Aleksey E Kuznetsov

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/1848232/publications.pdf

Version: 2024-02-01

75 papers	4,338 citations	201674 27 h-index	102487 66 g-index
84 all docs	84 docs citations	84 times ranked	3815 citing authors

#	Article	IF	Citations
1	Core-modified porphyrins: novel building blocks in chemistry. ChemistrySelect, 2023, 8, 1513-1543.	1.5	1
2	Reactive molecular dynamics of pyrolysis and combustion of alternative jet fuels: A ReaxFF study. Fuel, 2022, 310, 122157.	6.4	19
3	Review of research of nanocomposites based on graphene quantum dots. ChemistrySelect, 2022, 7, 605-628.	1.5	0
4	Imine-based Zwitterion: Synthesis, single-crystal characterization, and computational investigation. Journal of Molecular Structure, 2022, 1253, 132237.	3.6	22
5	Hexabenzocoronene functionalized with antiaromatic S- and Se-core-modified porphyrins (isophlorins): comparison with the dyad with regular porphyrin. Pure and Applied Chemistry, 2022, 94, 747-765.	1.9	0
6	Ultrasound versus Light: Exploring Photophysicochemical and Sonochemical Properties of Phthalocyanine-Based Therapeutics, Theoretical Study, and In Vitro Evaluations. ACS Applied Bio Materials, 2022, 5, 1139-1150.	4.6	32
7	Synthesis, single-crystal exploration, hirshfeld surface analysis, and DFT investigation of the thiosemicarbazones. Journal of Molecular Structure, 2022, 1262, 133088.	3.6	14
8	Reactive molecular dynamics and DFT simulations of FTDO explosive. Computational and Theoretical Chemistry, 2022, 1212, 113723.	2.5	8
9	DFT and single-crystal investigation of the pyrimethamine-based novel co-crystal salt: 2,4-diamino-5-(4-chlorophenyl)-6-ethylpyrimidin-1-ium-4-methylbenzoate hydrate (1:1:1) (DEMH). Journal of Molecular Structure, 2021, 1228, 129445.	3.6	32
10	DFT Investigation of the Î·6 â‡Œ Î·6-Inter-ring Haptotropic Rearrangement of the Group 8 Metals Complexes [(graphene)MCp]+ (M = Fe, Ru, Os). Journal of Physical Chemistry A, 2021, 125, 366-375.	2.5	1
11	Facile synthesis of Tb-decorated graphene oxide: electrochemical stability, hydrogen storage, and corrosion inhibition of Mg AZ13 alloy in 3.5% NaCl medium. RSC Advances, 2021, 11, 662-670.	3.6	1
12	Experimental and DFT studies of gadolinium decorated graphene oxide materials for their redox properties and as a corrosion inhibition barrier layer on Mg AZ13 alloy in a 3.5% NaCl environment. RSC Advances, 2021, 11, 22095-22105.	3.6	6
13	RMD simulations of ADN and ADN/GAP-based propellant. Journal of the Brazilian Society of Mechanical Sciences and Engineering, 2021, 43, 1.	1.6	5
14	2-Amino-6-methylpyridine based co-crystal salt formation using succinic acid: Single-crystal analysis and computational exploration. Journal of Molecular Structure, 2021, 1230, 129893.	3.6	29
15	A Rare Angular Trinuclear Mixed Valence Cobalt(III-II-III) Complex With Azido Bridges And Salpn-Type Schiff-Base Ligand: Synthesis, Crystal Structure And DFT Study. Journal of Molecular Structure, 2021, 1230, 129863.	3.6	3
16	exo- and endo-Complexes of Fe(0) with Carbon Allotropic Modifications on the Example of Fullerene Đ¡60: a Density Function Theory Study. Russian Journal of General Chemistry, 2021, 91, 828-834.	0.8	1
17	Combinatorial library design and virtual screening of cryptolepine derivatives against topoisomerase IIA by molecular docking and DFT studies. ChemistrySelect, 2021, 6, 221-246.	1.5	0
18	Synthesis, single-crystal exploration, and theoretical insights of arylsulfonylated 2-amino-6-methylpyrimidin derivatives. Journal of Molecular Structure, 2021, 1243, 130789.	3.6	13

