Anastassia N Alexandrova

List of Publications by Year in Descending Order

160 papers	5,136 citations	36 h-index	67 g-index
189 ext. papers	5,898 ext. citations	7 avg, IF	6.37 L-index

#	Paper	IF	Citations
160	Predicting Effects of Site-Directed Mutagenesis on Enzyme Kinetics by QM/MM and QM Calculations: A Case of Glutamate Carboxypeptidase II.. *Journal of Physical Chemistry B*, **2022**,	3.4	1
159	Interpreting the Operando X-ray Absorption Near-Edge Structure of Supported Cu and CuPd Clusters in Conditions of Oxidative Dehydrogenation of Propane: Dynamic Changes in Composition and Size. *Journal of Physical Chemistry C*, **2022**, 126, 1972-1981	3.8	1
158	Oxidation Dynamics of Supported Catalytic Cu Clusters: Coupling to Fluxionality. *ACS Catalysis*, **2022**, 12, 818-827	13.1	2
157	Theoretical Perspective on Spectroscopy of Fluxional Nanocatalysts.. *Journal of Physical Chemistry Letters*, **2022**, 13, 4321-4334	6.4	0
156	Electrocatalytic Methane Functionalization with d Early Transition Metals Under Ambient Conditions. *Angewandte Chemie - International Edition*, **2021**, 60, 26630-26638	16.4	0
155	Electrocatalytic Methane Functionalization with d0 Early Transition Metals Under Ambient Conditions. *Angewandte Chemie*, **2021**, 133, 26834	3.6	
154	Tribute to Alexander I. Boldyrev. *Journal of Physical Chemistry A*, **2021**, 125, 9261-9263	2.8	
153	Franck-Condon Tuning of Optical Cycling Centers by Organic Functionalization. *Physical Review Letters*, **2021**, 126, 123002	7.4	10
152	When Fluxionality Beats Size Selection: Acceleration of Ostwald Ripening of Sub-Nano Clusters. *Angewandte Chemie*, **2021**, 133, 12080-12089	3.6	
151	Optical Cycling Functionalization of Arenes. *Journal of Physical Chemistry Letters*, **2021**, 12, 3989-3995	6.4	5
150	Understanding the Hardness of Doped WB4.2. *Journal of Physical Chemistry C*, **2021**, 125, 9486-9496	3.8	3
149	When Fluxionality Beats Size Selection: Acceleration of Ostwald Ripening of Sub-Nano Clusters. *Angewandte Chemie - International Edition*, **2021**, 60, 11973-11982	16.4	7
148	Local Electric Fields as a Natural Switch of Heme-Iron Protein Reactivity. *ACS Catalysis*, **2021**, 11, 6534-6546	13.1	18
147	Visualizing the Dynamic Metalation State of New Delhi Metallo-β-lactamase-1 in Bacteria Using a Reversible Fluorescent Probe. *Journal of the American Chemical Society*, **2021**, 143, 8314-8323	16.4	7
146	Regularization of least squares problems in CHARMM parameter optimization by truncated singular value decompositions. *Journal of Chemical Physics*, **2021**, 154, 184101	3.9	0
145	Titr-DMD-A Rapid, Coarse-Grained Quasi-All-Atom Constant pH Molecular Dynamics Framework. *Journal of Chemical Theory and Computation*, **2021**, 17, 4538-4549	6.4	1
144	Suggesting Reviewers to Improve Your Manuscript. *Journal of Physical Chemistry C*, **2021**, 125, 14493-14494	3.8	1

143	Surface chemical trapping of optical cycling centers. *Physical Chemistry Chemical Physics*, **2021**, 23, 211-218	3.8	1
142	Global Activity Search Uncovers Reaction Induced Concomitant Catalyst Restructuring for Alkane Dissociation on Model Pt Catalysts. *ACS Catalysis*, **2021**, 11, 1877-1885	13.1	10
141	Heterogeneous Intramolecular Electric Field as a Descriptor of Diels-Alder Reactivity. *Journal of Physical Chemistry A*, **2021**, 125, 1289-1298	2.8	4
140	The Art of Reviewing Manuscripts. *Journal of Physical Chemistry C*, **2021**, 125, 16369-16370	3.8	
139	Contrasting Effects of Inhibitors Li and Be on Catalytic Cycle of Glycogen Synthase Kinase-3 *Journal of Physical Chemistry B*, **2021**, 125, 9480-9489	3.4	
