

Сведения, характеризующие научную ценность научных трудов, выдвигаемых на соискание премии, присуждаемой Санкт-Петербургским государственным университетом за научные труды в 2019 году

Автор: Новиков Александр Сергеевич (Scopus ID: 50262902200)

Название работы:

Компьютерное моделирование и теоретические исследования в органической, неорганической и металлоорганической химии: нековалентные взаимодействия, реакционная способность и катализ

Список опубликованных работ в 2015–2018 годах с указанием наукометрических показателей:

1. Popov R.A., Novikov A.S., Mikherdov A.S. “Synthesis of mixed-ligand nitrile and carbonyl–isocyanide complexes of platinum(II) and their reaction with p-toluenesulfonyl hydrazide” // *Russ. J. Gen. Chem.* 2018, V. 88. P. 2347. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 0.643/Q4 SJR/SNIP = 0.217/0.435 КВАРТИЛЬ ПО SJR: Q3
2. Novikov A.S., Ivanov D.M., Bikbaeva Z.M., Bokach N.A., Kukushkin V.Yu. “Noncovalent interactions involving iodofluorobenzenes: the interplay of halogen bonding and weak $lp(O)\cdots\pi$ -hole_{arene} interactions” // *Cryst. Growth Des.* 2018, V. 18. P. 7641. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 4.153/Q1 SJR/SNIP = 1.046/1.107 КВАРТИЛЬ ПО SJR: Q1
3. Adonin S.A., Gorokh I.D., Novikov A.S., Samsonenko D.G., Yushina I.V., Sokolov M.N., Fedin V.P. “Halobismuthates with halopyridinium cations: appearance or non-appearance of unusual colouring” // *CrystEngComm* 2018, V. 20. P. 7766. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 3.382/Q1 SJR/SNIP = 0.937/0.837 КВАРТИЛЬ ПО SJR: Q1
4. Gorokh I.D., Adonin S.A., Abramov P.A., Novikov A.S., Sokolov M.N., Fedin V.P. “New structural type in polybromide-bromometalate hybrids: $(Me_3NH)_3\{[Bi_2Br_9](Br_2)\}$ – crystal structure and theoretical studies of non-covalent $Br\cdots Br$ interactions” // *Inorg. Chem. Commun.* 2018, V. 98. P. 169. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 1.795/Q3 SJR/SNIP = 0.365/0.446 КВАРТИЛЬ ПО SJR: Q3
5. Kinzhalov M.A., Parfenova S.N., Novikov A.S., Katlenok E.A., Puzyk M.V., Avdontceva M.S., Bokach N.A. “Cyclometalated iridium(III) complexes featuring disubstituted cyanamides” // *ChemistrySelect* 2018, V. 3. P. 11875. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 1.716/Q3 SJR/SNIP = 0.445/0.445 КВАРТИЛЬ ПО SJR: Q2
6. Panova Y.S., Sheyanova A.V., Zolotareva N.V., Sushev V.V., Arapova A.V., Novikov A.S., Baranov E.V., Fukin G.K., Kornev A.N. “2,2'-Azobispyridine in phosphorus coordination chemistry: a new approach to 1,2,4,3-triazaphosphole derivatives” // *Eur. J. Inorg. Chem.* 2018, V. 2018. P. 4245. [Статье присвоен статус «Very Important Paper»] ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 2.578/Q2 SJR/SNIP = 0.736/0.601 КВАРТИЛЬ ПО SJR: Q2