#	Article	IF	Citations
19	Comparison of P- and As-core-modified porphyrins with the parental porphyrin: a computational study. Pure and Applied Chemistry, 2021, 93, 561-570.	1.9	2
20	DFT and single crystal analysis of the pyrimethamine-based novel co-crystal salt: 2,4-diamino-5-(4-chloro-phenyl)-6-ethylpyrimidin-1-ium:4-hydroxybenzoate:methanol:hydrate (1:1:1:1) (DEHMH). Journal of Molecular Structure, 2020, 1199, 127041.	3.6	59
21	Hexabenzocoronene functionalized with porphyrin and P-core-modified porphyrin: A comparative computational study. Computational and Theoretical Chemistry, 2020, 1188, 112973.	2.5	3
22	Spectroscopic studies, molecular structure optimization and investigation of structural and electrical properties of novel and biodegradable Chitosan-GO polymer nanocomposites. Journal of Materials Science, 2020, 55, 14829-14847.	3.7	67
23	Experimental and computational studies of graphene oxide covalently functionalized by octylamine: electrochemical stability, hydrogen evolution, and corrosion inhibition of the AZ13 Mg alloy in 3.5% NaCl. RSC Advances, 2020, 10, 11426-11434.	3.6	42
24	Structural, optical, and surface morphological studies of ethyl cellulose/graphene oxide nanocomposites. Polymer Composites, 2020, 41, 2792-2802.	4.6	85
25	Stability of di-butyl-dichalcogenide-capped gold nanoparticles: experimental data and theoretical insights. RSC Advances, 2020, 10, 6259-6270.	3.6	11
26	Experimental and DFT studies of porous carbon covalently functionalized by polyaniline as a corrosion inhibition barrier on nickel-based alloys in acidic media. RSC Advances, 2020, 10, 12151-12165.	3.6	8
27	Phthalocyanines core-modified by P and S and their complexes with fullerene C60: DFT study. Physical Sciences Reviews, 2019, 4, .	0.8	2
28	Stacks of Metalloporphyrins: Comparison of Experimental and Computational Results. Journal of Physical Chemistry B, 2019, 123, 10044-10060.	2.6	1
29	Computational investigations into the structural and electronic properties of Cd_nTe_n (n = 1â€“17) quantum dots. RSC Advances, 2019, 9, 5091-5099.	3.6	11
30	Experimental and computational studies of a graphene oxide barrier layer covalently functionalized with amino acids on Mg AZ13 alloy in salt medium. RSC Advances, 2019, 9, 32441-32447.	3.6	22
31	Experimental and DFT studies of carbon nanotubes covalently functionalized with an imidazole derivative for electrochemical stability and green corrosion inhibition as a barrier layer on the nickel alloy surface in a sulphuric acidic medium. RSC Advances, 2019, 9, 38677-38686.	3.6	7
32	Complexes between core-modified porphyrins ZnP(X)₄ (X = P and S) and small semiconductor nanoparticle Zn₆S₆: are they possible?. Physical Sciences Reviews, 2019, 4, .	0.8	3
33	9. Complexes between core-modified porphyrins ZnP(X)₄ (X = P and S) and small semiconductor nanoparticle Zn₆S₆: are they possible?. , 2018, , 135-146.		3
34	Three Ligands with Biomedical Importance: Binding to Small ZnS Quantum Dots. Journal of Physical Chemistry C, 2018, 122, 12454-12463.	3.1	2
35	Influence of an exciton-delocalizing ligand on the structural, electronic, and spectral features of the Cd₃₃S₃₃ quantum dot: insights from computational studies. Journal of Materials Chemistry C, 2018, 6, 8751-8761.	5.5	7
36	Phytotoxicity, structural and computational analysis of 2-methyl-1,5-diarylpentadienones. Journal of Molecular Structure, 2017, 1142, 239-247.	3.6	3