138	Revising Manuscripts: Trying to Make Everyone Happy. *Journal of Physical Chemistry C*, **2021**, 125, 18087-18088	3.8	1
137	Machine Learning to Predict Diels-Alder Reaction Barriers from the Reactant State Electron Density. *Journal of Chemical Theory and Computation*, **2021**, 17, 6203-6213	6.4	5
136	Advances in optimizing enzyme electrostatic preorganization. *Current Opinion in Structural Biology*, **2021**, 72, 1-8	8.1	8
135	Electrostatic regulation of blue copper sites. *Chemical Science*, **2021**, 12, 11406-11413	9.4	3
134	Electron Density Geometry and the Quantum Theory of Atoms in Molecules.. *Journal of Physical Chemistry A*, **2021**, 125, 10622-10631	2.8	1
133	Toxic and Physiological Metal Uptake and Release by Human Serum Transferrin. *Biophysical Journal*, **2020**, 118, 2979-2988	2.9	7
132	Stoichiometry-controllable optical defects in CuxIn2Sy quantum dots for energy harvesting. *Journal of Materials Chemistry A*, **2020**, 8, 12556-12565	13	6
131	Why Boron Nitride is such a Selective Catalyst for the Oxidative Dehydrogenation of Propane. *Angewandte Chemie - International Edition*, **2020**, 59, 16527-16535	16.4	37
130	Coking-Resistant Sub-Nano Dehydrogenation Catalysts: PtnSnx/SiO2 (n = 4, 7). *ACS Catalysis*, **2020**, 10, 4543-4558	13.1	24
129	Dynamical Bonding Driving Mixed Valency in a Metal Boride. *Angewandte Chemie - International Edition*, **2020**, 59, 10996-11002	16.4	3
128	Reagent-Triggered Isomerization of Fluxional Cluster Catalyst via Dynamic Coupling. *Journal of Physical Chemistry Letters*, **2020**, 11, 3089-3094	6.4	16
127	(Photo)Electrocatalytic CO2 Reduction at the Defective Anatase TiO2 (101) Surface. *ACS Catalysis*, **2020**, 10, 4048-4058	13.1	24
126	Why Boron Nitride is such a Selective Catalyst for the Oxidative Dehydrogenation of Propane. *Angewandte Chemie*, **2020**, 132, 16670-16678	3.6	3

125	Characteristics of Impactful Computational Contributions to The Journal of Physical Chemistry C. *Journal of Physical Chemistry C*, **2020**, 124, 13509-13510	3.8	3
124	Influence of Terminal Carboxyl Groups on the Structure and Reactivity of Functionalized m-Carboranethiolate Self-Assembled Monolayers. *Chemistry of Materials*, **2020**, 32, 6800-6809	9.6	3
123	Sn-modification of Pt/alumina model catalysts: Suppression of carbon deposition and enhanced thermal stability. *Journal of Chemical Physics*, **2020**, 152, 024702	3.9	20
122	Ensembles of Metastable States Govern Heterogeneous Catalysis on Dynamic Interfaces. *Accounts of Chemical Research*, **2020**, 53, 447-458	24.3	72
121	The Case for Enzymatic Competitive Metal Affinity Methods. *ACS Catalysis*, **2020**, 10, 2298-2307	13.1	5
120	CO Hydrogenation to Formate and Formic Acid by Bimetallic Palladium-Copper Hydride Clusters. *Journal of the American Chemical Society*, **2020**, 142, 7930-7936	16.4	34
119	Interpreting the Operando XANES of Surface-Supported Subnanometer Clusters: When Fluxionality, Oxidation State, and Size Effect Fight. *Journal of Physical Chemistry C*, **2020**, 124, 10057-10066	3.8	16
118	Oxidative Dehydrogenation of Cyclohexane by Cu vs Pd Clusters: Selectivity Control by Specific Cluster Dynamics. *ChemCatChem*, **2020**, 12, 1307-1315	5.2	14
117	Towards a Single Chemical Model for Understanding Lanthanide Hexaborides. *Angewandte Chemie*, **2020**, 132, 22873-22878	3.6	1
116	Towards a Single Chemical Model for Understanding Lanthanide Hexaborides. *Angewandte Chemie - International Edition*, **2020**, 59, 22684-22689	16.4	
115	Hydrogen Evolution on Restructured B-Rich WB: Metastable Surface States and Isolated Active Sites. *ACS Catalysis*, **2020**, 10, 13867-13877	13.1	10
