Curriculum Vitae

Dr. Alexander S. Novikov

Scopus ID: 50262902200

Web of Science ResearcherID: L-5001-2015

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

novikov@itmo.ru

Mobile: +7 981 958 0247

Personal Information

Nationality:

Russian

Date of birth:

June 6th, 1988

Place of birth:

Moscow, USSR

Languages:

Russian (native), English (fluent), Portuguese (intermediate)

Working Addresses:

Institute of Chemistry, Saint Petersburg State University, Universitetskii pr., 26, 198504, Petergof, St. Petersburg, Russia: Senior Researcher

Infochemistry Scientific Center, ITMO University, Lomonosova st., 9, 191002, St. Petersburg, Russia: Associate Research Professor and “Computational Chemistry” Group Leader

Research Interests

Fields of expertise:

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

Present investigation interests:

- ✓ Non-covalent interactions
- ✓ 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 (2018–2021); 20-33-70010 (2019–2021); 20-53-00006 (2020–2022)] (2016–present)

- Associate Research Professor and "Computational Chemistry" Group Leader at the Infochemistry Scientific Center, ITMO University (Saint Petersburg, Russia) (2020–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

Teaching in fields of General Chemistry; Quantum and Computational Chemistry (lectures, seminars, practical classes) at the ITMO University, Infochemistry Scientific Center [March 2020–present, Saint Petersburg, Russia]

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]

Teaching activity at the High-School level

Teaching Assistant at the High School №1319 with advanced learning of English [September–December 2009, Moscow, Russia]

Teaching Assistant at the High School №46 [February–March 2009, Moscow, Russia]

Publications (h-index in Google Scholar/Scopus/Web of Science = 31/28/28)

1. Shmelev N. Y., Okubazghi T. H., Abramov P. A., Komarov V. Y., Rakhmanova M. I., **Novikov A. S.**, Gushchin A. L. “Intramolecular aurophilic interactions in dinuclear gold(I) complexes with twisted bridging 2,2′-bipyridine ligands” // *Dalton Trans.* 2021, V. 50. P. 12448. [**Highlighted on cover**]
2. Abramov P. A., **Novikov A. S.**, Sokolov M. N. "Interactions of aromatic rings in the crystal structures of hybrid polyoxometalates and Ru clusters" // *CrystEngComm* 2021, V. 23. P. 6409.
3. Afanasenko A. M., Krutin D. V., Taishev A. E., **Novikov A. S.**, Chulkova T. G., Kolesnikov I. E., Kornyakov I. V., Panikorovskii T. L., Vereshchagin A. N., Elinson M. N. “The impact of the molecular structure on aggregation and solid state luminescence of 2,3-diarylfumaronitriles” // *J. Mol. Struct.* 2021, V. 1248. P. 131503.
4. Bondarenko M. A., **Novikov A. S.**, Chernova K. V., Sokolov M. N., Adonin S. A. “2-Methylpyridinium salt of pentaiodobenzoic acid: role of the halogen bond in the formation of a crystal packing” // *J. Struct. Chem.* 2021, V. 62. P. 1237.
5. Lukoyanov A. N., Fomenko I. S., Gongola M. I., Shul’pina L. S., Ikonnikov N. S., Shul’pin G. B., Ketkov S. Y., Fukin G. K., Rumyantcev R. V., **Novikov A. S.**, Nadolinny V. A., Sokolov M. N., Gushchin A. L. “Novel oxidovanadium complexes with redox-active R-mian and R-bian ligands: synthesis, structure, redox and catalytic properties” // *Molecules* 2021, V. 26. P. 5706.
6. Baykov S. V., Mikherdov A. S., **Novikov A. S.**, Geyl K. K., Tarasenko M. V., Gureev M. A., Boyarskiy V. P. “π–π noncovalent interaction involving 1,2,4- and 1,3,4-oxadiazole systems: the combined experimental, theoretical, and database study” // *Molecules* 2021, V. 26. P. 5672.
7. Toikka Y. N., Spiridonova D. V., **Novikov A. S.**, Bokach N. A. “Copper(II) prevents the saccarine-dialkylcyanamide coupling by forming mononuclear (saccharinate)(dialkylcyanamide)copper(II) complexes” // *Inorganics* 2021, V. 9. P. 69.
8. Deriabin K. V., Ignatova N. A., Kirichenko S. O., **Novikov A. S.**, Kryukova M. A., Kukushkin V. Yu., Islamova R. M. "Structural features of polymer ligand environments

dramatically affect the mechanical and room-temperature self-healing properties of cobalt(II)-incorporating polysiloxanes" // *Organometallics* 2021, V. 40. P. 2750.

