

Aleksey E Kuznetsov

List of Publications by Year in descending order

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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	A Fast Soluble Carbon-Free Molecular Water Oxidation Catalyst Based on Abundant Metals. <i>Science</i> , 2010, 328, 342-345.	12.6	1,354
2	Observation of All-Metal Aromatic Molecules. <i>Science</i> , 2001, 291, 859-861.	12.6	597
3	All-Metal Antiaromatic Molecule: Rectangular Al ₄ ⁻ in the Li ₃ Al ₄ ⁻ Anion. <i>Science</i> , 2003, 300, 622-625.	12.6	219
4	On the Aromaticity of Square Planar Ga ₄ ⁻ and In ₄ ⁻ in Gaseous NaGa ₄ ⁻ and NaIn ₄ ⁻ Clusters. <i>Journal of the American Chemical Society</i> , 2001, 123, 8825-8831.	13.7	217
5	Experimental and Theoretical Observations of Aromaticity in Heterocyclic XAl ₃ ⁻ (X=Si, Ge, Sn, Pb) Systems. <i>Angewandte Chemie - International Edition</i> , 2001, 40, 1867-1870.	13.8	147
6	Aromatic Mercury Clusters in Ancient Amalgams. <i>Angewandte Chemie - International Edition</i> , 2001, 40, 3369-3372.	13.8	140
7	On the Resonance Energy in New All-Metal Aromatic Molecules. <i>Inorganic Chemistry</i> , 2002, 41, 532-537.	4.0	139
8	Theoretical Evidence of Aromaticity in X ₃ ⁻ (X = B, Al, Ga) Species. <i>Structural Chemistry</i> , 2002, 13, 141-148.	2.0	130
9	Al ₆ ⁻ Fusion of Two Aromatic Al ₃ ⁻ Units. A Combined Photoelectron Spectroscopy and ab Initio Study of M+[Al ₆ ⁻] (M = Li, Na, K, Cu, and Au). <i>Journal of the American Chemical Society</i> , 2002, 124, 11791-11801.	13.7	124
10	Probing the Electronic Structure and Aromaticity of Pentapnictogen Cluster Anions Pn ₅ ⁻ (Pn = P, As, Sb, Bi, Po). <i>Journal of Physical Chemistry A</i> , 2002, 106, 5600-5606.	2.5	94
11	Dioxygen and Water Activation Processes on Multi-Ru-Substituted Polyoxometalates: Comparison with the Ru ₂ O ₂ Dimer. <i>Journal of the American Chemical Society</i> , 2009, 131, 6844-6854.	13.7	88
12	Structural, optical, and surface morphological studies of ethyl cellulose/graphene oxide nanocomposites. <i>Polymer Composites</i> , 2020, 41, 2792-2802.	4.6	85
13	Spectroscopic studies, molecular structure optimization and investigation of structural and electrical properties of novel and biodegradable Chitosan-GO polymer nanocomposites. <i>Journal of Materials Science</i> , 2020, 55, 14829-14847.	3.7	67
14	Peculiar Antiaromatic Inorganic Molecules of Tetrapnictogen in Na ⁺ Pn ₄ ⁻ (Pn = P, As, Sb) and Important Consequences for Hydrocarbons. <i>Inorganic Chemistry</i> , 2002, 41, 6062-6070.	4.0	66
15	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) (DEMHM). <i>Journal of Molecular Structure</i> , 2020, 1199, 127041.	3.6	59
16	Multiple Aromaticity and Antiaromaticity in Silicon Clusters. <i>ChemPhysChem</i> , 2004, 5, 1885-1891.	2.1	48
17	A single σ-bond captures 3, 4 and 5 atoms. <i>Chemical Physics Letters</i> , 2004, 388, 452-456.	2.6	45
18	Revealing substituent effects on the electronic structure and planarity of Ni-porphyrins. <i>Computational and Theoretical Chemistry</i> , 2012, 981, 73-85.	2.5	42