114	Promoting the Cleavage of C□O Bonds at the Interface between a Metal Oxide Cluster and a Co(0001) Support. *ACS Catalysis*, **2020**, 10, 14722-14731	13.1	2
113	Direct Look at the Electric Field in Ketosteroid Isomerase and Its Variants. *ACS Catalysis*, **2020**, 10, 9915-9924	13.1	14
112	Ambient methane functionalization initiated by electrochemical oxidation of a vanadium (V)-oxo dimer. *Nature Communications*, **2020**, 11, 3686	17.4	20
111	Can Fluxionality of Subnanometer Cluster Catalysts Solely Cause Non-Arrhenius Behavior in Catalysis?. *Journal of Physical Chemistry C*, **2020**, 124, 19556-19562	3.8	4
110	Alloying with Sn Suppresses Sintering of Size-Selected Subnano Pt Clusters on SiO2 with and without Adsorbates. *Chemistry of Materials*, **2020**, 32, 8595-8605	9.6	13
109	Fjord-Edge Graphene Nanoribbons with Site-Specific Nitrogen Substitution. *Journal of the American Chemical Society*, **2020**, 142, 18093-18102	16.4	11
108	Global Optimization of Adsorbate Covered Supported Cluster Catalysts: The Case of Pt7H10CH3 on □Al2O3. *ChemCatChem*, **2020**, 12, 762-770	5.2	6

107	Dynamical Bonding Driving Mixed Valency in a Metal Boride. *Angewandte Chemie*, **2020**, 132, 11089-11095	3.6	2
106	Structural Rearrangements of Subnanometer Cu Oxide Clusters Govern Catalytic Oxidation. *ACS Catalysis*, **2020**, 10, 5309-5317	13.1	24
105	Installation of internal electric fields by non-redox active cations in transition metal complexes. *Chemical Science*, **2019**, 10, 10135-10142	9.4	29
104	Dodecaborane-Based Dopants Designed to Shield Anion Electrostatics Lead to Increased Carrier Mobility in a Doped Conjugated Polymer. *Advanced Materials*, **2019**, 31, e1805647	24	60
103	Photooxidative Generation of Dodecaborate-Based Weakly Coordinating Anions. *Inorganic Chemistry*, **2019**, 58, 10516-10526	5.1	4
102	Preparation of Size- and Composition-Controlled PtnSnx/SiO2 (n = 4, 7, 24) Bimetallic Model Catalysts with Atomic Layer Deposition. *Journal of Physical Chemistry C*, **2019**, 123, 16194-16209	3.8	14
101	Surface-supported cluster catalysis: Ensembles of metastable states run the show. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2019**, 9, e1420	7.9	22
100	Germanium as key dopant to boost the catalytic performance of small platinum clusters for alkane dehydrogenation. *Journal of Catalysis*, **2019**, 374, 93-100	7.3	22
99	Uncovered Dynamic Coupling Resolves the Ambiguous Mechanism of Phenylalanine Hydroxylase Oxygen Binding. *Journal of Physical Chemistry B*, **2019**, 123, 4534-4539	3.4	7
98	Charge Density in Enzyme Active Site as a Descriptor of Electrostatic Preorganization. *Journal of Chemical Information and Modeling*, **2019**, 59, 2367-2373	6.1	15
97	Resonant and Selective Excitation of Photocatalytically Active Defect Sites in TiO. *ACS Applied Materials & Interfaces*, **2019**, 11, 10351-10355	9.5	1
96	Designing clusters for heterogeneous catalysis. *Physics Today*, **2019**, 72, 38-43	0.9	8
95	Strain to alter the covalency and superconductivity in transition metal diborides. *Journal of Materials Chemistry C*, **2019**, 7, 10700-10707	7.1	6
94	Heterogeneity in Local Chemical Bonding Explains Spectral Broadening in Quantum Dots with Cu Impurities. *Journal of Physical Chemistry C*, **2019**, 123, 5705-5713	3.8	8
93	Photoinduced Carrier Generation and Distribution in Solution-Deposited Titanyl Phthalocyanine Monolayers. *Chemistry of Materials*, **2019**, 31, 10109-10116	9.6	7