7. Baykov S.V., Dabranskaya U., Ivanov D.M., Novikov A.S., Boyarskiy V.P. "Pt/Pd and I/Br isostructural exchange provides formation of C–I•••Pd, C–Br•••Pt, and C–Br•••Pd metal-involving halogen bonding" // *Cryst. Growth Des.* 2018, V. 18. P. 5973. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 4.153/Q1 SJR/SNIP = 1.046/1.107 КВАРТИЛЬ ПО SJR: Q1
8. Osipyan A., Sapegin A., Novikov A.S., Krasavin M. "Rare medium-sized rings prepared via hydrolytic imidazoline ring expansion (HIRE)" // *J. Org. Chem.* 2018, V. 83. P. 9707 [Обложка журнала] ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 4.745/Q1 SJR/SNIP = 1.607/0.952 КВАРТИЛЬ ПО SJR: Q1
9. Novikov A.S. "Strong metallophilic interactions in nickel coordination compounds" // *Inorg. Chim. Acta* 2018, V. 483. P. 21. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 2.433/Q2 SJR/SNIP = 0.445/0.654 КВАРТИЛЬ ПО SJR: Q2
10. Kinzhalov M.A., Kashina M.V., Mikherdov A.S., Mozheeva E.A., Novikov A.S., Smirnov A.S., Ivanov D.M., Kryukova M.A., Ivanov A.Yu., Smirnov S.N., Kukushkin V.Yu., Luzyanin K.V. "Dramatically enhanced solubility of halide-containing organometallic species in diiodomethane: the role of solvent•••complex halogen bonding" // *Angew. Chem. Int. Ed.* 2018, V. 57. P. 12785. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 12.257/Q1 SJR/SNIP = 5.478/2.132 КВАРТИЛЬ ПО SJR: Q1
11. Kinzhalov M.A., Novikov A.S., Khoroshilova O.V., Bokach N.A. "The structure of 2-methylphenylcyanamide in the solid state" // *J. Struct. Chem.* 2018, V. 59, P. 1302. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 0.541/Q4 SJR/SNIP = 0.190/0.331 КВАРТИЛЬ ПО SJR: Q4
12. Burianova V.K., Bolotin D.S., Novikov A.S., Kolesnikov I.E., Suslonov V.V., Zhdanov A.P., Zhizhin K.Yu., Kuznetsov N.T. "Nucleophilic addition of hydrazine and benzophenone hydrazone to 2-acetonitrilium *closo*-decaborate cluster: structural and photophysical study" // *Inorg. Chim. Acta* 2018, V. 482. P. 838. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 2.433/Q2 SJR/SNIP = 0.445/0.654 КВАРТИЛЬ ПО SJR: Q2
13. Adonin S.A., Udalova L.I., Abramov P.A., Novikov A.S., Yushina I.V., Korolkov I.V., Semitut E.Yu., Derzhavskaya T.A., Stevenson K.J., Troshin P.A., Sokolov M.N., Fedin V.P. "A novel family of polyiodo-bromoantimonate(III) complexes: cation-driven self-assembly of photoconductive metal-polyhalide frameworks" // *Chem. Eur. J.* 2018, V. 24. P. 14707. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 5.16/Q1 SJR/SNIP = 1.842/0.972 КВАРТИЛЬ ПО SJR: Q1
14. Burianova V.K., Mikherdov A.S., Bolotin D.S., Novikov A.S., Mokolokolo P.P., Roodt A., Boyarskiy V.P., Suslonov V.V., Zhdanov A.P., Zhizhin K.Yu., Kuznetsov N.T. "Electrophilicity of aliphatic nitrilium *closo*-decaborate clusters: Hyperconjugation provides an unexpected inverse reactivity order" // *J. Organomet. Chem.* 2018, V. 870. P. 97. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 2.066/Q3 SJR/SNIP = 0.530/0.580 КВАРТИЛЬ ПО SJR: Q2
15. Usoltsev A.N., Adonin S.A., Abramov P.A., Novikov A.S., Shayapov V.R., Plyusnin P.E., Korolkov I.V., Sokolov M.N., Fedin V.P. "1D and 2D polybromotellurates (IV): structural studies and thermal stability" // *Eur. J. Inorg. Chem.* 2018, V. 2018. P. 3264. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 2.578/Q2 SJR/SNIP = 0.736/0.601 КВАРТИЛЬ ПО SJR: Q2
16. Rozhkov A.V., Novikov A.S., Ivanov D.M., Bolotin D.S., Bokach N.A., Kukushkin V.Yu. "Structure-directing weak interactions with 1,4-diiodotetrafluorobenzene convert