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19	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. <i>RSC Advances</i> , 2020, 10, 11426-11434.	3.6	42
20	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. <i>Journal of Physical Chemistry A</i> , 2010, 114, 535-542.	2.5	39
21	Polyoxometalates in the Design of Effective and Tunable Water Oxidation Catalysts. <i>Israel Journal of Chemistry</i> , 2011, 51, 238-246.	2.3	37
22	Structural and Electronic Properties of Bare and Capped Cd ₃₃ Se ₃₃ and Cd ₃₃ Te ₃₃ Quantum Dots. <i>Journal of Physical Chemistry C</i> , 2014, 118, 7094-7109.	3.1	32
23	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). <i>Journal of Molecular Structure</i> , 2021, 1228, 129445.	3.6	32
24	Ultrasound versus Light: Exploring Photophysicochemical and Sonochemical Properties of Phthalocyanine-Based Therapeutics, Theoretical Study, and In Vitro Evaluations. <i>ACS Applied Bio Materials</i> , 2022, 5, 1139-1150.	4.6	32
25	Structural and Electronic Properties of Bare and Capped Cd _n Se _n /Cd _n Te _n Nanoparticles (n = 6, 9). <i>Journal of Physical Chemistry C</i> , 2012, 116, 6817-6830.	3.1	31
26	Mechanism of the Divanadium-Substituted Polyoxotungstate [V ³⁺ -1,2-H ₂ SiV ₂ W ₁₀ O ₄₀] ⁴⁻ Catalyzed Olefin Epoxidation by H ₂ O ₂ : A Computational Study. <i>Inorganic Chemistry</i> , 2009, 48, 1871-1878.	4.0	29
27	2-Amino-6-methylpyridine based co-crystal salt formation using succinic acid: Single-crystal analysis and computational exploration. <i>Journal of Molecular Structure</i> , 2021, 1230, 129893.	3.6	29
28	Insights into the Mechanism of O ₂ Formation and Release from the Mn ₄ O ₄ L ₆ •Cubane Cluster. <i>Journal of Physical Chemistry A</i> , 2010, 114, 11417-11424.	2.5	27
29	Distance-Independent Charge Recombination Kinetics in Cytochrome <i>c</i> Cytochrome <i>c</i> Peroxidase Complexes: Compensating Changes in the Electronic Coupling and Reorganization Energies. <i>Journal of Physical Chemistry B</i> , 2013, 117, 9129-9141.	2.6	23
30	Experimental and computational studies of a graphene oxide barrier layer covalently functionalized with amino acids on Mg AZ13 alloy in salt medium. <i>RSC Advances</i> , 2019, 9, 32441-32447.	3.6	22
31	Imine-based Zwitterion: Synthesis, single-crystal characterization, and computational investigation. <i>Journal of Molecular Structure</i> , 2022, 1253, 132237.	3.6	22
32	Reactive molecular dynamics of pyrolysis and combustion of alternative jet fuels: A ReaxFF study. <i>Fuel</i> , 2022, 310, 122157.	6.4	19
33	Mass-selected Ag ₃ clusters soft-landed onto MgO/Mo(100): femtosecond photoemission and first-principles simulations. <i>European Physical Journal D</i> , 2007, 45, 477-483.	1.3	15
34	Synthesis, single-crystal exploration, hirshfeld surface analysis, and DFT investigation of the thiosemicarbazones. <i>Journal of Molecular Structure</i> , 2022, 1262, 133088.	3.6	14
35	Peculiar Transformation of a Nonaromatic Al ₄ Cl ₄ (NH ₃) ₄ into an Aromatic Na ₂ Al ₄ Cl ₄ (NH ₃) ₄ . <i>Inorganic Chemistry</i> , 2002, 41, 3596-3598.	4.0	13
36	Synthesis, single-crystal exploration, and theoretical insights of arylsulfonylated 2-amino-6-methylpyrimidin derivatives. <i>Journal of Molecular Structure</i> , 2021, 1243, 130789.	3.6	13