9. Sysoeva A. A., **Novikov A. S.**, Il'in M. V., Suslonov V. V., Bolotin D. S. "Predicting the catalytic activity of azolium-based halogen bond donors: an experimentally-verified theoretical study" // *Org. Biomol. Chem.* 2021, V. 19. P. 7611. [**Highlighted on cover**]
10. Bondarenko M. A., **Novikov A. S.**, Sukhikh T. S., Korolkov I. V., Sokolov M. N., Adonin S. A. "Mono- and binuclear Cu(II) 3,5-diiodosalicylates: structures and features of non-covalent interactions in crystalline state" // *J. Mol. Struct.* 2021, V. 1244. P. 130942.
11. Nesterov P. V., Shilovskikh V. V., Sokolov A. D., Gurzhiy V. V., **Novikov A. S.**, Timralieva A. A., Belogub E. V., Kondratyuk N. D., Orekhov N. D., Skorb E. V. "Encapsulation of rhodamine 6G dye molecules for affecting symmetry of supramolecular crystals of melamine-barbiturate" // *Symmetry* 2021, V. 13. P. 1119.
12. Imoro N., Shilovskikh V. V., Nesterov P. V., Timralieva A. A., Gets D., Nebalueva A., Lavrentev F. V., **Novikov A. S.**, Kondratyuk N. D., Orekhov N. D., Skorb E. V. "Biocompatible pH-degradable functional capsules based on melamine cyanurate self-assembly" // *ACS Omega* 2021, V. 6. P. 17267. [**Highlighted on cover**]
13. Khrustalev V. N., Grishina M. M., Matsulevich Z. V., Lukiyanova J. M., Borisova G. N., Osmanov V. K., **Novikov A. S.**, Kirichuk A. A., Solari E., Borisov A. V., Tskhovrebov A. G. "Novel cationic 1,2,4-selenadiazoles: synthesis via addition of 2-pyridylselenyl halides to unactivated nitriles, structures and four-center Se•••N contacts" // *Dalton Trans.* 2021, V. 50. P. 10689. [**Highlighted on cover**]
14. Rudnitskaya O. V., Tereshina T. A., Dobrokhotova E. V., Kultyshkina E. K., **Novikov A. S.**, Tskhovrebov A. G., Zubavichus Y. V., Khrustalev V. N. "Monoprotonated dimethyl sulfoxide, $[HOSMe_2]^+$: synthesis, crystal structure, spectroscopic and theoretical studies of $[HOSMe_2]_2[OsCl_6]\bullet 2H_2O$ // *ChemistrySelect* 2021, V. 6. P. 5211.
15. **Novikov A. S.**, Gushchin A. L. "Trinuclear molybdenum clusters with sulfide bridges as potential anionic receptors via chalcogen bonding" // *CrystEngComm* 2021, V. 23. P. 4607.
16. Vershinin M. A., Rakhmanova M. I., **Novikov A. S.**, Sokolov M. N., Adonin S. A. "Zn(II) heteroleptic halide complexes with 2-halopyridines: features of halogen bonding in solid state" // *Molecules* 2021, V. 26. P. 3393.
17. Rostovtseva V., Pulyalina A., Dubovenko R., Faykov I., Subbotina K., Saprykina N., **Novikov A.**, Vinogradova L., Polotskaya G. "Enhancing pervaporation membrane selectivity by incorporating star macromolecules modified with ionic liquid for intensification of lactic acid dehydration" // *Polymers* 2021, V. 13. P. 1811. [**Editor's Choice Article**]
18. Dodonov V. A., Kushnerova O. A., Baranov E. V., **Novikov A. S.**, Fedushkin I. L. "Activation and modification of carbon dioxide by redox-active low-valent gallium species" // *Dalton Trans.* 2021, V. 50. P. 8899.
19. Bondarenko M.A., **Novikov A.S.**, Adonin S.A. "Mononuclear Zn(II) 3,5-diiodosalicylate complex with 3-chloropyridine: synthesis and features of non-covalent interactions in the solid state" // *Russ. J. Inorg. Chem.* 2021. V. 66. P. 814.
20. Dubovtsev A.Yu., Zvereva V.V., Shcherbakov N.V., Dar'in D.V., **Novikov A.S.**, Kukushkin V.Yu. "Acid-catalyzed [2+2+2] cycloaddition of two cyanamides and one ynamide: highly regioselective synthesis of 2,4,6-triaminopyrimidines" // *Org. Biomol. Chem.* 2021, V. 19. P. 4577.

