Curriculum Vitae

Dr. Alexander S. Novikov

Scopus ID: 50262902200

Web of Science ResearcherID: L-5001-2015

E-mail: a.s.novikov@spbu.ru

Personal Information

Nationality:

Russian

Date of birth:

June, 6th, 1988

Place of birth:

Moscow, USSR

Affiliation:

Institute of Chemistry, Saint Petersburg State University, Universitetsky pr., 26, 198504, Stary Petergof, Russia – Senior Researcher

Research Interests

Fields of expertise:

- ✓ Quantum and Computational Chemistry
- ✓ Inorganic and Coordination Chemistry
- ✓ Organometallic Chemistry and Catalysis

Present investigation interests:

- ✓ Non-covalent interactions in coordination and organometallic chemistry
- ✓ Ligand reactivity and catalysis
- ✓ Functionalization of hydrocarbons

Degrees

2013

"Candidate of Sciences" degree (an equivalent to Ph.D.)

Degree was awarded on December, 12th, 2013 at the Saint Petersburg State University, Saint Petersburg, Russia

Specialty: "Inorganic Chemistry"

Title of the Ph.D. thesis: "Study of transition metal complexes featuring isocyanide ligands in cycloaddition with nitrones"

Highest marks for all Ph.D. exams and unanimous vote for awarding the scientific degree (*summa cum laude*)

2010

Diploma of Higher Education at the Department of Chemistry, Moscow State Pedagogical University, Moscow, Russia

Specialty: "Chemistry" with supplementary specialty "Pedagogy and Psychology"

Title of the diploma thesis: "Quantum chemical study of the structure and acidity of metals III A group aqua complexes"

The highest rank student ("red" diploma – *summa cum laude*) with excellent marks for all exams (the final media is 5.00 in the scale of 0–5)

Previous Employment

Department of Physical and Analytical Chemistry, University of Oviedo, Oviedo, Spain – Invited Lecturer (2019) *Topic: "Computer modeling in organometallic and coordination chemistry: catalysis, reactivity, and non-covalent interactions" course for PhD and MSc students*

Otto Schott Institute of Materials Research, Faculty of Physics and Astronomy, Friedrich Schiller University Jena, Jena, Germany – Visiting Researcher (2019) *Topic: Application of TURBOMOLE quantum chemical program package in multi-scale computational studies of structure, properties and reactivity of complex materials*

Department of Chemistry, University of Jyväskylä, Jyväskylä, Finland – Invited Lecturer (2019) *Topic: "Computer modeling in chemistry and materials science" course for PhD and MSc students*

Biocenter Oulu and Faculty of Biochemistry and Molecular Medicine, University of Oulu, Oulu, Finland – Invited Lecturer (2019) *Topic: "Density functional theory calculations in organometallic and coordination chemistry: reactivity, catalysis, and non-covalent interactions"*

Department of Chemistry, Uppsala University, Uppsala, Sweden – Invited Lecturer (2019) *Topic: "Density functional theory calculations in organometallic and coordination chemistry: reactivity, catalysis, and non-covalent interactions" course for PhD students*

Department of Chemistry, University of Jyväskylä, Jyväskylä, Finland – Invited Lecturer (2018) *Topic: "Materials modeling" course for PhD and MSc students*

Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa, Lisbon, Portugal – Visiting Researcher (2017) *Topic: Non-covalent interactions*

Department of Chemistry, University of Jyväskylä, Jyväskylä, Finland – Visiting Researcher / Invited Lecturer (2017) *Topic: Non-covalent interactions / "Quantum and Computational Chemistry" course for PhD students*

Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa, Lisbon, Portugal – Visiting Researcher (2016) *Topic: Non-covalent interactions*

Department of Chemistry, University of Jyväskylä, Jyväskylä, Finland – Visiting Researcher (2015) *Topic: Non-covalent interactions*

Institute of Chemistry, Saint Petersburg State University, Saint Petersburg, Russia – Postdoctoral Fellow (2014–2015) *Topic: Non-covalent interactions and catalysis*

Centro de Química Estrutural, Instituto Superior Técnico, Lisbon, Portugal – Postdoctoral Fellow (2014) *Topic: Catalysis*

Department of Chemistry, Moscow State Pedagogical University, Moscow, Russia – Engineer (2013–2014) *Topic: Computational chemistry*

Centro de Química Estrutural, Instituto Superior Técnico, Lisbon, Portugal – Research Grantee [Master] (2012–2013) *Topic: Catalysis*

Centro de Química Estrutural, Instituto Superior Técnico, Lisbon, Portugal – Research Grantee [BIC] (2011) *Topic: Organometallic chemistry*

Research Experience

- Senior Researcher at the Institute of Chemistry, Saint Petersburg State University (Saint Petersburg, Russia): PI of research project funded by Russian Science Foundation [19-73-00001 (2019–2021)] and two research projects funded by Russian Foundation for Basic Research [16-33-60063 (2016–2018); 16-33-00212 (2016–2017)], collaborator on several research projects funded by Russian Science Foundation [17-73-20185 (2017–2020), 14-43-00017(-P) (2014–2018)] and Russian Foundation for Basic Research [16-03-00441 (2016–2018); 18-33-00704 (2018–2019); 18-29-04006 (2018–2020); 20-33-70010 (2019–2021); 20-53-00006 (2020–2022)] (2016–present)