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37	Effects of S-containing ligands on the structure and electronic properties of CdnSen/CdnTen nanoparticles (n=3, 4, 6, and 9). <i>Chemical Physics</i> , 2012, 407, 97-109.	1.9	12
38	Metalloporphyrins with all the pyrrole nitrogens replaced with phosphorus atoms, MP(P) ₄ (M = Sc, Ti). <i>Tj ETQq0 0 Q rgBT /Overlock 10 T</i>	1.9	12
39	Structural isomerism of Ru(^{II})-carbonyl complexes: synthesis, characterization and their antitrypanosomal activities. <i>New Journal of Chemistry</i> , 2017, 41, 4468-4477.	2.8	12
40	Computational investigations into the structural and electronic properties of Cd _n Te _n (n = 1-17) quantum dots. <i>RSC Advances</i> , 2019, 9, 5091-5099.	3.6	11
41	Stability of di-butyl-dichalcogenide-capped gold nanoparticles: experimental data and theoretical insights. <i>RSC Advances</i> , 2020, 10, 6259-6270.	3.6	11
42	Optical properties of small silver clusters supported at MgO. <i>European Physical Journal D</i> , 2007, 45, 471-476.	1.3	10
43	The role of the heteroatom (X = Si, P, and S) on the reactivity of { ^{III} -(H ₂ O)RuIII(1/4-OH)2RuIII(H ₂ O)}[X _n W ₁₀ O ₃₆]} ⁿ⁻ with the O ₂ molecule. <i>Theoretical Chemistry Accounts</i> , 2011, 130, 197-207.	1.4	9
44	Computational design of ZnP(P) ₄ stacks: Three modes of binding. <i>Journal of Theoretical and Computational Chemistry</i> , 2016, 15, 1650043.	1.8	8
45	How the change of the ligand from L = porphine, P ₂ , to L = P ₄ -substituted porphine, P(P) ₄ , affects the electronic properties and the ML binding energies for the first-row transition metals M = Sc-Zn: Comparative study. <i>Chemical Physics</i> , 2016, 469-470, 38-48.	1.9	8
46	Experimental and DFT studies of porous carbon covalently functionalized by polyaniline as a corrosion inhibition barrier on nickel-based alloys in acidic media. <i>RSC Advances</i> , 2020, 10, 12151-12165.	3.6	8
47	Can MP(P) ₄ Compounds Form Complexes with C ₆₀ ?. <i>Journal of Applied Solution Chemistry and Modeling</i> , 2017, 6, 91-97.	0.4	8
48	Reactive molecular dynamics and DFT simulations of FTDO explosive. <i>Computational and Theoretical Chemistry</i> , 2022, 1212, 113723.	2.5	8
49	Influence of an exciton-delocalizing ligand on the structural, electronic, and spectral features of the Cd ₃₃ S ₃₃ quantum dot: insights from computational studies. <i>Journal of Materials Chemistry C</i> , 2018, 6, 8751-8761.	5.5	7
50	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. <i>RSC Advances</i> , 2019, 9, 38677-38686.	3.6	7
51	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. <i>RSC Advances</i> , 2021, 11, 22095-22105.	3.6	6
52	RMD simulations of ADN and ADN/GAP-based propellant. <i>Journal of the Brazilian Society of Mechanical Sciences and Engineering</i> , 2021, 43, 1.	1.6	5
53	Phytotoxicity, structural and computational analysis of 2-methyl-1,5-diarylpentadienones. <i>Journal of Molecular Structure</i> , 2017, 1142, 239-247.	3.6	3
54	9. Complexes between core-modified porphyrins ZnP(X) ₄ (X = P and S) and small semiconductor nanoparticle Zn ₆ S ₆ : are they possible?. , 2018, , 135-146.		3