21. Bondarenko M.A., **Novikov A.S.**, Korolkov I.V., Sokolov M.N., Adonin S.A. "Cu(II) 2-iodobenzoates: precursor-dependent formation of paddlewheel-like $[Cu_2(OOCR)_4L_2]$ or $[Cu_2L_4(OOCR)_2Cl_2]$ binuclear complexes" // *Inorg. Chim. Acta* 2021, V. 524. P. 120436.

22. Mukhacheva A.A., Komarov V.Yu., Kokovkin V.V., **Novikov A.S.**, Abramov P.A., Sokolov M.N. "Unusual π-π interactions directed by $[\{(C_6H_6)Ru\}_2W_8O_{30}(OH)_2]^{6-}$ hybrid anion" // *CrystEngComm* 2021, V. 23. P. 4125.

23. Usoltsev A.N., Korobeynikov N.A., Kolesov B.A., **Novikov A.S.**, Abramov P.A., Sokolov M.N., Adonin S.A. "Oxochloroselenate(IV) with Incorporated $\{Cl_2\}$: The Case of Strong Cl⋯Cl Halogen Bonding" // *Chem. Eur. J.* 2021, V. 27. P. 9292.

24. Nikitina A.A., Milichko V.A., **Novikov A.S.**, Larin A.O., Nandi P., Mirsaidov U., Andreeva D.V., Rybin M.V., Kivshar Y.S., Skorb E.V. "All-dielectric nanostructures with a thermoresponsible dynamic polymer shell" // *Angew. Chem. Int. Ed.* 2021, V. 60. P. 12737.

25. Bondarenko M.A., Abramov P.A., Plyusnin P.E., **Novikov A.S.**, Sokolov M.N., Adonin S.A. "Bromoantimonates with bis(pyridinium)-type dications obtained via oxidation by dibromine: diverse structural types and features of interactions pattern" // *Polyhedron* 2021, V. 202. P. 115217.

26. Tskhovrebov A.G., **Novikov A.S.**, Tupertsev B.S., Nazarov A.A., Antonets A.A., Astafiev A.A., Kritchenkov A.S., Kubasov A.S., Nenajdenko V.G., Khrustalev V.N. "Azoimidazole gold(III) complexes: synthesis, structural characterization and self-assembly in the solid state" // *Inorg. Chim. Acta* 2021, V. 522. P. 120373.

27. Khrustalev V.N., Savchenko A.O., Zhukova A.I., Chernikova N.Yu., Kurykin M.A., **Novikov A.S.**, Tskhovrebov A.G. "Attractive fluorine•••fluorine interactions between perfluorinated alkyl chains: a case of perfluorinated Cu(II) diiminate $Cu[C_2F_5–C(NH)–CF=C(NH)–CF_3]_2$" // *Z. Kristallogr. Cryst. Mater.* 2021, V. 236. P. 117.

28. Nelyubin A.V., Klyukin I.N., **Novikov A.S.**, Zhdanov A.P., Grigoriev M.S., Zhizhin K.Yu., Kuznetsov N.T. "Nucleophilic addition of amino acid esters to nitrilium derivatives of *closo*-decaborate anion" // *Mendeleev Commun.* 2021, V. 31. P. 201.

29. Shikhaliyev N.G., Maharramov A.M., Bagirova K.N., Suleymanova G.T., Tsyrenova B.D., Nenajdenko V.G., **Novikov A.S.**, Khrustalev V.N., Tskhovrebov A.G. "Supramolecular organic frameworks derived from bromoaryl-substituted dichlorodiazabutadienes via Cl•••Br halogen bonding" // *Mendeleev Commun.* 2021, V. 31. P. 191.