92	Pt cluster on alumina under a pressure of hydrogen: Support-dependent reconstruction from first-principles global optimization. *Journal of Chemical Physics*, **2019**, 151, 194703	3.9	20
91	Dynamic Phase Diagram of Catalytic Surface of Hexagonal Boron Nitride under Conditions of Oxidative Dehydrogenation of Propane. *Journal of Physical Chemistry Letters*, **2019**, 10, 20-25	6.4	38
90	Dynamics of Subnanometer Pt Clusters Can Break the Scaling Relationships in Catalysis. *Journal of Physical Chemistry Letters*, **2019**, 10, 460-467	6.4	45

89	Mechanism of CO2 Photocatalytic Reduction to Methane and Methanol on Defected Anatase TiO2 (101): A Density Functional Theory Study. *Journal of Physical Chemistry C*, **2019**, 123, 3505-3511	3.8	36
88	Understanding How Bonding Controls Strength Anisotropy in Hard Materials by Comparing the High-Pressure Behavior of Orthorhombic and Tetragonal Tungsten Monoboride. *Journal of Physical Chemistry C*, **2018**, 122, 5647-5656	3.8	10
87	Computational Design of Clusters for Catalysis. *Annual Review of Physical Chemistry*, **2018**, 69, 377-400	15.7	50
86	Acid-Base Control of Valency within Carboranedithiol Self-Assembled Monolayers: Molecules Do the Can-Can. *ACS Nano*, **2018**, 12, 2211-2221	16.7	15
85	Diborane Interactions with Pt7/Alumina: Preparation of Size-Controlled Borated Pt Model Catalysts. *Journal of Physical Chemistry C*, **2018**, 122, 1631-1644	3.8	13
84	Local Fluxionality of Surface-Deposited Cluster Catalysts: The Case of Pt on AlO. *Journal of Physical Chemistry Letters*, **2018**, 9, 1696-1702	6.4	50
83	Nanoalloying MgO-Deposited Pt Clusters with Si To Control the Selectivity of Alkane Dehydrogenation. *ACS Catalysis*, **2018**, 8, 8346-8356	13.1	20
82	Geometry Change in a Series of Zirconium Compounds during Lactide Ring-Opening Polymerization. *Organometallics*, **2018**, 37, 4040-4047	3.8	14
81	Multicenter Bonding Effects in Oxygen Vacancy in the Bulk and on the Surface of MgO. *Journal of Physical Chemistry C*, **2018**, 122, 11933-11937	3.8	10
80	Fluxionality of Catalytic Clusters: When It Matters and How to Address It. *ACS Catalysis*, **2017**, 7, 1905-1911	13.1	106
79	Prediction of Two-Dimensional Phase of Boron with Anisotropic Electric Conductivity. *Journal of Physical Chemistry Letters*, **2017**, 8, 1224-1228	6.4	32
78	SmB Cluster Anion: Covalency Involving f Orbitals. *Journal of Physical Chemistry A*, **2017**, 121, 1849-1854	2.8	36
77	Quantified electrostatic preorganization in enzymes using the geometry of the electron charge density. *Chemical Science*, **2017**, 8, 5010-5018	9.4	31
76	Ethylene Dehydrogenation on Pt4,7,8 Clusters on Al2O3: Strong Cluster Size Dependence Linked to Preferred Catalyst Morphologies. *ACS Catalysis*, **2017**, 7, 3322-3335	13.1	95
75	Divide-and-Conquer Chemical Bonding Models for Materials: A Tool for Materials Design at the Electronic Level. *Chemistry of Materials*, **2017**, 29, 8555-8565	9.6	4
74	Boron Switch for Selectivity of Catalytic Dehydrogenation on Size-Selected Pt Clusters on AlO. *Journal of the American Chemical Society*, **2017**, 139, 11568-11575	16.4	77
73	Mystery of Three Borides: Differential Metal-Boron Bonding Governing Superhard Structures. *Chemistry of Materials*, **2017**, 29, 9892-9896	9.6	37
72	Photoelectron spectroscopic and computational study of the PtMgH3,5(-) cluster anions. *Physical Chemistry Chemical Physics*, **2016**, 18, 19345-9	3.6	6

71	Ensemble-Average Representation of Pt Clusters in Conditions of Catalysis Accessed through GPU Accelerated Deep Neural Network Fitting Global Optimization. *Journal of Chemical Theory and Computation*, **2016**, 12, 6213-6226	6.4	81
