in Ionic Liquid //* ECS Transactions. **33** (28) (2011) 43-55.
29. Vladimir V. Matveev, Mikhail Zubkov, Erkki Laehderantab, Petri Ingman, **Oleg N. Kalugin** & Ashok K. Adya. *Composition of Ni^{2+} cation solvation shell in $NiCl_2$-methanol solution by multinuclear NMR* // Phys. Chem. Liq., **49** (6) (2011), 746-752.
30. O. O. Postupna, Y. V. Kolesnik, **O. N. Kalugin**, and O. V. Prezhdo. *Microscopic Structure and Dynamics of $LiBF_4$ solutions in Cyclic and Linear Carbonates* // J. Phys. Chem. B **115** (2011) 14563-14571.

31. **Oleg N. Kalugin**, Vira N. Agieienko, Natalya A. Otroshko. *Ion association and solvation in solutions of Mg^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+} and Ni^{2+} perchlorates in acetonitrile: Conductometric study* // J. Mol. Liq. **165** (2012) 78-86.
32. Chaban V.V., Voroshylova I.V., **Kalugin O.N.**, Prezhdo O.V. *Acetonitrile boosts conductivity of imidazolium ionic liquids*. // J. Phys. Chem. B. **116** (2012) 7719-7727.
33. **O.N. Kalugin**, Iu.V. Voroshylova, A.V. Riabchunova, E.V. Lukinova, V.V. Chaban. *Conductometric study of binary systems based on ionic liquids and acetonitrile in a wide concentration range s* // Elecrochim. Acta. **105** (2013) 188-199.
34. B.A. Marekha, **O. N. Kalugin**, M. Bria, R. Buchner, A. Idrissi . *Translational Diffusion in Mixtures of Imidazolium ILs with Polar Aprotic Molecular Solvents*. // J. Phys. Chem. B. **118**(2014) 5509-5517.
35. V. N. Agieienko, Y.V. Kolesnik, **O. N. Kalugin**. *Structure, solvation, and dynamics of Mg^{2+}, Ca^{2+}, Sr^{2+}, and Ba^{2+} complexes with 3-hydroxyflavone and perchlorate anion in acetonitrile medium: A molecular dynamics simulation study*. // J. Chem. Phys. **140** (2014) 194501.
36. V. N. Agieienko, **O. N. Kalugin**. *Complexation of $Ni(ClO_4)_2$ and $Mg(ClO_4)_2$ with 3-hydroxyflavone in acetonitrile medium: conductometric, spectroscopic and quantum chemical investigation*. // J. Phys. Chem. B. **118** (2014) 12251-12262.
37. O. M. Korsun, **O. N. Kalugin**, O. V. Prezhdo. *Control of Carbon Nanotube Electronic Properties by Lithium Cation Intercalation.* // J. Phys. Chem. Let. **5** (2014) 4129–4133.
38. I.A. Golenya, E. Gumienna-Kontecka, M. Haukka, O.M. Korsun, **O.N. Kalugin** and I. O. Fritsky. *Copper(II) complexes of 3- and 4-picolinehydroxamic acids: from mononuclear compounds to 1D- and 2D-coordination polymers*. // CrystEngComm. **16** (2014) 1904.
39. A. Kyrychenko, O. M. Korsun, Iu. I. Gubin, S. M. Kovalenko, and **O. N. Kalugin**. *Atomistic Simulations of Coating of Silver Nanoparticles with Poly(vinylpyrrolidone) Oligomers: Effect of Oligomer Chain Length* // J. Phys. Chem. C, **119 (14) (**2015)7888.
40. B. A. Marekha, M. Bria, M. Moreau, I. De Waele, F.-A. Miannay, Ye. Smortsova, T. Takamuku, **O. N. Kalugin,** M. Kiselev, A. Idrissi. *Intermolecular interactions in mixtures of 1-n-butyl-3-methylimidazolium acetate and water: Insights from IR, Raman, NMR spectroscopy and quantum chemistry calculations* // J. Mol. Liquids, **210** Part B (2015) 227.
41. B. A. Marekha, **O.N. Kalugin**, M. Bria and A. Idrissi. *Probing structural patterns of ion association and solvation in mixtures of imidazolium ionic liquids with acetonitrile by means of relative ^{1}H and ^{13}C NMR chemical shifts* // Phys.Chem.Chem.Phys., **17** (2015) 23183.
42. B. A. Marekha, V. A. Koverga, M. Moreau, M. Kiselev, T. Takamuku, **O. N. Kalugin** and A. Idrissia. *Intermolecular interactions, ion solvation, and association in mixtures of 1-n-butyl-3-methylimidazolium hexafluorophosphate and gamma-butyrolactone: insights from Raman spectroscopy* // J. Raman Spectrosc. **46** (2015) 339.
43. Iu. V. Voroshylova, S. R. Smaga, E. V. Lukinova, V. V. Chaban, **O.N. Kalugin**. *Conductivity and association of imidazolium and pyridinium based ionic liquids in methanol* // J. Mol. Liquids **203** (2015) 7.
44. Marekha B. A., **Kalugin O. N**., Idrissi A. Non-covalent interactions in ionic liquid ion pairs and ion pair dimers: A quantum chemical calculation analysis. // Phys. Chem. Chem. Phys., **17(26)** (2015), 16846.
45. Korsun, O. M.; **Kalugin, O. N.;** Vasenko, A. S.; Prezhdo, O. V. *Electronic Properties of Carbon Nanotubes Intercalated with Li^{+} and Mg^{2+}: Effects of Ion Charge and Ion Solvation* // J. Phys. Chem. **120 (46) (**2016**)** 26514.
46. Y. Smortsova, F.-A. Miannay, H. Ohera, B. Marekha, J. Dubois, M. Sliwa, **O. Kalugin**, A. Idrissi. *Solvation dynamics and rotation of coumarin 153 in a new ionic liquid/molecular solvent mixture model: [BMIM][TFSI]/propylene carbonate* // J. Mol. Liq. (2016). DOI: 10.1016/j.molliq.2016.10.008.
47. B. A. Marekha, V. A. Koverga, E. Chesneau, **O. N. Kalugin**, T. Takamuku, P. Jedlovszky, A. Idrissi. *Local Structure in Terms of Nearest-Neighbor Approach in 1-Butyl-3- methylimidazolium-Based Ionic Liquids: MD Simulations* // J. Phys. Chem. B. **120(22)** (2016) 5029. DOI: 10.1021/acs.jpcb.6b04066.
48. O. M. Korsun, **O. N. Kalugin**, I. O. Fritsky, O. V. Prezhdo. *Ion Association in Aprotic Solvents for Lithium Ion Batteries Requires Discrete−Continuum Approach: Lithium Bis(oxalato)borate in Ethylene Carbonate Based Mixtures* // J. Phys. Chem C.**120(30)** (2016) 16545. DOI: 10.1021/acs.jpcc.6b05963.
49. Agieienko, V. N.; Otroshko, N. A.; **Kalugin, O. N.,** Complexation of the alkaline earth metals perchlorates with 3-hydroxyflavone in acetonitrile: Precise conductometric treatment. *J Mol Liq* **2017**; *245*, 27-34. DOI: 10.1016/j.molliq.2017.05.141
50. Koverga, V. A.; Korsun, O. M.; **Kalugin, O. N**.; Marekha, B. A.; Idrissi, A., A new potential model for acetonitrile: Insight into the local structure organization. *J Mol Liq* **2017,** *233*, 251-261; DOI: 10.1016/j.molliq.2017.03.025
51. Kyrychenko, A.; Pasko, D. A.; **Kalugin, O. N**., Poly(vinyl alcohol) as a water protecting agent for silver nanoparticles: The role of polymer size and structure. *Phys. Chem. Chem. Phys.* **2017,** *19* (13), 8742-8756; DOI: 10.1039/c6cp05562a
52. Marekha, B. A.; **Kalugin, O. N**.; Bria, M.; Takamuku, T.; Gadžurić, S.; Idrissi, A., Competition between Cation–Solvent and Cation–Anion Interactions in Imidazolium Ionic Liquids with Polar Aprotic Solvents. *ChemPhysChem* **2017,** *18* (7), 718-721; DOI: 10.1002/cphc.201601445
53. Smortsova, Y.; Miannay, F. A.; Oher, H.; Marekha, B.; Dubois, J.; Sliwa, M.; **Kalugin, O**.; Idrissi, A., Solvation dynamics and rotation of coumarin 153 in a new ionic liquid/molecular solvent mixture model: [BMIM][TFSI]/propylene carbonate. *J Mol Liq* **2017,** *226*, 48-55; 10.1016/j.molliq.2016.10.008
54. Smortsova, Y.; Oher, H.; Miannay, F. A.; Vanel, R.; Dubois, J.; **Kalugin, O.;** Idrissi, A., Solvatochromic effects on a class of indoline derivatives organic photosensitizers: About the influence of hydrogen-bond acceptor and donor abilities parameters. *J Mol Liq* **2017,** *245*,76-84; DOI: 10.1016/j.molliq.2017.06.052
55. Vovchynskyi, I. S.; Kolesnik, Y. V.; Filatov, Y. I.; **Kalugin, O. N.,** Molecular modelling on solutions of 1-1′-spirobipirrolidinium tetrafluoroborate in acetonitrile. *J Mol Liq* **2017,** *235*, 60-67. DOI: 10.1016/j.molliq.2016.12.029.

