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Working Address:

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

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
- ✓ Reaction mechanisms
- ✓ Machine learning, artificial intelligence and big data analysis in chemistry

Teaching activity at the University level

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

Supervising activity

Supervising of PhD-projects and co-supervising of students' research projects in the ITMO University, Infochemistry Scientific Center [2020–present, Saint Petersburg, Russia]

Publications (h-index in Google Scholar = 40)

1. Timralieva A. A., Moskalenko I. V., Nesterov P. V., Shilovskikh V. V., **Novikov A. S.**, Konstantinova E. A., Kokorin A. I., Skorb E. V. “Melamine Barbiturate as a Light-Induced Nanostructured Supramolecular Material for a Bioinspired Oxygen and Organic Radical Trap and Stabilization” // *ACS Omega* 2023, V. 8. P. 8276.
2. Bondarenko M. A., Zherebtsov D. A., **Novikov A. S.**, Fedin V. P., Adonin S. A. “Two-dimensional Cu(II) 5-iodoisophthalate with a 1,2-bis(4-pyridyl)ethylene linker: crystal structure and features of electronic structure” // *J. Struct. Chem.* 2023, V. 64. P. 112.
3. **Novikov A. S.** “Non-Covalent Interactions in Polymers” // *Polymers* 2023, V. 15. P. 1139.
4. Derkach K. V., Gureev M. A., Babushkina A. A., Mikhaylov V. N., Zakharova I. O., Bakhtyukov A. A., Sorokoumov V. N., **Novikov A. S.**, Krasavin M., Shpakov A. O., Balova I. A. “Dual PTP1B/TC-PTP Inhibitors: Biological Evaluation of 3-(Hydroxymethyl)cinnoline-4(1H)-Ones” // *Int. J. Mol. Sci.* 2023, V. 24. P. 4498.
5. **Novikov, A. S.** “Theoretical Studies and Computer Modeling of Supramolecular Chemical Systems: Structure, Properties and Reactivity” // *Chem. Proc.* 2022, V. 12. P. 88.
6. Вершинин М. А., **Новиков А. С.**, Адонин С. А. “Галогенидные комплексы [(2-Br-5-MePy)$_2$ZnX$_2$] (X = Cl, Br): строение и особенности нековалентных взаимодействий в кристаллической структуре” // *Коорд. Хим.* 2023, V. 49. In press. DOI: 10.31857/S0132344X22600369.
7. T. M. Tamer, M. El M. Tantawi, A. Brussevich, A. Nebalueva, **A. Novikov**, I. Moskalenko, M. M. Abu-Serie, M. A. Hassan, S. Ulasevich, E. V. Skorb “Functionalization of chitosan with poly aromatic hydroxyl molecules for improving its antibacterial and antioxidant properties: practical and theoretical studies” // *Int. J. Biol. Macromol.* 2023, V. 234. P. 123687.
8. **Novikov A. S.** “Recent progress in theoretical studies and computer modeling of non-covalent interactions” // *Crystals* 2023, V. 13. P. 361.
9. Sheina E. S., Shestakova T. S., Deev S. L., Khalymbadzha I. A., Slepukhin P. A., Eltsov O. S., **Novikov A. S.**, Shevyrin V. A., Charushin V. N., Chupakhin O. N. “Mesomeric betaines based on adamantylated 1,2,4-triazolo[4,3-a]pyrimidin-5-ones: synthesis, structure and conversion into anionic N-heterocyclic carbenes” // *Chem. Asian J.* 2023, In press. DOI: http://10.1002/asia.202201306.
10. Загузин А. С., Спиридонова Д. В., **Новиков А. С.**, Рахманова М. И., Жеребцов Д. А., Федин В. П., Адонин С. А. “Двухмерный координационный полимер на основе Zn^{II} и 5-иодизофталата: синтез, строение и особенности электронного строения” // *Изв. АН. Сер. Хим.* 2023, Т. 1. С. 177.
11. Klyukin I. N., Kolbunova A. V., **Novikov A. S.**, Nelyubin A. V., Zhdanov A. P., Kubasov A. S., Selivanov N. A., Bykov A. Y., Zhizhin K. Y., Kuznetsov N. T. “Synthesis of disubstituted carboxonium derivatives of *closo*-decaborate anion [2,6-$B_{10}H_8O_2CC_6H_5]^-$: theoretical and experimental study” // *Molecules* 2023, V. 28. P. 1757.
12. Artem’ev A. V., Doronina E. P., Rakhmanova M. I., Hei X., Stass D. V., Tarasova O. A., Bagryanskaya I. Yu., Samsonenko D. G., **Novikov A. S.**, Nedolya N. A., Li J. “A family of CuI-based 1D polymers showing colorful short-lived TADF and phosphorescence induced by photo- and X-ray irradiation” // *Dalton Trans.* 2023, In press. DOI: 10.1039/D3DT00035D