30. Voinova V.V., Klyukin I.N., **Novikov A.S.**, Koz'menkova A.Ya., Zhdanov A.P., Zhizhin K.Yu., Kuznetsov N.T. "Electrochemical properties of the *closo*-decaborate anion $[B_{10}H_{10}]^{2-}$ and a new method for preparation of the $[B_{20}H_{18}]^{2-}$ anion" // *Russ. J. Inorg. Chem.* 2021, V. 66. P. 295.

31. Tskhovrebov A.G., **Novikov A.S.**, Khrustalev V.N. "Identification of supramolecular dimers in the crystal structure of (Z)-1-(((5-fluoropyridin-2-yl)amino)methylene)naphthalen-2(1H)-one via $C(sp^2)$–H•••F hydrogen bonding: a combined experimental and theoretical study" // *J. Struct. Chem.* 2021, V. 62. P. 460.

32. Usoltsev A.N., Korobeynikov N.A., Kolesov B.A., **Novikov A.S.**, Samsonenko D.G., Fedin V.P., Sokolov M.N., Adonin S.A. "Rule, not exclusion: formation of dichlorine-containing supramolecular complexes with chlorometalates(IV)" // *Inorg. Chem.* 2021, V. 60. P. 4171.

33. Bondarenko M.A., **Novikov A.S.**, Sakhapov I.F., Sokolov M.N., Adonin S.A. “Heteroleptic Cu(I) halide complexes with perchlorinated 1,10-phenanthroline” // *J. Mol. Struct.* 2021, V. 1234. P. 130199.

34. Klyukin I.N., Vlasova Y.S., **Novikov A.S.**, Zhdanov A.P., Zhizhin K.Y., Kuznetsov N.T. “Theoretical study of *closo*-borate anions $[B_nH_n]^{2-}$ (n = 5–12): bonding, atomic charges, and reactivity analysis” // *Symmetry* 2021, V. 13. P. 464.

35. Baykov S.V., Presnukhina S.I., **Novikov A.S.**, Shetnev A.A., Boyarskiy V.P., Kukushkin V.Yu. “2,5-Dibromothiophenes: halogen bond involving packing patterns and their relevance to solid-state polymerization” // *Cryst. Growth Des.*, 2021, V. 21. P. 2526.

36. **Novikov A.S.** “IsoStar program suite for studies of noncovalent interactions in crystals of chemical compounds” // *Crystals* 2021, V. 11. P. 162.

37. Ivanov A.S., Nikolaev K.G., **Novikov A.S.**, Yurchenko S.O., Novoselov K.S., Andreeva D.V., Skorb E.V. “Programmable soft-matter electronics” // *J. Phys. Chem. Lett.* 2021, V. 12. P. 2017.

38. Jiménez-Grávalos F., Gallegos M., Pendás Á. M., **Novikov A.S.** “Challenging the electrostatic σ-hole picture of halogen bonding using minimal models and the interacting quantum atoms approach” // *J. Comput. Chem.* 2021, V. 42. P. 676.

39. Usoltsev A.N., Sukhikh T.S., **Novikov A.S.**, Shayapov V.R., Pishchur D.P., Korolkov I.V., Sakhapov I.F., Fedin V.P., Sokolov M.N., Adonin S.A. “Unexpected polymorphism in bromoantimonate(III) complexes and its effect on optical properties” // *Inorg. Chem.* 2021, V. 60. P. 2797.

40. Katkova S.A., Luzyanin K.V., **Novikov A.S.**, Kinzhalov M.A. “Modulation of luminescence properties for [cyclometalated]-Pt^{II}(isocyanide) complexes upon co-crystallisation with halosubstituted perfluorinated arenes” // *New J. Chem.* 2021, V. 45. P. 2948.

41. Bondarenko M.A., **Novikov A.S.**, Abramov P.A., Sakhapov I.F., Sokolov M.N., Adonin S.A. “2,3,4,5-Tetraiodopyrrole as a building block for halogen bonding: formation of supramolecular hybrids with organic iodide salts in solid state” // *J. Mol. Struct.* 2021, V. 1230. P. 129931.

42. Voinova V.V., Selivanov N.A., Plyushchenko I.V., Vokuev M.F., Bykov A.Y., Klyukin I.N., **Novikov A.S.**, Zhdanov A.P., Grigoriev M.S., Rodin I.A., Zhizhin K.Yu., Kuznetsov N.T. “Fused 1,2-diboraoxazoles based on *closo*-decaborate anion–novel members of diboroheterocycle class” // *Molecules* 2021, V. 26. P. 248.