- Short-term visit to the research group of Prof. Ángel Martín Pendás at the Department of Physical and Analytical Chemistry, University of Oviedo (Oviedo, Spain) [Erasmus+ International Credit Mobility] (2019)

- Internship (Visiting Researcher) at the Otto Schott Institute of Materials Research, Faculty of Physics and Astronomy, Friedrich Schiller University Jena (Jena, Germany) under supervision of Prof. Marek Sierka [Inter-university exchange cooperation agreement between Saint Petersburg State University and Friedrich Schiller University Jena / DAAD] (2019)

- Short-term visit to the research group of Prof. Matti Haukka at the Department of Chemistry, University of Jyväskylä (Jyväskylä, Finland) [Inter-university exchange cooperation agreement between Saint Petersburg State University and University of Jyväskylä / Finnish-Russian Student and Teacher Exchange Programme (FIRST+)] (2019)

- Short-term visit to the research group of Dr. André H. Juffer at the Biocenter Oulu and Faculty of Biochemistry and Molecular Medicine, University of Oulu (Oulu, Finland) [Finnish-Russian Student and Teacher Exchange Programme (FIRST+)] (2019)

- Short-term visit to the research group of Prof. Kersti Hermansson at the Department of Chemistry, Uppsala University (Uppsala, Sweden) [Erasmus+ International Credit Mobility] (2019)

- Short-term visit to the research group of Prof. Matti Haukka at the Department of Chemistry, University of Jyväskylä (Jyväskylä, Finland) [Finnish-Russian Student and Teacher Exchange Programme (FIRST+)] (2018)

- Internship (Visiting Researcher) at the Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa (Lisbon, Portugal) under supervision of Prof. M.L. Kuznetsov [Joint fellowship program of Saint Petersburg State University and Santander Bank] (2017)

- Internship (Visiting Researcher) at the Department of Chemistry, University of Jyväskylä (Jyväskylä, Finland) under supervision of Prof. Matti Haukka [Finnish-Russian Student and Teacher Exchange Programme (FIRST)] (2017)

- Internship (Visiting Researcher) at the Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa (Lisbon, Portugal) under supervision of Prof. M.L. Kuznetsov [Joint fellowship program of Saint Petersburg State University and Santander Bank] (2016)

- Research grant contract (Post-Doctoral Scholarship) at the Institute of Chemistry, Saint Petersburg State University, (Saint Petersburg/Stary Petergof, Russia) under supervision of Prof. V.Yu. Kukushkin [Grant 12.50.1190.2014, Saint Petersburg State University, Russia] (2014–2015)

- Research contract (Visiting Researcher) at the Department of Chemistry, University of Jyväskylä (Jyväskylä, Finland) under supervision of Prof. Matti Haukka (2015)

- Research grant contract (Post-Doctoral Scholarship) at the Centro de Química Estrutural, Instituto Superior Técnico (Lisbon, Portugal) under supervision of Dr. M.L. Kuznetsov and Prof. A.J.L. Pombeiro [Project PTDC/QUI-OUI/119561/2010 (RD 0188), Fundação para a Ciência e a Tecnologia, Portugal] (2014)

- Research grant contract (Research Scholarship – Master) at the Centro de Química Estrutural, Instituto Superior Técnico (Lisbon, Portugal) under supervision of Dr. M.L. Kuznetsov and Prof. A.J.L. Pombeiro [Project PTDC/QUI-OUI/119561/2010 (RD 0188), Fundação para a Ciência e a Tecnologia, Portugal] (2012–2013)

- Research scholarship contract (Scientific initiation grants – BIC) at the Centro de Química Estrutural, Instituto Superior Técnico (Lisbon, Portugal) under supervision of Dr. M.L. Kuznetsov and Prof. A.J.L. Pombeiro [Project PTDC/QUI-OUI/102150/2008 (proj.3552), Fundação para a Ciência e a Tecnologia, Portugal] (2011)

Teaching Activities

Teaching activity at the University level

Lecture and practical course "Computer modeling in organometallic and coordination chemistry: catalysis, reactivity, and non-covalent interactions" for PhD and MSc students at the University of Oviedo, Department of Physical and Analytical Chemistry [October, 2019, Oviedo, Spain]

Lecture and practical course "Computer modeling in chemistry and materials science" for PhD and MSc students at the University of Jyväskylä, Department of Chemistry [June, 2019, Jyväskylä, Finland]

Lecture "Density functional theory calculations in organometallic and coordination chemistry: reactivity, catalysis, and non-covalent interactions" at the University of Oulu, Biocenter Oulu and Faculty of Biochemistry and Molecular Medicine [May, 2019, Oulu, Finland]

Lecture and practical course "Density functional theory calculations in organometallic and coordination chemistry: reactivity, catalysis, and non-covalent interactions" for PhD students at the Uppsala University, Department of Chemistry [May, 2019, Uppsala, Sweden]

Lecture course "Materials modeling" for PhD and MSc students at the University of Jyväskylä, Department of Chemistry [April, 2018, Jyväskylä, Finland]

Practical course "Quantum and Computational Chemistry" for PhD students at the University of Jyväskylä, Department of Chemistry [June, 2017, Jyväskylä, Finland]

Lecture course "Bioinorganic Chemistry" for Master in Chemistry students at the Moscow State Pedagogical University, Department of Chemistry [November, 2013, Moscow, Russia]

Lecture course "Toxicological Chemistry" for Master in Chemistry students in the Moscow State Pedagogical University, Department of Chemistry [February–May, 2012, Moscow, Russia]