13. **Novikov A. S.** "Non-covalent catalysts" // *Catalysts* 2023, V. 13. P. 339.
14. Lavrenova L. G., Ivanova A. I., Glinskaya L. A., Artem'ev A. V., Lavrov A. N., **Novikov A. S.**, Abramov P. A. "Halogen bonding channels for magnetic exchange in Cu(II) complexes with 2,5-di(methylthio)-1,3,4-thiadiazole" // *Chem. Asian J.* 2023, In press. DOI: 10.1002/asia.202201200
15. Kukhtenko E. V., Lavrentev F. V., Shilovskikh V. V., Zyrianova P. I., Koltsov S. I., Ivanov A. S., **Novikov A. S.**, Muravev A. A., Nikolaev K. G., Andreeva D. V., Skorb E. V. "Periodic self-assembly of poly(ethyleneimine)–poly(4-styrenesulfonate) complex coacervate membranes" // *Polymers* 2023, V. 15. P. 45.
16. **Novikov A. S.** "Recent progress in the theoretical studies of the noncovalent interactions of supramolecular complexes with polyhalides and halometalates" // *Compounds* 2023, V. 3. P. 27.
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18. Savintseva L., Avdoshin A., Ignatov S., **Novikov A.** "Theoretical study of charge mobility in crystal porphine and a computer design of a porphine-based semiconductive discotic liquid mesophase" // *Int. J. Mol. Sci.* 2023, V. 24. P. 736.
19. Grzhegorzhevskii K., Tonkushina M., Gushchin P., Gagarin I., Ermoshin A., Belova K., Prokofyeva A., Ostroushko A., **Novikov A.** "Association of Keplerate-type polyoxometalate $\{Mo_{72}Fe_{30}\}$ with tetracycline: nature of binding sites and antimicrobial action" // *Inorganics* 2023, V. 11. P. 9.
20. Polonnikov D. A., Il'in M. V., Safinskaya Y. V., Aliyarova I. S., **Novikov A. S.**, Bolotin D. S. "(Pre)association as a crucial step for computational prediction and analysis of the catalytic activity of σ-hole donating organocatalysts" // *Org. Chem. Front.* 2023, V. 10. P. 169.
21. Sadieva L. K., Kovalev I. S., Taniya O. S., Platonov V. A., **Novikov A. S.**, Berseneva V. S., Santra S., Zyryanov G. V., Ranu B. C., Charushin V. N. "Bola-type PEG-linked polyaromatic hydrocarbon-based chemosensors for the "turn-off" excimer fluorescence detection of nitro-analytes/explosives in aqueous solutions" // *Dyes and Pigments* 2023, V. 210. P. 111014.
22. **Novikov A. S.** "Plethora of non-covalent interactions in coordination and organometallic chemistry are modern smart tool for materials science, catalysis, and drugs design" // *Int. J. Mol. Sci.* 2022, V. 23. P. 14767.
23. Sharapov A. D., Fatykhov R. F., Khalymbadzha I. A., Valieva M. I., Nikonov I. L., Taniya O. S., Kopchuk D. S., Zyryanov G. V., Potapova A. P., **Novikov A. S.**, Sharutin V. V., Chupakhin O. N. "Fluorescent pyranoindole congeners: synthesis and photophysical properties of pyrano[3,2-*f*], [2,3-*g*], [2,3-*f*], and [2,3-*e*]indoles" // *Molecules* 2022, V. 27. P. 8867.
24. Miroshnichenko A. S., Deriabin K. V., Rashevskii A. A., Suslonov V. V., **Novikov A. S.**, Mukhin I. S., Islamova R. M. "Structural features of Eu^{3+} and Tb^{3+}-bipyridinedicarboxamide complexes" // *Polymers* 2022, V. 14. P. 5540.
25. Klyukin I. N., Kolbunova A. V., **Novikov A. S.**, Zhdanov A. P., Zhizhin K. Y., Kuznetsov N. T. "Theoretical insight into B–C chemical bonding in *closo*-borate $[B_nH_{n-1}CH_3]^{2-}$ (n = 6, 10, 12) and monocarborane $[CB_nH_nCH_3]^-$ (n = 5, 9, 11) anions" // *Inorganics* 2022, V. 10. P. 186.