43. Aliyarova I.S., Ivanov D.M., Soldatova N.S., **Novikov A.S.**, Postnikov P.S., Yusubov M.S., Kukushkin V.Yu. “Bifurcated halogen bonding involving diaryliodonium cations as iodine(III)-based double-σ-hole donors” // *Cryst. Growth Des.* 2021, V. 21. P. 1136.

44. Yunusova S.N., **Novikov A.S.**, Soldatova N.S., Vovk M.A., Bolotin D.S. “Iodonium salts as efficient iodine(III)-based noncovalent organocatalysts for Knorr-type reactions” // *RSC Adv.* 2021, V. 11. P. 4574.

45. Bondarenko M.A., Rakhmanova M.I., Plyusnin P.E., Abramov P.A., **Novikov A.S.**, Rajakumar K., Sokolov M.N., Adonin S.A. “Heteroleptic Zn(II) 3,5-diiodosalicylates: structures, luminescence and features of non-covalent interactions in solid state” // *Polyhedron* 2021, V. 194. P. 114895.

46. Popov R.A., Mikherdov A.S., **Novikov A.S.**, Myznikov L.V., Boyarskiy V.P. “Pd^{II}- and Pt^{II}-mediated coupling of aryl isocyanides with N-heterocyclic thiones” // *New J. Chem.* 2021, V. 45. P. 1785.

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205. Kinzhalov M.A., **Novikov A.S.**, Luzyanin K.V., Haukka M., Pombeiro A.J.L., Kukushkin V.Yu. "Pd^{II}-mediated integration of isocyanides and azide ion might proceed via formal 1,3-dipolar cycloaddition between RNCs ligands and uncomplexed azide" // *New J. Chem.* 2016, V. 40. P. 521.

206. Ivanov D.M., Kirina Y.V., **Novikov A.S.**, Starova G.L., Kukushkin V.Yu. "Efficient π-stacking with benzene provides 2D assembly of *trans*-[$PtCl_2$(*p*-$CF_3C_6H_4CN)_2$]" // *J. Mol. Struct.* 2016, V. 1104. P. 19.

207. Andrusenko E.V., Kabin E.V., **Novikov A.S.**, Bokach N.A., Starova G.L., Zolotarev A.A., Kukushkin V.Yu. "Highly reactive Ni^{II}-bound nitrile–oxime coupling intermediate stabilized by substituting conventional nitriles with a dialkylcyanamide" // *Eur. J. Inorg. Chem.* 2015, V. 2015. P. 4894.

208. **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.

209. 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.

210. Bolotin D.S., Demakova M.Ya., **Novikov A.S.**, Avdontceva M.S., Kuznetsov M.L., Bokach N.A., Kukushkin V.Yu. "Bifunctional reactivity of amidoximes observed upon nucleophilic addition to metal-activated nitriles" // *Inorg. Chem.* 2015. V. 54. P. 4039.

211. 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.

212. **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.

213. **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.

214. **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.

215. **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.

216. **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* (Russia)

Member of the Expert Council of the *Gennady Komissarov Foundation for Support of Young Scientists* (Russia)

Reviewer of grant research proposals for the *National Science Centre* (Poland)

Reviewer of grant research proposals for the *National Research Foundation* (South Africa)

Guest Editor of the Special Issue "Non-covalent interactions in crystals" in *Zeitschrift für Kristallographie – Crystalline Materials* (De Gruyter)

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 "New Trends in King Saud University in Crystals" in *Crystals* (MDPI)
https://www.mdpi.com/journal/crystals/special_issues/King_Saud_University

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 *Compounds* (MDPI)
https://www.mdpi.com/journal/compounds/editors