Publications (h-index in Scopus/Web of Science = 22/23 on 07.09.2020)

1. **Novikov A.S.** "Non-covalent interactions in coordination and organometallic chemistry" // *Crystals* 2020, V. 10. P. 537.
2. Mikherdov A.S., **Novikov A.S.**, Boyarskiy V.P., Kukushkin V.Yu. "The halogen bond with isocyano carbon reduces isocyanide odor" // *Nat. Commun.* 2020, V. 11. P. 2921. [**Featured in Editors' Highlights webpage**]
3. **Novikov A.S.** "Why [2 + 2]-cycloaddition reactions between isocyanates and imines do not occur in Pd-activation conditions?" // *Inorg. Chim. Acta* 2020, V. 510. P. 119758.
4. Usoltsev A.N., Adonin S.A., Kolesov B.A., **Novikov A.S.**, Fedin V.P., Sokolov M.N. "Opening the third century of polyhalide chemistry: thermally stable complex with "trapped" dichlorine" // *Chem. Eur. J.* 2020, In press. DOI: 10.1002/chem.202002014
5. Adonin S.A., Usoltsev A.N., **Novikov A.S.**, Kolesov B.A., Fedin V.P., Sokolov M.N. "One- and two-dimensional iodine-rich iodobismuthate(III) complexes: structure, optical properties and features of halogen bonding in the solid state" // *Inorg. Chem.* 2020, V. 59. P. 3290.
6. Efimenko Z.M., **Novikov A.S.**, Ivanov D.M., Piskunov A.V., Vereshchagin A.A., Levin O.V., Bokach N.A., Kukushkin V.Yu. "The (dioximate)Ni^{II}/I_2 system: ligand oxidation and binding modes of triiodide species" // *Inorg. Chem.* 2020, V. 59. P. 2316.
7. Chupina A.V., Shayapov V.R., **Novikov A.S.**, Volchek V.V., Benassi E., Abramov P.A., Sokolov M.N. "$[\{AgL\}_2Mo_8O_{26}]^{n-}$ complexes: a combined experimental and theoretical study" // *Dalton Trans.* 2020, V. 49. P. 1522.
8. Bolotin D.S., Il'in M.V., Suslonov V.V., **Novikov A.S.** "Symmetrical noncovalent interactions Br•••Br observed in crystal structure of exotic primary peroxide" // *Symmetry* 2020, V. 12. P. 637.
9. Ivanov D.M., Baykov S.V., **Novikov A.S.**, Romanenko G., Bokach N.A., Evarestov R.A., Kukushkin V.Yu. "Noncovalent sulfoxide–nitrile coupling involving four-center heteroleptic dipole–dipole interactions between the sulfinyl and nitrile groups" // *Cryst. Growth Des.* 2020, V. 20. P. 3417.
10. Paul A., Martins L.M.D.R.S., Karmakar A., Kuznetsov M.L., **Novikov A.S.**, Guedes da Silva M.F.C., Pombeiro A.J.L. "Environmentally benign benzyl alcohol oxidation and C-C coupling catalysed by amide functionalized 3D Co(II) and Zn(II) metal organic frameworks" // *J. Catal.* 2020, V. 385. P. 324.
11. Ostras' A.S., Ivanov D.M., **Novikov A.S.**, Tolstoy P.M. "Phosphine oxides as spectroscopic halogen bond descriptors: IR and NMR correlations with interatomic distances and complexation energy" // *Molecules* 2020, V. 25. P. 1406.
12. Pulyalina A., Faykov I., Nesterova V., Goikhman M., Podeshvo I., Loretsyan N., **Novikov A.**, Gofman I., Toikka A., Polotskaya G. "Novel polyester amide membranes containing biquinoline units and complex with Cu(I): synthesis, characterization, and approbation for n-heptane isolation from organic mixtures" // *Polymers* 2020, V. 12. P. 645.
13. Buldakov A.V., Kinzhalov M.A., Kryukova M.A., Ivanov D.M., **Novikov A.S.**, Smirnov A.S., Starova G.L., Bokach N.A., Kukushkin V.Yu. "Isomorphous series of Pd^{II}-containing halogen-bond donors exhibiting Cl/Br/I triple halogen isostructural exchange" // *Cryst. Growth Des.* 2020, V. 20. P. 1975.

14. Sharutin V.V., Sharutina O.K., **Novikov A.S.**, Adonin S.A. “Substituent-dependent reactivity of triarylantimony(III) toward I_2: isolation of $[Ar_3SbI]^+$ salt” // *New J. Chem.* 2020, V. 44. P. 14339.

15. Usoltsev A.N., Korobeynikov N.A., **Novikov A.S.**, Plyusnin P.E., Fedin V.P., Sokolov M.N., Adonin S.A. “Hybrid chlorobismuthate(III) “trapping” Br_2 unit: crystal structure and theoretical investigation of non-covalent Cl•••Br interactions in $(1\text{-MePy})_3\{[Bi_2Cl_9](Br_2)\}$” // *Inorg. Chim. Acta* 2020, V. 513. P. 119932.