- 1D-arrays of $[M^{II}(\text{acac})_2]$ species into 3D-networks” // *Cryst. Growth Des.* 2018, V. 18. P. 3626. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 4.153/Q1 SJR/SNIP = 1.046/1.107 КВАРТИЛЬ ПО SJR: Q1
17. Mikherdov A.S., Kinzhalov M.A., Novikov A.S., Boyarskiy V.P., Boyarskaya I.A., Avdontceva M.S., Kukushkin V.Yu. “Ligation-enhanced π -hole $\cdots\pi$ interactions involving isocyanides. Effect of π -hole $\cdots\pi$ non-covalent bonding on conformational stabilization of acyclic diaminocarbene ligands” // *Inorg. Chem.* 2018, V. 57. P. 6722. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 4.85/Q1 SJR/SNIP = 1.501/1.092 КВАРТИЛЬ ПО SJR: Q1
18. Dmitriev V.A., Efremova M.M., Novikov A.S., Zarubaev V.V., Slita A.V., Galochkina A.V., Starova G.L., Ivanov A.V., Molchanov A.P. “Highly efficient and stereoselective cycloaddition of nitrones to indolyl- and pyrrolylacrylates” // *Tetrahedron Lett.* 2018, V. 59. P. 2327. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 2.259/Q2 SJR/SNIP = 0.621/0.576 КВАРТИЛЬ ПО SJR: Q2
19. Adonin S.A., Bondarenko M.A., Abramov P.A., Novikov A.S., Plyusnin P.E., Sokolov M.N., Fedin V.P. “Bromo- and polybromoantimonates (V): structural and theoretical studies of hybrid halogen-rich halometalate frameworks” // *Chem. Eur. J.* 2018, V. 24. P. 10165. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 5.16/Q1 SJR/SNIP = 1.842/0.972 КВАРТИЛЬ ПО SJR: Q1
20. Kinzhalov M.A., Katkova S.A., Doronina E.P., Novikov A.S., Eliseev I.I., Pichev V.A., Kukinov A.A., Starova G.L., Bokach N.A. “Red photo- and electroluminescent half-lantern cyclometalated dinuclear platinum(II) complex” // *Z. Kristallogr. Cryst. Mater.* 2018, V. 233. P. 795. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 1.09/Q3 SJR/SNIP = 0.393/0.512 КВАРТИЛЬ ПО SJR: Q2
21. Burianova V.K., Bolotin D.S., Mikherdov A.S., Novikov A.S., Mokolokolo P.P., Roodt A., Boyarskiy V.P., Dar'in D., Krasavin M., Suslonov V.V., Zhdanov A.P., Zhizhin K.Yu., Kuznetsov N.T. “Mechanism of generation of *closo*-decaborato amidrazones. Intramolecular non-covalent B–H $\cdots\pi$ (Ph) interaction determines stabilization of the configuration around the amidrazone C=N bond” // *New J. Chem.* 2018, V. 42. P. 8693. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 3.069/Q2 SJR/SNIP = 0.716/0.724 КВАРТИЛЬ ПО SJR: Q1
22. Novikov A.S. “Theoretical studies of cycloaddition to metal-activated substrates with isocyanide ligands” // *Russ. J. Coord. Chem.* 2018, V. 44. P. 252. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 0.636/Q4 SJR/SNIP = 0.206/0.314 КВАРТИЛЬ ПО SJR: Q3
23. Mikherdov A.S., Novikov A.S., Kinzhalov M.A., Zolotarev A.A., Boyarskiy V.P. “Intra-/intermolecular bifurcated chalcogen bonding in crystal structure of thiazole/thiadiazole derived binuclear (diaminocarbene)Pd^{II} complexes” // *Crystals* 2018, V. 8. P. 112. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 2.061/Q2 SJR/SNIP = 0.497/0.695 КВАРТИЛЬ ПО SJR: Q2
24. Novikov A.S., Bolotin D.S. “Tautomerism of amidoximes and other oxime species” // *J. Phys. Org. Chem.* 2018, V. 31. P. e3772. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 1.53/Q3 SJR/SNIP = 0.421/0.509 КВАРТИЛЬ ПО SJR: Q3
25. Mikherdov A.S., Novikov A.S., Kinzhalov M.A., Boyarskiy V.P., Starova G.L., Ivanov A.Yu., Kukushkin V.Yu. “Halides held by bifurcated chalcogen–hydrogen bonds. Effect of $\mu_{(S,N-H)}Cl$ contacts on dimerization of Cl(Carbene)Pd^{II} species” // *Inorg. Chem.* 2018, V. 57. P. 3420. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 4.85/Q1 SJR/SNIP = 1.501/1.092 КВАРТИЛЬ ПО SJR: Q1

