

**Сведения, характеризующие научную ценность научных трудов, выдвигаемых на соискание премии, присуждаемой Санкт-Петербургским государственным университетом за научные труды в 2018 году**

Автор: Новиков Александр Сергеевич

Название работы:

Компьютерное моделирование и теоретические исследования в координационной и металлоорганической химии: межмолекулярные взаимодействия, реакционная способность и катализ

Список опубликованных работ в 2015–2017 годах с указанием импакт-факторов соответствующих научных журналов (IF):

1. 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 Br<sub>2</sub> linkers” // *Eur. J. Inorg. Chem.* 2017, V. 2017. P. 4925. **IF = 2.507**
2. 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. **IF = 3.201**
3. 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. **IF = 4.7**
4. 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. **IF = 1.505**
5. 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<sup>II</sup> and Pt<sup>II</sup> complexes formed upon addition of N,N'-diphenylguanidine to metal-activated isocyanides” // *Organometallics* 2017, V. 36. P. 4145. **IF = 4.051**
6. Kinzhalov M.A., Legkoduikh 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. **IF = 4.051**
7. 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. **IF = 5.16**
8. 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. **IF = 3.304**
9. Il'in 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<sup>II</sup>, Ni<sup>II</sup>, Pd<sup>II</sup>, and Pt<sup>II</sup>)” // *Inorg. Chim. Acta* 2017, V. 467. P. 372. **IF = 2.264**
  10. Bikbaeva Z.M., **Novikov A.S.**, Suslonov V.V., Bokach N.A., Kukushkin V.Yu. “Metal-mediated reactions between dialkylcyanamides and acetamidoxime generate unusual (nitrosoguanidinate)nickel(II) complexes” // *Dalton Trans.* 2017, V. 46. P. 10090. **IF = 4.099**
  11. 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. **IF = 1.263**
  12. 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 benzyldenecyclopropane: An experimental and theoretical study” // *Tetrahedron* 2017, V. 73. P. 3025. **IF = 2.377**
  13. Anisimova T.B., Kinzhalov M.A., Guedes da Silva M.F.C., **Novikov A.S.**, Kukushkin V.Yu., Pombeiro 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. **IF = 3.201**
  14. **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. **IF = 3.304**
  15. 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. Журнал начал выходить в 2016 году, в связи с этим его IF ещё не определён
  16. Melekhova A.A., **Novikov A.S.**, Rostovskii N.V., Sakharov P.A., Panikorovskii T.L., Bokach N.A. “Open-chain hemiketal is stabilized by coordination to a copper(II)” // *Inorg. Chem. Commun.* 2017, V. 79. P. 82. **IF = 1.81**
  17. Ivanov D.M., Kinzhalov M.A., **Novikov A.S.**, Ananyev I.V., Romanova A.A., Boyarskiy V.P., Haukka M., Kukushkin V.Yu. “The H<sub>2</sub>C(X)–X···X<sup>–</sup> (X = Cl, Br) halogen bonding of dihalomethanes” // *Cryst. Growth Des.* 2017, V. 17. P. 1353. **IF = 3.972**
  18. Bolotin D.S., Il'in M.V., **Novikov A.S.**, Bokach N.A., Suslonov V.V., Kukushkin V.Yu. “Trinuclear (aminonitronate)Zn<sup>II</sup> complexes as key intermediates in zinc(II)-mediated generation of 1,2,4-Oxadiazoles from amidoximes and nitriles” // *New J. Chem.* 2017, V. 41. P. 1940. **IF = 3.201**
  19. Kinzhalov M.A., **Novikov A.S.**, Chernyshev A.N., Suslonov V.V. “Intermolecular hydrogen bonding H···Cl<sup>–</sup> in the solid palladium(II)-diaminocarbene complexes” // *Z. Kristallogr. Cryst. Mater.* 2017, V. 232. P. 299. **IF = 1.263**
  20. Andrusenko E.V., Kabin E.V., **Novikov A.S.**, Bokach N.A., Starova G.L., Kukushkin V.Yu. “Metal-mediated generation of triazapentadienate-terminated di- and trinuclear  $\mu_2$ -pyrazolate Ni<sup>II</sup> species and control of their nuclearity” // *New J. Chem.* 2017, V. 41. P. 316. **IF = 3.201**