16. Usoltsev A.N., Korobeynikov N.A., **Novikov A.S.**, Shayapov V.R., Korolkov I.V., Samsonenko D.G., Fedin V.P., Sokolov M.N., Adonin S.A. “One-dimensional supramolecular hybrid iodobismuthate$(1\text{-EtPy})_3\{[Bi_2I_9](I_2)_{0.75}\}$: structural features and theoretical studies of I•••I non-covalent interactions” // *J. Clust. Sci.* 2020, In press. DOI: 10.1007/s10876-020-01843-2

17. Klyukin I.N., **Novikov A.S.**, Zhdanov A.P., Zhizhin K.Yu., Kuznetsov N.T. “Theoretical study of *closo*-borate derivatives of general type $[B_nH_{n-1}COR]^{2-}$ (n = 6, 10, 12; R = H, CH_3, NH_2, OH, OCH_3) – borylated analogue of organic carbonyl compounds” // *Polyhedron* 2020, V. 187. P. 114682.

18. Nelyubin A.V., Selivanov N.A., Bykov A.Yu., Klyukin I.N., **Novikov A.S.**, Zhdanov A.P., Zhizhin K.Yu., Kuznetsov N.T. ”N-borylated hydroxylamines $[B_{12}H_{11}NH_2OH]^-$ as a novel type of substituted derivative of the *closo*-dodecaborate anion” // *Russ. J. Inorg. Chem.* 2020, V. 65. P. 719.

19. Adonin S.A., **Novikov A.S.**, Smirnova Yu.K., Tushakova Z.R., Fedin V.P. "Heteroligand Cu(II) complexes with 2-halogenopyridines: crystal structure and features of halogen•••halogen contacts in the solid state" // *J. Struct. Chem.* 2020, V. 61. P. 712.

20. Suslonov V.V., Eliseeva A.A., **Novikov A.S.**, Ivanov D.M., Dubovtsev A.Yu., Bokach N.A., Kukushkin V.Yu. “Tetrachloroplatinate(II) anion as a square-planar tecton for crystal engineering involving halogen bonding” // *CrystEngComm* 2020, V. 22. P. 4180.

21. Kryukova M.A., Sapegin A.V., **Novikov A.S.**, Krasavin M., Ivanov D.M. “New crystal forms for biologically active compounds. Part 2: anastrozole as N-substituted 1,2,4-triazole in halogen bonding and lp-π interactions with 1,4-diiodotetrafluorobenzene” // *Crystals* 2020, V. 10. P. 371.

22. Yunusova S.N., **Novikov A.S.**, Khoroshilov O.V., Kolesnikov I.E., Demakova M.Ya., Bolotin D.S. “Solid-state fluorescent 1,2,4-triazole zinc(II) complexes: self-organization via bifurcated $(N–H)_2$•••Cl contacts” // *Inorg. Chim. Acta* 2020, V. 510. P. 119660.

23. Adonin S.A., Bondarenko M.A., **Novikov A.S.**, Sokolov M.N. “Halogen bonding in isostructural Co(II) complexes with 2-halopyridines” // *Crystals* 2020, V. 10. P. 289.

24. Bondarenko M.A., Adonin S.A., **Novikov A.S.**, Sokolov M.N., Fedin V.P. “Supramolecular bromoantimonate(V) polybromide $(2,6\text{-BrPyH})_3[SbBr_6]\{(Br_2)Br\}\cdot 2H_2O$: specific features of halogen•••halogen contacts in the crystal structure” // *Russ. J. Coord. Chem.* 2020, V. 46. P. 302.

25. Soldatova N.S., Suslonov V.V., Kissler T.Yu., Ivanov D.M., **Novikov A.S.**, Yusubov M.S., Postnikov P.S., Kukushkin V.Yu. “Halogen bonding provides heterooctameric supramolecular aggregation of diaryliodonium thiocyanate” // *Crystals* 2020, V. 10. P. 230.

26. Efremova M.M., Molchanov A.P., **Novikov A.S.**, Starova G.L., Muryleva A.A., Slita A.V., Zarubaev V.V. “1,3-Dipolar cycloaddition of *N*-allyl substituted polycyclic derivatives of isoindole-1,3-dione with nitrones and nitrile oxides: An experimental and theoretical investigation” // *Tetrahedron* 2020, V. 76. P. 131104.

27. Klyukin I.N., **Novikov A.S.**, Zhdanov A.P., Zhizhin K.Yu., Kuznetsov N.T. "Theoretical study of monocarbonyl derivatives of *closo*-borate anions $[B_nH_{n-1}CO]^-$ (n = 6, 10, 12): bonding and reactivity analysis" // *Mendeleev Commun.* 2020, V. 30. P. 88.

28. Usoltsev A.N., **Novikov A.S.**, Kolesov B.A., Chernova K.V., Plyusnin P.E., Fedin V.P., Sokolov M.N., Adonin S.A. "Halogen•••halogen contacts in triiodide salts of pyridinium-derived cations: theoretical and spectroscopic studies" // *J. Mol. Struct.* 2020, V. 1209. P. 127949.

29. Mikhaylov V.N., Sorokoumov V.N., **Novikov A.S.**, Melnik M.V., Tskhovrebov A.G., Balova I.A. "Intramolecular hydrogen bonding stabilizes *trans*-configuration in a mixed carbene/isocyanide Pd^{II} complexes" // *J. Organomet. Chem.* 2020, V. 912. P. 121174.

30. Usoltsev A.N., Adonin S.A., **Novikov A.S.**, Abramov P.A., Sokolov M.N., Fedin V.P. "Chlorotellurate(IV) supramolecular associates with "trapped" Br_2: features of non-covalent halogen•••halogen interactions in crystalline phases" // *CrystEngComm* 2020, V. 22. P. 1985.