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), *Chemistry – A European Journal* (John Wiley & Sons), *Journal of Computational Chemistry* (John Wiley & Sons), *Journal of Heterocyclic Chemistry* (John Wiley & Sons), *Crystal Research & Technology* (John Wiley & Sons), *Molecules* (MDPI), *Crystals* (MDPI), *Materials* (MDPI), *Viruses* (MDPI), *International Journal of Molecular Sciences* (MDPI), *Inorganics* (MDPI), *Chemosensors* (MDPI), *Symmetry* (MDPI), *Mathematics* (MDPI), *Biology* (MDPI), *Entropy* (MDPI), *Processes* (MDPI), *Vaccines* (MDPI), *Nanomaterials* (MDPI), *Pharmaceuticals* (MDPI), *Sustainability* (MDPI), *Zeitschrift für Kristallographie – Crystalline Materials* (De Gruyter), *Current Organic Chemistry* (Bentham Science), *Frontiers in Chemistry* (Frontiers), *Coordination Chemistry Review* (Elsevier), *Applied Catalysis B: Environmental* (Elsevier), *International Journal of Hydrogen Energy* (Elsevier), *International Journal of Biological Macromolecules* (Elsevier), *Journal of Materials Research and Technology* (Elsevier), *Materials Letters* (Elsevier), *Food Chemistry* (Elsevier), *Physica E: Low-dimensional Systems and Nanostructures* (Elsevier), *Inorganica Chimica Acta* (Elsevier), *Solid State Sciences* (Elsevier), *Journal of Solid State Chemistry* (Elsevier), *Diamond and Related Materials* (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), *Arabian Journal of Chemistry* (Elsevier), *Carbohydrate Research* (Elsevier), *Surfaces and Interfaces* (Elsevier), *Optik* (Elsevier), *Data in Brief* (Elsevier), *Chemical Data Collections* (Elsevier), *Journal of Coordination Chemistry* (Taylor & Francis), *Structural Chemistry* (Springer), *Chemical Papers* (Springer), *Research on Chemical Intermediates* (Springer), *Reaction Kinetics, Mechanisms and Catalysis* (Springer), *Journal of Molecular Modeling* (Springer), *Chemistry Africa* (Springer), *Russian Journal of Inorganic Chemistry* (Pleiades Publishing)

12th International Conference on Chemistry for Young Scientists "Mendeleev 2021" (Saint Petersburg, Russia, 06–10 September 2021) – *Chairman of section "Computer modelling and cheminformatics", Member of the program and organization committees*

4th International Symposium on Halogen Bonding (Virtual event due to COVID-19 pandemic, Stellenbosch, South Africa, 02–05 November 2020) – *Member of the international advisory board*

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*

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

Laureate of the Scientific Works Competition named after Academician Ya. K. Syrkin (quantum chemistry, theory of molecules structure and chemical bonds), Kurnakov Institute of General and Inorganic Chemistry of the Russian Academy of Sciences, Moscow, Russia (2020)

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 "Intramolecular aurophilic interactions in dinuclear gold(I) complexes with twisted bridging 2,2′-bipyridine ligands" was recognized by the editorial board of *Dalton Transactions* as ***one of the most significant articles of the issue and its graphical abstract was placed on the cover*** of 36th issue 2021 (DOI: 10.1039/d1dt02164h).

The paper by Alexander S. Novikov and colleagues "Predicting the catalytic activity of azolium-based halogen bond donors: an experimentally-verified theoretical study" was recognized by the editorial board of *Organic & Biomolecular Chemistry* as ***one of the most significant articles of the issue and its graphical abstract was placed on the cover*** of 35th issue 2021 (DOI: 10.1039/d1ob01158h).

The paper by Alexander S. Novikov and colleagues "Enhancing pervaporation membrane selectivity by incorporating star macromolecules modified with ionic liquid for intensification of lactic acid dehydration" was selected by the academic editors of *Polymers* as one of the ***Editor's Choice Articles*** (DOI: 10.3390/polym13111811).

The paper by Alexander S. Novikov and colleagues "Novel cationic 1,2,4-selenadiazoles: synthesis via addition of 2-pyridylselenyl halides to unactivated nitriles, structures and four-center Se•••N contacts" was recognized by the editorial board of *Dalton Transactions* as ***one of the most significant articles of the issue and its graphical abstract was placed on the cover*** of 31th issue 2021 (DOI: 10.1039/D1DT01322J).

The paper by Alexander S. Novikov and colleagues "Biocompatible pH-degradable functional capsules based on melamine cyanurate self-assembly" was recognized by the editorial board of *ACS Omega* as ***one of the most significant articles of the issue and its graphical abstract was placed on the cover*** of 27th issue 2021 (DOI: 10.1021/acsomega.1c01124).

The paper by Alexander S. Novikov and colleagues “Opening the third century of polyhalide chemistry: thermally stable complex with “trapped” dichlorine” was recognized by the editorial board of *Chemistry – A European Journal* as ***Hot Paper*** (DOI: 10.1002/chem.202002014).

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).