21. Mikherdov A.S., Kinzhalov M.A., **Novikov A.S.**, Boyarskiy V.P., Boyarskaya I.A., Dar'in D.V., Starova G.L., Kukushkin V.Yu. "Difference in energy between two distinct types of chalcogen bonds drives regioisomerization of binuclear (diaminocarbene)Pd<sup>II</sup> complexes" // *J. Am. Chem. Soc.* 2016, V. 138. P. 14129. **IF = 14.357**
22. Bolotin D.S., Burianova V.K., **Novikov A.S.**, Demakova M.Ya., Pretorius C., Mokolokolo P.P., Roodt A., Bokach N.A., Suslonov V.V., Zhdanov A.P., Zhizhin K.Yu., Kuznetsov N.T., Kukushkin V.Yu. "Nucleophilicity of oximes based upon addition to a nitrilium closo-decaborate cluster" // *Organometallics* 2016, V. 35. P. 3612. **IF = 4.051**
23. Kolari K., Sahamies J., Kalenius E., **Novikov A.S.**, Kukushkin V.Yu., Haukka M. "Metallophilic interactions in polymeric group 11 thiols" // *Solid State Sciences* 2016, V. 60. P. 92. **IF = 1.861**
24. Ivanov D.M., **Novikov A.S.**, Starova G.L., Haukka M., Kukushkin V.Yu. "A family of heterotetrameric clusters of chloride species and halomethanes held by two halogen and two hydrogen bonds" // *CrystEngComm* 2016, V. 18. P. 5278. [Анонс статьи попал на обложку журнала] **IF = 3.304**
25. Afanasenko A.M., Avdontceva M.S., **Novikov A.S.**, Chulkova T.G. "Halogen and hydrogen bonding in *cis*-dichlorobis(propionitrile)platinum(II) chloroform monosolvate" // *Z. Kristallogr. Cryst. Mater.* 2016, V. 231. P. 435. **IF = 1.263**
26. Melekhova A.A., **Novikov A.S.**, Bokach N.A., Avdonceva M.S., Kukushkin V.Yu. "Characterization of Cu-ligand bonds in tris-pyrazolymethane isocyanide copper(I) complexes based upon combined X-ray diffraction and theoretical study" // *Inorg. Chim. Acta* 2016, V. 450. P. 140. **IF = 2.264**
27. Mikhaylov V.N., Sorokoumov V.N., Korvinson K.A., **Novikov A.S.**, Balova I.A. "Synthesis and simple immobilization of palladium(II) acyclic diaminocarbene complexes on polystyrene-support as efficient catalysts for Sonogashira and Suzuki-Miyaura cross-coupling" // *Organometallics* 2016, V. 35. P. 1684. **IF = 4.051**
28. Serebryanskaya T.V., **Novikov A.S.**, Gushchin P.V., Haukka M., Asfin R.E., Tolstoy P.M., Kukushkin V.Yu. "Identification and H(D)-bond energies of C–H(D)···Cl interactions in chloride–haloalkane clusters: combined X-ray crystallographic, spectroscopic, and theoretical study" // *Phys. Chem. Chem. Phys.* 2016, V. 18. P. 14104. **IF = 3.906**
29. Andrusenko E.V., **Novikov A.S.**, Starova G.L., Bokach N.A. "Three-dimensional hydrogen bonding network in the structures of (dimethylcyanamide)cobalt(II) complexes" // *Inorg. Chim. Acta* 2016, V. 447. P. 142. **IF = 2.264**
30. Ivanov D.M., **Novikov A.S.**, Ananyev I.V., Kirina Y.V., Kukushkin V.Yu. "Halogen bonding between metal centers and halocarbons" // *Chem. Commun.* 2016, V. 52. P. 5565. **IF = 6.29**
31. Bolotin D.S., **Novikov A.S.**, Kolesnikov I.E., Suslonov V.V., Novozhilov Y., Ronzhina O., Dorogov M., Krasavin M., Kukushkin V.Yu. "Phosphorescent platinum(II) complexes featuring chelated acetoxime pyrazoles: synthetic, structural, and photophysical study" // *ChemistrySelect* 2016, V. 3. P. 456. **IF = 1.505**
32. Ding X., Tuikka M.J., Hirva P., Kukushkin V.Yu., **Novikov A.S.**, Haukka M. "Fine-tuning halogen bonding properties of diiodine through halogen-halogen charge transfer – Extended [Ru(2,2'-bipyridine)(CO)<sub>2</sub>X<sub>2</sub>]**I**<sub>2</sub> systems (X= Cl, Br, I)" // *CrystEngComm* 2016, V. 18. P. 1987. **IF = 3.304**
33. **Novikov A.S.**, Kuznetsov M.L., Rocha B.G.M., Pombeiro A.J.L., Shul'pin G.B. "Oxidation of olefins with H<sub>2</sub>O<sub>2</sub> 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. **IF = 5.365**
34. Kulish K.I., **Novikov A.S.**, Tolstoy P.M., Bolotin D.S., Bokach N.A., Zolotarev A.A., Kukushkin V.Yu. “Solid state and dynamic solution structures of O-carbamidine amidoximes gives further insight into the mechanism of zinc(II)-mediated generation of 1,2,4-oxadiazoles” // *J. Mol. Struct.* 2016, V. 1111. P. 142. **IF = 2.011**
35. Ivanov D.M., Gushchin P.V., **Novikov A.S.**, Avdontceva M.S., Zolotarev A.A., Starova G.L., Chen Y.-T., Liu S.-H., Chou P.-T., Kukushkin V.Yu. “Platinum(II)-mediated double coupling of 2,3-diphenylmaleimidine with nitrile functionalities giving annulated triazapentadiene PANT systems” // *Eur. J. Inorg. Chem.* 2016, V. 2016. P. 1480. [Анонс статьи попал на обложку журнала] **IF = 2.507**
36. Kinzhalov M.A., **Novikov A.S.**, Luzyanin K.V., Haukka M., Pombeiro A.J.L., Kukushkin V.Yu. “Pd<sup>II</sup>-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. **IF = 3.201**
37. Ivanov D.M., Kirina Y.V., **Novikov A.S.**, Starova G.L., Kukushkin V.Yu. “Efficient  $\pi$ -stacking with benzene provides 2D assembly of *trans*-[PtCl<sub>2</sub>(*p*-CF<sub>3</sub>C<sub>6</sub>H<sub>4</sub>CN)<sub>2</sub>]” // *J. Mol. Struct.* 2016, V. 1104. P. 19. **IF = 2.011**
38. Andrusenko E.V., Kabin E.V., **Novikov A.S.**, Bokach N.A., Starova G.L., Zolotarev A.A., Kukushkin V.Yu. “Highly reactive Ni<sup>II</sup>-bound nitrile–oxime coupling intermediate stabilized by substituting conventional nitriles with a dialkylcyanamide” // *Eur. J. Inorg. Chem.* 2015, V. 2015. P. 4894. **IF = 2.507**
39. **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. **IF = 1.946**
40. 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. **IF = 2.264**
41. 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. **IF = 4.7**
42. 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. **IF = 4.099**

Суммарный IF = 137.465