31. Usoltsev A.N., Adonin S.A., **Novikov A.S.**, Sokolov M.N., Fedin V.P. "Two-dimensional coordination polymer {[Bi(Pyz)I_3]}: structure and analysis of the packing using the Hirshfeld surface method" // *Russ. J. Coord. Chem.* 2020, V. 46. P. 23.

32. Adonin S.A., **Novikov A.S.**, Fedin V.P. "Crystal structure of the heteroligand complex [(2-Br-5-MePy)$_2$$CoCl_2$]·(2-Br-5-MePy): formation of supramolecular associates due to the halogen bond" // *Russ. J. Coord. Chem.* 2020, V. 46. P. 37.

33. Adonin S.A., **Novikov A.S.**, Fedin V.P. "Heteroleptic binuclear iodoacetate copper(II) complexes with 3-bromopyridine and 4-ethylpyridine: crystal structures and peculiarities of contacts halogen•••halogen" // *Russ. J. Coord. Chem.* 2020, V. 46. P. 119.

34. Bolotin D.S., Soldatova N.S., Demakova M.Y., **Novikov A.S.**, Ivanov D.M., Aliyarova I.S., Sapegin A., Krasavin M. "Pentacoordinated silver(I) complex featuring 8-phenylquinoline ligands: interplay of coordination bonds, semicoordination, and stacking interactions" // *Inorg. Chim. Acta* 2020, V. 504. P. 119453.

35. Mikshiev V.Y., Pozharskii A.F., Filarowski A., **Novikov A.S.**, Antonov A.S., Tolstoy P.M., Vovk M.A., Khoroshilova O.V. "How strong is hydrogen bonding to amide nitrogen?" // *ChemPhysChem* 2020, V. 21. P. 651. [**Very Important Paper status**]

36. Mikherdov A.S., Katkova S.A., **Novikov A.S.**, Efremova M.M., Reutskaya E.Yu., Kinzhalov M.A. "(Isocyano group)•••lone pair interactions involving coordinated isocyanides: experimental, theoretical and CSD study" // *CrystEngComm* 2020, V. 22. P. 1154.

37. Nikolaev K.G., Ulasevich S.A., Luneva O., Orlova O.Yu., Vasileva D., Vasilev S., **Novikov A.S.**, Skorb E.V. "Humidity-driven transparent holographic free-standing polyelectrolyte films" // *ACS Appl. Polym. Mater.* 2020, V. 2. P. 105.

38. Repina O.V., **Novikov A.S.**, Khoroshilova O.V., Kritchenkov A.S., Vasin A.A., Tskhovrebov A.G. "Lasagna-like supramolecular polymers derived from the Pd^{II} osazone complexes via C(sp^2)–H•••Hal hydrogen bonding" // *Inorg. Chim. Acta* 2020, V. 502. P. 119378.

39. Baykov S.V., Filimonov S.I., Rozhkov A.V., **Novikov A.S.**, Ananyev I.V., Ivanov D.M., Kukushkin V.Yu. "Reverse sandwich structures from interplay between lone pair–π-hole atom-directed C•••d_z^2[M] and halogen bond interactions" // *Cryst. Growth Des.* 2020, V. 20. P. 995.

40. Il'in M.V., Lesnikova L.A., Bolotin D.S., **Novikov A.S.**, Suslonov V.V., Kukushkin V.Yu. "One-pot route to *N*-acyl ureas: a formal four-component hydrolytic reaction

involving aminonitrones and isocyanide dibromides" // *New J. Chem.* 2020, V. 44. P. 1253.

41. Eliseeva A.A., Ivanov D.M., **Novikov A.S.**, Rozhkov A.V., Kornyakov I.V., Dubovtsev A.Yu., Kukushkin V.Yu. "Hexaiododiplatinate(II) as a useful supramolecular synthon for halogen bond involving crystal engineering" // *Dalton Trans.* 2020, V. 49. P. 356.
42. Adonin S.A., **Novikov A.S.**, Chernova K.V., Vinnik D.A., Taskaev S.V., Korolkov I.V., Ilyina E.V., Pavlov A.A., Novikov V.V., Sokolov M.N., Fedin V.P. "Heteroleptic copper(II) complexes with 2-bromo-5-methylpyridine: structures, features of non-covalent interactions and magnetic behavior" // *Inorg. Chim. Acta* 2020, V. 502. P. 119333.
43. Adonin S.A., Bondarenko M.A., **Novikov A.S.**, Plyusnin P.E., Korolkov I.V., Sokolov M.N., Fedin V.P. "Five new Sb(V) bromide complexes and their polybromide derivatives with pyridinium-type cations: structures, thermal stability and features of halogen•••halogen contacts in solid state" // *Inorg. Chim. Acta* 2020, V. 502. P. 119278.
44. Rozhkov A.V., Ivanov D.M., **Novikov A.S.**, Ananyev I.V., Bokach N.A., Kukushkin V.Yu. "Metal-involving halogen bond Ar–I•••[$d_z^2Pt^{II}$] in a platinum acetylacetonate complex" // *CrystEngComm* 2020, V. 22. P. 554.
45. Gorokh I.D., Adonin S.A., Usoltsev A.N., **Novikov A.S.**, Samsonenko D.G., Zakharov S.V., Sokolov M.N., Fedin V.P. "Bromide complexes of bismuth with 4-bromobenzyl-substituted cations of pyridinium family" // *J. Mol. Struct.* 2020, V. 1199. P. 126955.
46. Kostenko E.A., Baykov S.V., **Novikov A.S.**, Boyarskiy V.P. "Nucleophilic properties of the positively charged metal center in the solid state structure of palladium(II)-terpyridine complex" // *J. Mol. Struct.* 2020, V. 1199. P. 126957.
47. Afanasenko A.M., **Novikov A.S.**, Chulkova T.G., Grigoriev Y.M., Kolesnikov I.E., Selivanov S.I., Starova G.L., Zolotarev A.A., Vereshchagin A.N., Elinson M.N. "Intermolecular interactions-photophysical properties relationships in phenanthrene-9,10-dicarbonitrile assemblies" // *J. Mol. Struct.* 2020, V. 1199. P. 126789.
48. Teterina P.S., Efremova M.M., Sirotkina E.V., **Novikov A.S.**, Khoroshilova O.V., Molchanov A.P. "A highly efficient and stereoselective cycloaddition of nitrones to *N*-arylitaconimides" // *Tetrahedron Lett.* 2019, V. 60. P. 151063.
49. Klyukin I.N., **Novikov A.S.**, Zhdanov A.P., Zhizhin K.Yu., Kuznetsov N.T. "QTAIM analysis of mono-hydroxy derivatives of *closo*-borate anions $[B_nH_{n-1}OH]^{2-}$ (n = 6, 10, 12)" // *Russ. J. Inorg. Chem.* 2019. V. 64. P. 1825.
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mediated generation of 1,2,4-Oxadiazoles from amidoximes and nitriles" // *New J. Chem.* 2017, V. 41. P. 1940.