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29. Lorits E. M., Gubar E. A., **Novikov A. S.** “Design of the algorithm for packaging of water molecules in a fixed volume” // *Symmetry* 2022, V. 14. P. 2453.

30. Starnovskaya E. S., Kopchuk D. S., Khasanov A. F., Taniya O. S., Nikonov I. L., Valieva M. I., Pavlyuk D. E., **Novikov A. S.**, Zyryanov G. V., Chupakhin O. N. “Synthesis and photophysical properties of α-(N-biphenyl)-substituted 2,2′-bipyridine-based push–pull fluorophores“ // *Molecules* 2022, V. 27. P. 6879.

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35. Nebalueva A. S., Timralieva A. A., Sadovnichii R. V., **Novikov A. S.**, Zhukov M. V., Aglikov A. S., Muravev A. A., Sviridova T. V., Boyarskiy V. P., Kholkin A. L., Skorb E. V. “Piezo-responsive hydrogen-bonded frameworks based on vanillin-barbiturate conjugates” // *Molecules* 2022, V. 27. P. 5659.

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Kirichuk A. A., Peregudov A. S., Kritchenkov A. S., Tskhovrebov A. G. “Facile access to 2-selenoxo-1,2,3,4-tetrahydro-4-quinazolinone scaffolds and corresponding diselenides via cyclization between methyl anthranilate and isoselenocyanates: synthesis and structural features” // *Molecules* 2022, V. 27. P. 5799.