70	4th International Conference on Chemical Bonding. *Journal of Physical Chemistry A*, **2016**, 120, 9353-9356	2.8	1
69	Predictive methods for computational metalloenzyme redesign - a test case with carboxypeptidase A. *Physical Chemistry Chemical Physics*, **2016**, 18, 31744-31756	3.6	11
68	Aromaticity in polyhydride complexes of Ru, Ir, Os, and Pt. *Physical Chemistry Chemical Physics*, **2016**, 18, 11644-52	3.6	4
67	Visible-Light-Induced Olefin Activation Using 3D Aromatic Boron-Rich Cluster Photooxidants. *Journal of the American Chemical Society*, **2016**, 138, 6952-5	16.4	75
66	Histone Deacetylase 8: Characterization of Physiological Divalent Metal Catalysis. *Journal of Physical Chemistry B*, **2016**, 120, 5884-95	3.4	16
65	Oxygen Vacancies of Anatase(101): Extreme Sensitivity to the Density Functional Theory Method. *Journal of Chemical Theory and Computation*, **2016**, 12, 2889-95	6.4	29
64	Metallic and Magnetic 2D Materials Containing Planar Tetracoordinated C and N. *Journal of Physical Chemistry C*, **2016**, 120, 21685-21690	3.8	10
63	Use of QM/DMD as a Multiscale Approach to Modeling Metalloenzymes. *Methods in Enzymology*, **2016**, 577, 319-39	1.7	1
62	Pt Zn Clusters on Stoichiometric MgO(100) and TiO2(110): Dramatically Different Sintering Behavior. *Journal of Physical Chemistry C*, **2015**, 119, 6047-6055	3.8	15
61	AFFCK: Adaptive Force-Field-Assisted ab Initio Coalescence Kick Method for Global Minimum Search. *Journal of Chemical Theory and Computation*, **2015**, 11, 2385-93	6.4	31
60	Origin of extraordinary stability of square-planar carbon atoms in surface carbides of cobalt and nickel. *Angewandte Chemie - International Edition*, **2015**, 54, 5312-6	16.4	55
59	Computational treatment of metalloproteins. *Journal of Physical Chemistry B*, **2015**, 119, 5945-56	3.4	14
58	Artificial Photosynthesis on TiO2-Passivated InP Nanopillars. *Nano Letters*, **2015**, 15, 6177-81	11.5	67
57	Conservative tryptophan mutants of the protein tyrosine phosphatase YopH exhibit impaired WPD-loop function and crystallize with divanadate esters in their active sites. *Biochemistry*, **2015**, 54, 6490-500	3.2	10
56	Alloying Pt Sub-nano-clusters with Boron: Sintering Preventative and Coke Antagonist?. *ACS Catalysis*, **2015**, 5, 5719-5727	13.1	35
55	Microscopic Study of Atomic Layer Deposition of TiO2 on GaAs and Its Photocatalytic Application. *Chemistry of Materials*, **2015**, 27, 7977-7981	9.6	25
54	Photoelectron spectroscopic and theoretical study of the [HPd(η(2)-H2)](-) cluster anion. *Journal of Chemical Physics*, **2015**, 143, 094307	3.9	20

53	Origin of Extraordinary Stability of Square-Planar Carbon Atoms in Surface Carbides of Cobalt and Nickel. *Angewandte Chemie*, **2015**, 127, 5402-5406	3.6	4
52	Assessing the Bonding Properties of Individual Molecular Orbitals. *Journal of Physical Chemistry A*, **2015**, 119, 12862-7	2.8	11
51	The mechanism of the Pd-catalyzed formation of coumarins: a theoretical study. *Physical Chemistry Chemical Physics*, **2015**, 17, 1347-53	3.6	8
50	Rutile-Deposited PtPd clusters: A Hypothesis Regarding the Stability at 50/50 Ratio. *ACS Catalysis*, **2014**, 4, 3570-3580	13.1	27
49	PtZnH5(-), A Aromatic Cluster. *Journal of Physical Chemistry Letters*, **2014**, 5, 1596-601	6.4	48
48	Pure and Zn-doped Pt clusters go flat and upright on MgO(100). *Physical Chemistry Chemical Physics* , **2014**, 16, 26436-42	3.6	13
47	Mysteries of metals in metalloenzymes. *Accounts of Chemical Research*, **2014**, 47, 3110-7	24.3	87