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complexes featuring chelated acetoxime pyrazoles: synthetic, structural, and photophysical study" // *ChemistrySelect* 2016, V. 3. P. 456.

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147. **Novikov A.S.**, Kuznetsov M.L., Rocha B.G.M., Pombeiro A.J.L., Shul'pin G.B. "Oxidation of olefins with H_2O_2 catalysed by salts of Group III metals (Ga, In, Sc, Y and La): epoxidation versus hydroperoxidation" // *RSC Catal. Sci. Tech.* 2016, V. 6. P. 1343.

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153. **Novikov A.S.** "1,3-Dipolar cycloaddition of nitrones to transition metal-bound isocyanides: DFT and HSAB principle theoretical model together with analysis of vibrational spectra" // *J. Organomet. Chem.* 2015, V. 797. P. 8.

154. Melekhova A.A., **Novikov A.S.**, Luzyanin K.V., Bokach N.A., Starova G.L., Gurzhiy V.V., Kukushkin V.Yu. "Tris-Isocyanide copper(I) complexes: synthetic, structural, and theoretical study" // *Inorg. Chim. Acta* 2015. V. 434. P. 31.

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156. Serebryanskaya T.V., **Novikov A.S.**, Gushchin P.V., Zolotarev A.A., Gurzhiy V.V., Kukushkin V.Yu. "Coupling of platinated triguanides with platinum-activated nitriles as a novel strategy for generation of dimetallic systems" // *Dalton Trans.* 2015. V. 44. P. 6003.

157. **Novikov A.S.**, Kuznetsov M.L., Pombeiro A.J.L., Bokach N.A., Shul'pin G.B. "Generation of HO$^{\bullet}$ radical from hydrogen peroxide catalyzed by aqua-complexes of the group III metals $[M(H_2O)_n]^{3+}$ (M = Ga, In, Sc, Y, La): a theoretical study" // *ACS Catal.* 2013. V. 3. P. 1195.

158. **Novikov A.S.**, Kuznetsov M.L., Pombeiro A.J.L. “Theory of the formation and decomposition of N-heterocyclic aminooxycarbenes through metal-assisted [2+3]-dipolar cycloaddition/retro-cycloaddition” // *Chem. Eur. J.* 2013. V. 19. P. 2874.

159. **Novikov A.S.**, Dement`ev A.I., Medvedev Yu.N. “Theoretical study of the reactivity of Rh(I) and Rh(III) bis(isonitrile) complexes in cycloaddition reactions with nitrones” // *Russ. J. Inorg. Chem.* 2013. V. 58. P. 320.

160. **Novikov A.S.**, Dement`ev A.I., Medvedev Yu.N. “Theoretical study of Rh(I) and Rh(III) bis(isonitrile) complexes as promising reagents for synthesis of N-heterocyclic carbenes” // *Russ. J. Inorg. Chem.* 2012. V. 57. P. 1576.

161. **Novikov A.S.**, Kuznetsov M.L. “Theoretical study of Re(IV) and Ru(II) bis-isocyanide complexes and their reactivity in cycloaddition reactions with nitrones” // *Inorg. Chim. Acta* 2012. V. 380. P. 78.