39. Demyanov Y. V., Sadykov E. H., Rakhmanova M. I., **Novikov A. S.**, Bagryanskaya I. Y., Artem’ev A. V. “Tris(2-pyridyl)arsine as a new platform for design of luminescent Cu(I) and Ag(I) complexes” // *Molecules* 2022, V. 27. P. 6059.
40. Bondarenko M. A., **Novikov A. S.**, Sokolov M. N., Adonin S. A. “Heteroleptic Zn(II)–pentaiodobenzoate complexes: structures and features of halogen–halogen non-covalent interactions in solid state” // *Inorganics* 2022, V. 10. P. 151.
41. Il’in M. V., **Novikov A. S.**, Bolotin D. S. “Sulfonium and selenonium salts as noncovalent organocatalysts for the multicomponent Groebke–Blackburn–Bienaymé reaction” // *J. Org. Chem.* 2022, V. 87. P. 10199.
42. Nenajdenko V. G., Shikhaliyev N. G., Maharramov A. M., Atakishiyeva G. T., Niyazova A. A., Mammadova N. A., **Novikov A. S.**, Buslov I. V., Khrustalev V. N., Tskhovrebov A. G. “Structural organization of dibromodiazadienes in the crystal and identification of Br···O halogen bonding involving the nitro group” // *Molecules* 2022, V. 27. P. 5110.
43. Muravev A. A., Ovsyannikov A. S., Konorov G. V., Islamov D. R., Usachev K. S., **Novikov A. S.**, Solovieva S. E., Antipin I. S. “Thermodynamic vs. kinetic control in synthesis of O-donor 2,5-substituted furan and 3,5-substituted pyrazole from heteropropargyl precursor” // *Molecules* 2022, V. 27. P. 5178.
44. Korobeynikov N. A., Usoltsev A. N., **Novikov A. S.**, Abramov P. A., Sokolov M. N., Adonin S. A. “Selenium(IV) polybromide complexes: structural diversity driven by halogen and chalcogen bonding” // *Molecules* 2022, V. 27. P. 5355.
45. Mezenov Y. A., Bruyere S., Krasilin A., Khrapova E., Bachinin S. V., Alekseevskiy P. V., Shipiloskikh S., Boulet P., Hupont S., Nomine A., Vigolo B., **Novikov A. S.**, Belmonte T., Milichko V. A. “Insights into solid-to-solid transformation of MOF amorphous phases” // *Inorg. Chem.* 2022, V. 61. P. 13992.
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48. **Novikov A. S.** “Self-healing polymers” // *Polymers*, 2022, V. 14. P. 2261.
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50. Petrov P. A., Filippova E. A., Sukhikh T. S., **Novikov A. S.**, Sokolov M. N. “Sterically hindered tellurium(IV) catecholate as a Lewis acid” // *Inorg. Chem.* 2022, V. 61. P. 9184.

51. Pulyalina A., Grekov K., Tataurova V., Senchukova A., **Novikov A.**, Faykov I., Polotskaya G. “Effect of ionic liquid on formation of copolyimide ultrafiltration membranes with improved rejection of La^{3+}” // *Sci. Rep.* 2022, V. 12. P. 8200.

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55. Shmelev N. Y., Okubazghi T. H., Abramov P. A., Rakhmanova M. I., **Novikov A. S.**, Sokolov M. N., Gushchin A. L. “Asymmetric coordination mode of phenanthroline-like ligands in gold(I) complexes: a case of the antichelate effect” // *Cryst. Growth Des.* 2022, V. 22. P. 3882.

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Hobby

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

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 Dmitry S. Bolotin "Xenon derivatives as aerogen bond-donating catalysts for organic transformations: a theoretical study on the metaphorical "spherical cow in a vacuum" provides insights into noncovalent organocatalysis" was recognized by the editorial board of *J. Org. Chem.* as ***one of the most significant articles of the issue and its graphical abstract was placed on the cover*** of 4th issue 2023 (DOI: 10.1021/acs.joc.2c00680).

The paper by Alexander S. Novikov and colleagues "Diaryliodoniums as hybrid hydrogen- and halogen-bond-donating organocatalysts for the Groebke–Blackburn–Bienaymé reaction" was recognized by the editorial board of *J. Org. Chem.* as ***one of the most significant articles of the***

issue and its graphical abstract was placed on the cover of 7th issue 2022 (DOI: 10.1021/acs.joc.1c02885).

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 “Theoretical study of *closo*-borate anions $[B_nH_n]^{2-}$ (n = 5–12): bonding, atomic charges, and reactivity analysis” was selected by the academic editors of *Symmetry* as one of the ***Editor's Choice Articles*** (DOI: 10.3390/sym13030464).

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 “Programmable soft-matter electronics” was recognized by the editorial board of *The Journal of Physical Chemistry Letters* as ***one of the most significant articles of the issue and its graphical abstract was placed on the cover*** of 7th issue 2021 (DOI: 10.1021/acs.jpclett.1c00007).

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).