#	Article	IF	Citations
37	Structural isomerism of Ru(<scp>ii</scp>)-carbonyl complexes: synthesis, characterization and their antitrypanosomal activities. New Journal of Chemistry, 2017, 41, 4468-4477.	2.8	12
38	Design of Novel Classes of Building Blocks for Nanotechnology: Coreâ€Modified Metalloporphyrins and Their Derivatives. , 2017, , .		1
39	Can MP(P)4 Compounds Form Complexes with C60?. Journal of Applied Solution Chemistry and Modeling, 2017, 6, 91-97.	0.4	8
40	Computational design of ZnP(P)₄ stacks: Three modes of binding. Journal of Theoretical and Computational Chemistry, 2016, 15, 1650043.	1.8	8
41	How the change of the ligand from L = porphine, P 2â^ , to L = P 4 -substituted porphine, P(P) 4 2â^ , affects the electronic properties and the Mâ€“L binding energies for the first-row transition metals M = Scâ€“Zn: Comparative study. Chemical Physics, 2016, 469-470, 38-48.	1.9	8
42	Metalloporphyrins with all the pyrrole nitrogens replaced with phosphorus atoms, MP(P)4 (M = Sc, Ti,) Tj ETQq0 0 0 rgBT /Overlock 10 T	1.9	12
43	Anti-Mycobacterium tuberculosisand Cytotoxicity Activities of Ruthenium(II)/Bipyridine/Diphosphine/Pyrimidine-2-thiolate Complexes: The Role of the Non-CoordinatedN-Atom. Journal of the Brazilian Chemical Society, 2015, , .	0.6	1
44	Structural and Electronic Properties of Bare and Capped Cd₃₃Se₃₃ and Cd₃₃Te₃₃ Quantum Dots. Journal of Physical Chemistry C, 2014, 118, 7094-7109.	3.1	32
45	Distance-Independent Charge Recombination Kinetics in Cytochrome câ€“Cytochrome c Peroxidase Complexes: Compensating Changes in the Electronic Coupling and Reorganization Energies. Journal of Physical Chemistry B, 2013, 117, 9129-9141.	2.6	23
46	Effects of S-containing ligands on the structure and electronic properties of CdnSen/CdnTen nanoparticles (n=3, 4, 6, and 9). Chemical Physics, 2012, 407, 97-109.	1.9	12
47	Revealing substituent effects on the electronic structure and planarity of Ni-porphyrins. Computational and Theoretical Chemistry, 2012, 981, 73-85.	2.5	42
48	Structural and Electronic Properties of Bare and Capped Cd_nSe_n/Cd_nTe_n Nanoparticles (n = 6, 9). Journal of Physical Chemistry C, 2012, 116, 6817-6830.	3.1	31
49	Polyoxometalates in the Design of Effective and Tunable Water Oxidation Catalysts. Israel Journal of Chemistry, 2011, 51, 238-246.	2.3	37
50	The role of the heteroatom (XÂ=ÂSiIV, PV, and SVI) on the reactivity of {Î³-[(H2O)RuIII(Î¼-OH)2RuIII(H2O)][Xn+W10O36]}(8â^'n)â^' with the O2 molecule. Theoretical Chemistry Accounts, 2011, 130, 197-207.	1.4	9
51	Insights into the Mechanism of O₂ Formation and Release from the Mn₄O₄L₆ â€œCubaneâ€•Cluster. Journal of Physical Chemistry A, 2010, 114, 11417-11424.	2.5	27
52	Computational Studies of the Geometry and Electronic Structure of an All-Inorganic and Homogeneous Tetra-Ru-Polyoxotungstate Catalyst for Water Oxidation and Its Four Subsequent One-Electron Oxidized Forms. Journal of Physical Chemistry A, 2010, 114, 535-542.	2.5	39
53	Does the MgO(100)-Support Facilitate the Reaction of Nitrogen and Hydrogen Molecules Catalyzed by Zr2Pd2 Clusters? A Computational Study. Inorganic Chemistry, 2010, 49, 2557-2567.	4.0	0
54	A Fast Soluble Carbon-Free Molecular Water Oxidation Catalyst Based on Abundant Metals. Science, 2010, 328, 342-345.	12.6	1,354