Other Activities

Expert of the *Russian Science Foundation* in fields of Quantum Chemistry, Computer Modeling, and Supramolecular Chemistry

Reviewer of grants from the *National Research Foundation* (South Africa)

Guest Editor of the Special Issue "Computational Insights into Industrial Chemistry" in *Computation* (MDPI)
https://www.mdpi.com/journal/computation/special_issues/CIIC

Guest Editor of the Special Issue “Non-covalent Interactions in Coordination and Organometallic Chemistry” in *Crystals* (MDPI)
https://www.mdpi.com/journal/crystals/special_issues/organometallic_compounds

Guest Editor of the Special Issue “Symmetry in Quantum and Computational Chemistry” in *Symmetry* (MDPI)
https://www.mdpi.com/journal/symmetry/special_issues/Symmetry_Quantum_Computational_Chemistry

Editorial Board member in *Computation* (MDPI): Computational Chemistry Section
https://www.mdpi.com/journal/computation/sectioneditors/computational-chemistry

Reviewer of manuscripts for *The Journal of Organic Chemistry* (American Chemical Society), *Langmuir* (American Chemical Society), *Physical Chemistry Chemical Physics* (Royal Society of Chemistry), *CrystEngComm* (Royal Society of Chemistry), *New Journal of Chemistry* (Royal

Society of Chemistry), *Molecules* (MDPI), *Crystals* (MDPI), *Materials* (MDPI), *International Journal of Molecular Sciences* (MDPI), *Chemosensors* (MDPI), *Symmetry* (MDPI), *Mathematics* (MDPI), *Entropy* (MDPI), *Processes* (MDPI), *Zeitschrift für Kristallographie – Crystalline Materials* (De Gruyter), *Current Organic Chemistry* (Bentham Science), *Applied Catalysis B: Environmental* (Elsevier), *International Journal of Hydrogen Energy* (Elsevier), *Journal of Materials Research and Technology* (Elsevier), *Materials Letters* (Elsevier), *Physica E: Low-dimensional Systems and Nanostructures* (Elsevier), *Inorganica Chimica Acta* (Elsevier), *Solid State Sciences* (Elsevier), *Computational and Theoretical Chemistry* (Elsevier), *Materials Chemistry and Physics* (Elsevier), *Journal of Luminescence* (Elsevier), *Materials Today Communications* (Elsevier), *Chemical Physics Letters* (Elsevier), *Journal of Molecular Structure* (Elsevier), *Journal of Molecular Graphics and Modelling* (Elsevier), *Carbohydrate Research* (Elsevier), *Surfaces and Interfaces* (Elsevier), *Optik* (Elsevier), etc.

British Council sponsored workshop "Dynamic self-assembly and quorum effects in chemistry and biology predicted by non-linear modelling algorithms" (Liverpool, United Kingdom, 20–23 October 2019) – *Invited speaker*

11th International Conference on Chemistry for Young Scientists "Mendeleev 2019" (Saint Petersburg, Russia, 09–13 September 2019) – *Chairman of section "Computer modeling and cheminformatics", Plenary speaker*

1st International Conference on Noncovalent Interactions (Lisbon, Portugal, 02–06 September 2019) – *Invited lecturer*

International Workshop on Chemical Crystallography and Structural Biology "The Second Struchkov Meeting" (Moscow, Russia, 13–16 November 2018) – *Invited speaker*

The Russian Cluster of Conferences on Inorganic Chemistry "InorgChem 2018" (Astrakhan, Russia, 17–21 September 2018) – *Member of the program and organization committees (8th International Russian Science Foundation Symposium on Organometallic Chemistry Incorporating Elements of School-Conference)*

Visit of teacher and student delegation from the University of Jyväskylä (Jyväskylä, Finland) at the Saint Petersburg State University (Saint Petersburg, Russia) within the framework of

Finnish–Russian student and teacher international exchange mobility program FIRST+ (17–24 March 2018) – *Principal curator, Plenary lecturer*

27th International Chugaev Conference on Coordination Chemistry (Nizhny Novgorod, Russia, 02–06 October 2017) – *Chairman of section 9 (7th Russian Science Foundation Symposium on Organometallic Chemistry Incorporating Elements of School-Conference), Member of the organization committee*

8th Russian Youth School-Conference "Quantum chemical calculations: structure and reactivity of organic and inorganic molecules" (Ivanovo, Russia, 24–26 April 2017) – *Plenary lecturer*

10th International Chemistry Conference for Young Scientists "Mendeleev 2017" (Saint Petersburg, Russia, 04–07 April 2017) – *Chairman of section "Computer modeling"*, *Member of the organization committee*

Cluster of Conferences "OrgChem-2016" (Saint Petersburg / Repino, Russia, 27 June–02 July 2016) – *Member of the organization committee (6th International Russian Science Foundation Symposium on Organometallic Chemistry Incorporating Elements of School-Conference)*

9th International Chemistry Conference for Young Scientists "Mendeleev 2015" (Saint Petersburg, Russia, 07–10 April 2015) – *Chairman of section "Quantum chemistry and computer modeling", Member of the program and organization committees*

Hobby

- Psychology
- History of Middle Ages
- Hiking and surf (preferably mountains and plateaus of Iberian Peninsula / Atlantic Ocean)

Training

25th Jyväskylä Summer School (Jyväskylä, Finland, 05–21, August 2015)
Attended the courses:

- CH1: Ion Mobility Mass Spectrometry
- CH2: Biomolecular NMR-spectroscopy

- CH4: Optical Molecular Spectroscopy, from Gas Phase to Condensed Phase, from Static Spectra to Dynamics

Awards

One of the best presentations at the *International Workshop on Chemical Crystallography and Structural Biology "The Second Struchkov Meeting"*, Moscow, Russia, 13–16 November 2018.