26. Adonin S.A., Gorokh I.D., Novikov A.S., Samsonenko D.G., Plyusnin P.E., Sokolov M.N., Fedin V.P. "Bromine-rich complexes of bismuth: experimental and theoretical studies" // *Dalton Trans.* 2018, V. 47. P. 2683. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 4.052/Q1 SJR/SNIP = 1.120/0.900 КВАРТИЛЬ ПО SJR: Q1
27. Bulatova M., Melekhova A.A., Novikov A.S., Ivanov D.M., Bokach N.A. "Redox reactive (RNC)Cu^{II} species stabilized in the solid state via halogen bond with I₂" // *Z. Kristallogr. Cryst. Mater.* 2018, V. 233. P. 371. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 1.09/Q3 SJR/SNIP = 0.393/0.512 КВАРТИЛЬ ПО SJR: Q2
28. Novikov A.S. "Theoretical confirmation of existence of X•••Au non-covalent contacts" // *Inorg. Chim. Acta* 2018, V. 471. P. 126. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 2.433/Q2 SJR/SNIP = 0.445/0.654 КВАРТИЛЬ ПО SJR: Q2
29. Efremova M.M., Novikov A.S., Kostikov R.R., Panikorovsky T.L., Ivanov A.V., Molchanov A.P. "Regio- and diastereoselectivity of the cycloaddition of nitrones with N-propadienyldole and pyrroles" // *Tetrahedron* 2018, V. 74. P. 174. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 2.379/Q2 SJR/SNIP = 0.709/0.656 КВАРТИЛЬ ПО SJR: Q2
30. Adonin S.A., Gorokh I.D., Novikov A.S., Samsonenko D.G., Korolkov I.V., Sokolov M.N., Fedin V.P. "Bromobismuthates: cation-induced structural diversity and Hirshfeld surface analysis of cation-anion contacts" // *Polyhedron* 2018, V. 139. P. 282. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 2.284/Q2 SJR/SNIP = 0.426/0.613 КВАРТИЛЬ ПО SJR: Q2
31. Adonin S.A., Gorokh I.D., Abramov P.A., Novikov A.S., Korolkov I.V., Sokolov M.N., Fedin V.P. "Chlorobismuthates trapping dibromine: formation of two-dimensional supramolecular polyhalide networks with Br₂ linkers" // *Eur. J. Inorg. Chem.* 2017, V. 2017. P. 4925. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 2.578/Q2 SJR/SNIP = 0.736/0.601 КВАРТИЛЬ ПО SJR: Q2
32. Melekhova A.A., Novikov A.S., Panikorovskii T.L., Bokach N.A., Kukushkin V.Yu. "Novel family of homoleptic copper(I) complexes featuring disubstituted cyanamides: combined synthetic, structural, and theoretical study" // *New J. Chem.* 2017, V. 41. P. 14557. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 3.069/Q2 SJR/SNIP = 0.716/0.724 КВАРТИЛЬ ПО SJR: Q1
33. Bikbaeva Z.M., Ivanov D.M., Novikov A.S., Ananyev I.V., Bokach N.A., Kukushkin V.Yu. "Electrophilic–nucleophilic dualism of nickel(II) toward Ni•••I non-covalent interactions: semicoordination of iodine centers via electron belt and halogen bonding via σ-Hole" // *Inorg. Chem.* 2017, V. 56. P. 13562. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 4.85/Q1 SJR/SNIP = 1.501/1.092 КВАРТИЛЬ ПО SJR: Q1
34. Bolotin D.S., Bikbaeva Z.M., Novikov A.S., Suslonov V.V., Bokach N.A. "A dimetallic aminonitrone nickel(II) complex: further insights into metal-mediated nucleophilic activation of amidoximes" // *ChemistrySelect* 2017, V. 2. P. 9674. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 1.716/Q3 SJR/SNIP = 0.445/0.445 КВАРТИЛЬ ПО SJR: Q2
35. Katkova S.A., Kinzhalov M.A., Tolstoy P.M., Novikov A.S., Boyarskiy V.P., Ananyan A.Yu., Gushchin P.V., Haukka M., Zolotarev A.A., Ivanov A.Yu., Zlotzky S.S., Kukushkin V.Yu. "Diversity of isomerization patterns and protolytic forms in aminocarbene Pd^{II} and Pt^{II} complexes formed upon addition of N,N'-diphenylguanidine to metal-activated isocyanides" // *Organometallics* 2017, V. 36. P. 4145. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 4.1/Q1 SJR/SNIP = 1.473/0.838 КВАРТИЛЬ ПО SJR: Q1