#	Article	IF	Citations
55	Mechanism of the Divanadium-Substituted Polyoxotungstate [Î³-1,2-H₂SiV₂W₁₀O₄₀]^{4â^'}Catalyzed Olefin Epoxidation by H₂O₂: A Computational Study. Inorganic Chemistry, 2009, 48, 1871-1878.	4.0	29
56	Dioxygen and Water Activation Processes on Multi-Ru-Substituted Polyoxometalates: Comparison with the â€œBlue-Dimerâ€•Water Oxidation Catalyst. Journal of the American Chemical Society, 2009, 131, 6844-6854.	13.7	88
57	Optical properties of small silver clusters supported at MgO. European Physical Journal D, 2007, 45, 471-476.	1.3	10
58	Mass-selected Ag3 clusters soft-landed onto MgO/Mo(100): femtosecond photoemission and first-principles simulations. European Physical Journal D, 2007, 45, 477-483.	1.3	15
59	Multiple Aromaticity and Antiaromaticity in Silicon Clusters. ChemPhysChem, 2004, 5, 1885-1891.	2.1	48
60	A single Ï€-bond captures 3, 4 and 5 atoms. Chemical Physics Letters, 2004, 388, 452-456.	2.6	45
61	All-Metal Antiaromatic Molecule: Rectangular Al4-4 in the Li3Al-4 Anion.. ChemInform, 2003, 34, no.	0.0	0
62	All-Metal Antiaromatic Molecule: Rectangular Al44- in the Li3Al4- Anion. Science, 2003, 300, 622-625.	12.6	219
63	Peculiar Transformation of a Nonaromatic Al4Cl4(NH3)4into an Aromatic Na2Al4Cl4(NH3)4. Inorganic Chemistry, 2002, 41, 3596-3598.	4.0	13
64	Peculiar Antiaromatic Inorganic Molecules of Tetrapnictogen in Na+Pn4-(Pn = P, As, Sb) and Important Consequences for Hydrocarbons. Inorganic Chemistry, 2002, 41, 6062-6070.	4.0	66
65	Al62- â^' Fusion of Two Aromatic Al3- Units. A Combined Photoelectron Spectroscopy and ab Initio Study of M+[Al62-] (M = Li, Na, K, Cu, and Au). Journal of the American Chemical Society, 2002, 124, 11791-11801.	13.7	124
66	On the Resonance Energy in New All-Metal Aromatic Molecules. Inorganic Chemistry, 2002, 41, 532-537.	4.0	139
67	Probing the Electronic Structure and Aromaticity of Pentapnictogen Cluster Anions Pn5-(Pn = P, As,) Tj ETQq1 1 0.784314 rgBT /Over Chemistry A, 2002, 106, 5600-5606.	2.5	94
68	Theoretical Evidence of Aromaticity in X3 â^' (X = B, Al, Ga) Species. Structural Chemistry, 2002, 13, 141-148.	2.0	130
69	Observation of All-Metal Aromatic Molecules. Science, 2001, 291, 859-861.	12.6	597
70	On the Aromaticity of Square Planar Ga42- and In42- in Gaseous NaGa4- and NaIn4- Clusters. Journal of the American Chemical Society, 2001, 123, 8825-8831.	13.7	217
71	Experimental and Theoretical Observations of Aromaticity in Heterocyclic XAl3â^' (X=Si, Ge, Sn, Pb) Systems. Angewandte Chemie - International Edition, 2001, 40, 1867-1870.	13.8	147
72	Aromatic Mercury Clusters in Ancient Amalgams. Angewandte Chemie - International Edition, 2001, 40, 3369-3372.	13.8	140

#	Article	IF	Citations
73	Experimental and Theoretical Observations of Aromaticity in Heterocyclic XAl3 (X=Si, Ge, Sn, Pb) Systems. Angewandte Chemie - International Edition, 2001, 40, 1867-1870.	13.8	3
74	Facile Synthesis and Characterization of Symmetric N-[(Phenylcarbonyl) carbamothioyl]benzamide Thiourea: Experimental and Theoretical Investigations. Journal of the Brazilian Chemical Society, 0, , .	0.6	2
75	Diethyl Selenodiglycolate: An Eco-Friendly Synthetic Antioxidant with Potential Application to Inflammatory Disorders. Journal of the Brazilian Chemical Society, 0, , .	0.6	0