56. Blazhynska M.M., Kyrychenko A., **Kalugin O.N.** Molecular dynamics simulation of the size-dependent morphological stability of cubic shape silver nanoparticles . Molecular Simulation**, 2018**, *44(12)*, 981-991. DOI: 10.1080/08927022.2018.1469751.
57. **O. N. Kalugin**, A.V. Riabchunova, Iu. V. Voroshylova, V.V. Chaban, B.A. Marekha, V.A. Koverga, A. Idrissi. Transport Properties and Ion Aggregation in Mixtures of Room Temperature Ionic Liquids with Aprotic Dipolar Solvents. In: Bulavin L., Chalyi A. (eds) Modern Problems of Molecular Physics. Springer Proceedings in Physics, Springer, Cham, **2018**, *197*, Chap. 5, 67-109. DOI: 10.1007/978-3-319-61109-9_5
58. V. Koverga, **Oleg N. Kalugin**, F.- A. Miannay, Ye. Smortsova, K. Golviznina, B. Marekha, P. Jedlovsky and A. Idrissi. The local structure in the BmimPF6/acetonitrile mixture: the charge distribution effect. *PCCP* **2018,** *20(34)*, 1463-9076. DOI: 10.1039/c8cp03546f
59. A. Kyrychenko, M. M. Blazhynska, M. V. Slavgorodska**, O. N. Kalugin**. Stimuli-responsive adsorption of poly(acrylic acid) onto silver nanoparticles: Role of polymer chain length and degree of ionization. *J Mol Liq* **2019**, *276*, 243–254. DOI: /10.1016/j.molliq.2018.11.130.
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13. Linguistic ability **Native languages:** Ukrainian, Russian

Other language proficiency on scale of 1 (basic) to 3 (fluent) for reading, writing and speaking:
English 3, 3, 3; French: 1, 1, 1; German: 1, 1, 1.

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