Yu. T. Struchkov Prize for young scientists from the Former Soviet Union for the best research works in the field of X-ray crystallography (2017)

Academia Europaea Award (Academy of Europe) for young Russian scientists in Chemistry field (2016)

Grant for young scientists from the Government of Saint Petersburg (2016)

Fellowships of Saint Petersburg State University and Santander Bank (visits to Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa, Lisbon, Portugal; September–October 2016 and August–September 2017)

Diploma for the best poster presentation at the *IV All-Russian Conference on Organic Chemistry and XVIII Youth School-Conference on Organic Chemistry*, Moscow, Russia, 22–27 November 2015

Diploma for the best poster presentation at the *International Youth Scientific Forum "Lomonosov-2015"*, Moscow, Russia, 13–17 April 2015

Diploma for active participation in the discussions at the *VI All-Russian Youth School-Conference "Quantum Chemical Calculations: The Structure and Reactivity of Organic and Inorganic Molecules"*, Ivanovo, Russia, 30 September–4 October 2013

Diploma for the best work at the *International Youth Scientific Forum "Lomonosov-2013"*, Moscow, Russia, 08–13 April 2013

2009/2010 academic years – the ***Special State Stipend*** from the Government of Russian Federation for talented students

The paper by Alexander S. Novikov and colleagues "The halogen bond with isocyano carbon reduces isocyanide odor" was featured in a *Nature Communications* **Editors' Highlights webpage** (DOI: 10.1038/s41467-020-16748-x).

The paper by Alexander S. Novikov and colleagues "How strong is hydrogen bonding to amide nitrogen?" was recognized by the editorial board of *ChemPhysChem* as ***VIP (Very Important Paper) based on referees' suggestions*** (DOI: 10.1002/cphc.201901104).

The paper by Alexander S. Novikov and colleagues "Polymeric lead(II) iodoacetate: Pb•••I and I•••I non-covalent interactions in solid state" was recognized by the editorial board of *European*

Journal of Inorganic Chemistry as ***one of the most significant articles of the issue and its graphical abstract was placed on the cover*** of 39-40th issue 2019 (DOI: 10.1002/ejic.201900349).

The paper by Alexander S. Novikov and colleagues “Gold-catalyzed functionalization of semicarbazides with terminal alkynes to achieve substituted semicarbazones” published in *Eur. J. Org. Chem.* (DOI: 10.1002/ejoc.201901108) was included by Wiley-VCH in **Hot Topic: Gold collection**.

The paper by Alexander S. Novikov and colleagues "Four-center nodes: supramolecular synthons based on cyclic halogen bonding" was recognized by the editorial board of *Chemistry – A European Journal* as ***one of the most significant articles of the issue and its graphical abstract was placed on the cover*** of 60th issue 2019 (DOI: 10.1002/chem.201902264).

The paper by Alexander S. Novikov and colleagues “(Isocyano group π-hole)•••[d_z^2-M^{II}] interactions at (isocyanide)[M^{II}] complexes, where positively charged metal centers (d^8M = Pt, Pd) act as nucleophiles” was recognized by the editorial board of *Chemistry – A European Journal* as ***Hot Paper*** (DOI: 10.1002/chem.201901187).

The paper by Alexander S. Novikov and colleagues “Reverse arene sandwich structures based upon π-hole•••[M^{II}](d^8M = Pt, Pd) interactions, where positively charged metal centers play the role of a nucleophile” was recognized by the editorial board of *Angewandte Chemie* as ***one of the most significant articles of the issue and its graphical abstract was placed on the cover*** of 13th issue 2019 (DOI: 10.1002/anie.201814062).

The paper by Alexander S. Novikov and colleagues “Re-thinking hydrolytic imidazoline ring expansion: a common approach to the preparation of medium-sized rings via side chain insertion into [1.4]oxa- and [1.4]thiazepinone scaffold” was recognized by the editorial board of *The Journal of Organic Chemistry* as ***one of the most significant articles of the issue and its graphical abstract was placed on the cover*** of 4th issue 2019 (DOI:10.1021/acs.joc.8b02805).

The paper by Alexander S. Novikov and colleagues “2,2′-Azobispyridine in phosphorus coordination chemistry: a new approach to 1,2,4,3-triazaphosphole derivatives” was recognized by the editorial board of *European Journal of Inorganic Chemistry* as ***VIP (Very Important Paper) based on referees' suggestions*** (DOI: 10.1002/ejic.201800831).

The paper by Alexander S. Novikov and colleagues “Rare medium-sized rings prepared via hydrolytic imidazoline ring expansion (HIRE)” was recognized by the editorial board of *The Journal of Organic Chemistry* as ***one of the most significant articles of the issue and its graphical abstract was placed on the cover*** of 17th issue 2018 (DOI:10.1021/acs.joc.8b01210).

The paper by Alexander S. Novikov and colleagues “Platinum(II)-mediated double coupling of 2,3-diphenylmaleimidine with nitrile functionalities giving annulated triazapentadiene PANT systems” was recognized by the editorial board of *European Journal of Inorganic Chemistry* as ***one of the most significant articles of the issue and its graphical abstract was placed on the cover*** of 10th issue 2016 (DOI: 10.1002/ejic.201501398).

The paper by Alexander S. Novikov and colleagues “A family of heterotetrameric clusters of chloride species and halomethanes held by two halogen and two hydrogen bonds” was recognized by the editorial board of *CrystEngComm* as ***one of the most significant articles of the issue and its graphical abstract was placed on the cover*** of 28th issue 2016 (DOI: 10.1039/c6ce01179a).

Referees