46	Co2+ acireductone dioxygenase: Fe2+ mechanism, Ni2+ mechanism, or something else?. *Chemical Physics Letters*, **2014**, 604, 77-82	2.5	10
45	Sub-Nano Clusters: The Last Frontier of Inorganic Chemistry. *Advances in Chemical Physics*, **2014**, 73-100		1
44	The PtAl(-) and PtAl2(-) anions: theoretical and photoelectron spectroscopic characterization. *Journal of Chemical Physics*, **2014**, 140, 164316	3.9	8
43	Cu,Zn-superoxide dismutase without Zn is folded but catalytically inactive. *Journal of Molecular Biology*, **2014**, 426, 4112-4124	6.5	35
42	The same in the bulk but different as clusters: X3Y3 (X = B, Al, Ga; Y = P, As). *Chemical Physics Letters*, **2013**, 588, 37-42	2.5	5
41	Metal-dependent activity of Fe and Ni acireductone dioxygenases: how two electrons reroute the catalytic pathway. *Journal of Molecular Biology*, **2013**, 425, 3007-18	6.5	30
40	The Role of the Flexible L43-S54 Protein Loop in the CcrA Metallo-Lactamase in Binding Structurally Dissimilar Lactam Antibiotics. *Journal of Chemical Theory and Computation*, **2013**, 9, 730-7	6.4	20
39	The Golden Crown: A Single Au Atom that Boosts the CO Oxidation Catalyzed by a Palladium Cluster on Titania Surfaces. *Journal of Physical Chemistry Letters*, **2013**, 4, 2250-2255	6.4	40
38	Tug of war between AO-hybridization and aromaticity in dictating structures of Li-doped alkali clusters. *Chemical Physics Letters*, **2012**, 533, 1-5	2.5	14
37	B13+ : a photodriven molecular Wankel engine. *Angewandte Chemie - International Edition*, **2012**, 51, 8512-5	16.4	64
36	Hybrid dynamics simulation engine for metalloproteins. *Biophysical Journal*, **2012**, 103, 767-76	2.9	22

35	Selected AB4(2-/-) (A = C, Si, Ge; B = Al, Ga, In) ions: a battle between covalency and aromaticity, and prediction of square planar Si in SiIn4(2-/-). *Physical Chemistry Chemical Physics*, **2012**, 14, 14815-21	3.6	29
34	Double Aromaticity in a Surface-Deposited Cluster: Pd4 on TiO2 (110). *Journal of Physical Chemistry Letters*, **2012**, 3, 751-4	6.4	20
33	Molecular basis for nanoscopic membrane curvature generation from quantum mechanical models and synthetic transporter sequences. *Journal of the American Chemical Society*, **2012**, 134, 19207-16	16.4	58
32	Why urease is a di-nickel enzyme whereas the CcrA lactamase is a di-zinc enzyme. *Journal of Physical Chemistry B*, **2012**, 116, 10649-56	3.4	25
31	B13+: A Photodriven Molecular Wankel Engine. *Angewandte Chemie*, **2012**, 124, 8640-8643	3.6	8
30	How metal substitution affects the enzymatic activity of catechol-o-methyltransferase. *PLoS ONE*, **2012**, 7, e47172	3.7	21
29	On the mechanism and rate of spontaneous decomposition of amino acids. *Journal of Physical Chemistry B*, **2011**, 115, 13624-32	3.4	19
28	Structure, stability, and mobility of small Pd clusters on the stoichiometric and defective TiO2 (110) surfaces. *Journal of Chemical Physics*, **2011**, 135, 174702	3.9	30
27	Computational design and characterisation of artificial enzymes for Kemp elimination. *Molecular Simulation*, **2011**, 37, 557-571	2	3
26	Lithium cluster anions: photoelectron spectroscopy and ab initio calculations. *Journal of Chemical Physics*, **2011**, 134, 044322	3.9	34
25	Persistent Covalency and Planarity in the BnAl6 2and LiBnAl6 (n = 0) Cluster Ions. *Journal of Physical Chemistry Letters*, **2011**, 2, 2046-2051	6.4	31
24	Rigid substructure search. *Bioinformatics*, **2011**, 27, 1327-9	7.2	24
23	H (H2O)n clusters: microsolvation of the hydrogen atom via molecular ab initio gradient embedded genetic algorithm (GEGA). *Journal of Physical Chemistry A*, **2010**, 114, 12591-9	2.8	57