36. Kinzhalov M.A., Legkodukh A.S., Anisimova T.B., Novikov A.S., Suslonov V.V., Luzyanin K.V., Kukushkin V.Yu. "Tetrazol-5-ylidene gold(III) complexes from sequential [2 + 3] cycloaddition of azide to metal-bound isocyanides and N4-alkylation" // *Organometallics* 2017, V. 36. P. 3974. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 4.1/Q1 SJR/SNIP = 1.473/0.838 КВАРТИЛЬ ПО SJR: Q1
37. Adonin S.A., Gorokh I.D., Novikov A.S., Abramov P.A., Sokolov M.N., Fedin V.P. "Halogen contacts-induced unusual coloring in Bi(III) bromide complex: anion-to-cation charge transfer via Br•••Br interactions" // *Chem. Eur. J.* 2017, V. 23. P. 15612. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 5.16/Q1 SJR/SNIP = 1.842/0.972 КВАРТИЛЬ ПО SJR: Q1
38. Usoltsev A.N., Adonin S.A., Novikov A.S., Samsonenko D.G., Sokolov M.N., Fedin V.P. "One-dimensional polymeric polybromotellurates (IV): structural and theoretical insights into halogen•••halogen contacts" // *CrystEngComm* 2017, V. 19. P. 5940. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 3.382/Q1 SJR/SNIP = 0.937/0.837 КВАРТИЛЬ ПО SJR: Q1
39. П'ин M.V., Bolotin D.S., Novikov A.S., Suslonov V.V., Chezhina N.V., Bubnov M.P., Cherkasov V.K., Venter G.J.S., Roodt A. "Square-planar aminonitronate transition metal complexes (M = Cu^{II}, Ni^{II}, Pd^{II}, and Pt^{II})" // *Inorg. Chim. Acta* 2017, V. 467. P. 372. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 2.433/Q2 SJR/SNIP = 0.445/0.654 КВАРТИЛЬ ПО SJR: Q2
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41. Kinzhalov M.A., Eremina A.A., Ivanov D.M., Novikov A.S., Katlenok E.A., Balashev K.P., Suslonov V.V. "Halogen and chalcogen bonding in dichloromethane solvate of cyclometalated iridium(III)-isocyanide complex" // *Z. Kristallogr. Cryst. Mater.* 2017, V. 232. P. 797. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 1.09/Q3 SJR/SNIP = 0.393/0.512 КВАРТИЛЬ ПО SJR: Q2
42. Sirotkina E.V., Efremova M.M., Novikov A.S., Zarubaev V.V., Orshanskaya I.R., Starova G.L., Kostikov R.R., Molchanov A.P. "Regio- and diastereoselectivity of the cycloaddition of aldonitrones with benzylidencyclopropane: An experimental and theoretical study" // *Tetrahedron* 2017, V. 73. P. 3025. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 2.379/Q2 SJR/SNIP = 0.709/0.656 КВАРТИЛЬ ПО SJR: Q2
43. Anisimova T.B., Kinzhalov M.A., Guedes da Silva M.F.C., Novikov A.S., Kukushkin V.Yu., Pompeiro A.J.L., Luzyanin K.V. "Addition of N-nucleophiles to gold(III)-bound isocyanides leading to short-lived gold(III) acyclic diaminocarbene complexes" // *New J. Chem.* 2017, V. 41. P. 3246. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 3.069/Q2 SJR/SNIP = 0.716/0.724 КВАРТИЛЬ ПО SJR: Q1
44. Novikov A.S., Ivanov D.M., Avdontceva M.S., Kukushkin V.Yu. "Diiodomethane as halogen bond donor toward metal-bound halides" // *CrystEngComm* 2017, V. 19. P. 2517. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 3.382/Q1 SJR/SNIP = 0.937/0.837 КВАРТИЛЬ ПО SJR: Q1
45. Melekhova A.A., Smirnov A.S., Novikov A.S., Panikorovskii T.L., Bokach N.A., Kukushkin V.Yu. "Copper(I)-catalyzed 1,3-dipolar cycloaddition of ketonitrones to dialkylcyanamides. A step toward sustainable generation of 2,3-dihydro-1,2,4-

- oxadiazoles” // *ACS Omega* 2017, V. 2. P. 1380. ИМПАКТ-ФАКТОР/КВАРТИЛЬ (JCR) = 2.584/Q2 SJR/SNIP = 0.754/0.673 КВАРТИЛЬ ПО SJR: Q1
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Суммарный ИМПАКТ-ФАКТОР (JCR) = 234.458