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55	Complexes between core-modified porphyrins $ZnP(X)_4$ (X = P and S) and small semiconductor nanoparticle Zn_6S_6 : are they possible?. <i>Physical Sciences Reviews</i> , 2019, 4, .	0.8	3
56	Hexabenzocoronene functionalized with porphyrin and P-core-modified porphyrin: A comparative computational study. <i>Computational and Theoretical Chemistry</i> , 2020, 1188, 112973.	2.5	3
57	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. <i>Journal of Molecular Structure</i> , 2021, 1230, 129863.	3.6	3
58	Experimental and Theoretical Observations of Aromaticity in Heterocyclic XAl_3 (X=Si, Ge, Sn, Pb) Systems. <i>Angewandte Chemie - International Edition</i> , 2001, 40, 1867-1870.	13.8	3
59	Facile Synthesis and Characterization of Symmetric N-[(Phenylcarbonyl) carbamothioyl]benzamide Thiourea: Experimental and Theoretical Investigations. <i>Journal of the Brazilian Chemical Society</i> , 0, , .	0.6	2
60	Three Ligands with Biomedical Importance: Binding to Small ZnS Quantum Dots. <i>Journal of Physical Chemistry C</i> , 2018, 122, 12454-12463.	3.1	2
61	Phthalocyanines core-modified by P and S and their complexes with fullerene C60: DFT study. <i>Physical Sciences Reviews</i> , 2019, 4, .	0.8	2
62	Comparison of P- and As-core-modified porphyrins with the parental porphyrin: a computational study. <i>Pure and Applied Chemistry</i> , 2021, 93, 561-570.	1.9	2
63	Design of Novel Classes of Building Blocks for Nanotechnology: Core-Modified Metalloporphyrins and Their Derivatives. , 2017, , .		1
64	Stacks of Metalloporphyrins: Comparison of Experimental and Computational Results. <i>Journal of Physical Chemistry B</i> , 2019, 123, 10044-10060.	2.6	1
65	DFT Investigation of the $\hat{I}6 \hat{\alpha} \hat{\epsilon} \hat{I}6$ -Inter-ring Haptotropic Rearrangement of the Group 8 Metals Complexes [(graphene)MCp] ⁺ (M = Fe, Ru, Os). <i>Journal of Physical Chemistry A</i> , 2021, 125, 366-375.	2.5	1
66	Facile synthesis of Tb-decorated graphene oxide: electrochemical stability, hydrogen storage, and corrosion inhibition of Mg AZ13 alloy in 3.5% NaCl medium. <i>RSC Advances</i> , 2021, 11, 662-670.	3.6	1
67	exo- and endo-Complexes of Fe(0) with Carbon Allotropic Modifications on the Example of Fullerene $\hat{D}j60$: a Density Function Theory Study. <i>Russian Journal of General Chemistry</i> , 2021, 91, 828-834.	0.8	1
68	Core-modified porphyrins: novel building blocks in chemistry. <i>ChemistrySelect</i> , 2023, 8, 1513-1543.	1.5	1
69	Anti-Mycobacterium tuberculosis and Cytotoxicity Activities of Ruthenium(II)/Bipyridine/Diphosphine/Pyrimidine-2-thiolate Complexes: The Role of the Non-Coordinated N-Atom. <i>Journal of the Brazilian Chemical Society</i> , 2015, , .	0.6	1
70	All-Metal Antiaromatic Molecule: Rectangular Al ₄ -4 in the Li ₃ Al ₄ Anion.. <i>ChemInform</i> , 2003, 34, no.	0.0	0
71	Does the MgO(100)-Support Facilitate the Reaction of Nitrogen and Hydrogen Molecules Catalyzed by Zr ₂ Pd ₂ Clusters? A Computational Study. <i>Inorganic Chemistry</i> , 2010, 49, 2557-2567.	4.0	0
72	Combinatorial library design and virtual screening of cryptolepine derivatives against topoisomerase IIA by molecular docking and DFT studies. <i>ChemistrySelect</i> , 2021, 6, 221-246.	1.5	0

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73	Diethyl Selenodiglycolate: An Eco-Friendly Synthetic Antioxidant with Potential Application to Inflammatory Disorders. Journal of the Brazilian Chemical Society, 0, , .	0.6	0
74	Review of research of nanocomposites based on graphene quantum dots. ChemistrySelect, 2022, 7, 605-628.	1.5	0
75	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