22	Photochemistry of DNA fragments via semiclassical nonadiabatic dynamics. *Journal of Physical Chemistry B*, **2010**, 114, 12116-28	3.4	51
21	Promiscuous DNA alkyladenine glycosylase dramatically favors a bound lesion over undamaged adenine. *Biophysical Chemistry*, **2010**, 152, 118-27	3.5	8
20	Vibrational predissociation spectra of the , n=3 10, 12 clusters: Even dd alternation in the core ion. *International Journal of Mass Spectrometry*, **2009**, 283, 94-99	1.9	10
19	Origin of the activity drop with the E50D variant of catalytic antibody 34E4 for Kemp elimination. *Journal of Physical Chemistry B*, **2009**, 113, 497-504	3.4	22
18	Catalytic mechanism and performance of computationally designed enzymes for Kemp elimination. *Journal of the American Chemical Society*, **2008**, 130, 15907-15	16.4	80

17	Why urea eliminates ammonia rather than hydrolyzes in aqueous solution. *Journal of Physical Chemistry B*, **2007**, 111, 720-30	3.4	75
16	On the structure and chemical bonding of Si6(2-) and Si6(2-) in NaSi6(-) upon Na+ coordination. *Journal of Chemical Physics*, **2006**, 124, 124305	3.9	28
15	All-boron aromatic clusters as potential new inorganic ligands and building blocks in chemistry. *Coordination Chemistry Reviews*, **2006**, 250, 2811-2866	23.2	509
14	Theoretical study of hydrogenation of the doubly aromatic B7- cluster. *Journal of Molecular Modeling*, **2006**, 12, 569-76	2	46
13	Cu3C4-: a new sandwich molecule with two revolving C2(2-) units. *Journal of Physical Chemistry A*, **2005**, 109, 562-70	2.8	27
12	Search for the Lin(0/+1/-1) (n = 5-7) Lowest-Energy Structures Using the ab Initio Gradient Embedded Genetic Algorithm (GEGA). Elucidation of the Chemical Bonding in the Lithium Clusters. *Journal of Chemical Theory and Computation*, **2005**, 1, 566-80	6.4	181
11	Photoelectron spectroscopy and ab initio study of the doubly antiaromatic B(6) (2-) dianion in the LiB(6) (-) cluster. *Journal of Chemical Physics*, **2005**, 122, 54313	3.9	92
10	Arachno, nido, and closo aromatic isomers of the Li6B6H6 molecule. *Inorganic Chemistry*, **2004**, 43, 3588-92	5.1	24
9	Molecular wheel B8(2-) as a new inorganic ligand. photoelectron spectroscopy and ab initio characterization of LiB8(-). *Inorganic Chemistry*, **2004**, 43, 3552-4	5.1	135
8	Structure of the Na(x)Cl(x+1) (-) (x=1-4) clusters via ab initio genetic algorithm and photoelectron spectroscopy. *Journal of Chemical Physics*, **2004**, 121, 5709-19	3.9	247
7	Hepta- and Octacoordinate Boron in Molecular Wheels of Eight- and Nine-Atom Boron Clusters: Observation and Confirmation. *Angewandte Chemie*, **2003**, 115, 6186-6190	3.6	65
6	Structure and Bonding in B6- and B6: Planarity and Antiaromaticity. *Journal of Physical Chemistry A*, **2003**, 107, 1359-1369	2.8	175
5	Photoelectron Spectroscopy and ab Initio Study of B3- and B4- Anions and Their Neutrals. *Journal of Physical Chemistry A*, **2003**, 107, 9319-9328	2.8	169
4	Aromaticity and Antiaromaticity in Alkali Metal and Alkaline Earth Metal Small Clusters. *Journal of Physical Chemistry A*, **2003**, 107, 554-560	2.8	178
3	Flattening the b(6)h(6)(2-) octahedron Ab initio prediction of a new family of planar all-boron aromatic molecules. *Journal of the American Chemical Society*, **2003**, 125, 10786-7	16.4	56
2	Hydrogen Trioxide Anion: A Possible Atmospheric Intermediate and Path to Oxygen-Rich Molecules. *Journal of Physical Chemistry A*, **2003**, 107, 1203-1206	2.8	9
1	Electronic structure and chemical bonding of B5 and B5 by photoelectron spectroscopy and ab initio calculations. *Journal of Chemical Physics*, **2002**, 117, 7917-7924	3.9	193