Anastassia N Alexandrova

List of Publications by Citations

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	All-boron aromatic clusters as potential new inorganic ligands and building blocks in chemistry. *Coordination Chemistry Reviews*, **2006**, 250, 2811-2866	23.2	509
159	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
158	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
157	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
156	Aromaticity and Antiaromaticity in Alkali Metal and Alkaline Earth Metal Small Clusters. *Journal of Physical Chemistry A*, **2003**, 107, 554-560	2.8	178
155	Structure and Bonding in B6- and B6: Planarity and Antiaromaticity. *Journal of Physical Chemistry A*, **2003**, 107, 1359-1369	2.8	175
154	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
153	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
152	Fluxionality of Catalytic Clusters: When It Matters and How to Address It. *ACS Catalysis*, **2017**, 7, 1905-1911	13.1	106
151	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
150	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
149	Mysteries of metals in metalloenzymes. *Accounts of Chemical Research*, **2014**, 47, 3110-7	24.3	87
148	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
147	Catalytic mechanism and performance of computationally designed enzymes for Kemp elimination. *Journal of the American Chemical Society*, **2008**, 130, 15907-15	16.4	80
146	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
145	Why urea eliminates ammonia rather than hydrolyzes in aqueous solution. *Journal of Physical Chemistry B*, **2007**, 111, 720-30	3.4	75
144	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

143	Ensembles of Metastable States Govern Heterogeneous Catalysis on Dynamic Interfaces. *Accounts of Chemical Research*, **2020**, 53, 447-458	24.3	72
142	Artificial Photosynthesis on TiO2-Passivated InP Nanopillars. *Nano Letters*, **2015**, 15, 6177-81	11.5	67
141	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
140	B13+ : a photodriven molecular Wankel engine. *Angewandte Chemie - International Edition*, **2012**, 51, 8512-5	16.4	64
139	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
138	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
137	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
136	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
135	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
134	Photochemistry of DNA fragments via semiclassical nonadiabatic dynamics. *Journal of Physical Chemistry B*, **2010**, 114, 12116-28	3.4	51
133	Computational Design of Clusters for Catalysis. *Annual Review of Physical Chemistry*, **2018**, 69, 377-400	15.7	50
132	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
131	PtZnH5(-), A □Aromatic Cluster. *Journal of Physical Chemistry Letters*, **2014**, 5, 1596-601	6.4	48
130	Theoretical study of hydrogenation of the doubly aromatic B7- cluster. *Journal of Molecular Modeling*, **2006**, 12, 569-76	2	46
129	Dynamics of Subnanometer Pt Clusters Can Break the Scaling Relationships in Catalysis. *Journal of Physical Chemistry Letters*, **2019**, 10, 460-467	6.4	45
128	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
127	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
126	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

125	Mystery of Three Borides: Differential Metal-Boron Bonding Governing Superhard Structures. *Chemistry of Materials*, **2017**, 29, 9892-9896	9.6	37
124	SmB Cluster Anion: Covalency Involving f Orbitals. *Journal of Physical Chemistry A*, **2017**, 121, 1849-1854	2.8	36
123	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
122	Alloying Pt Sub-nano-clusters with Boron: Sintering Preventative and Coke Antagonist?. *ACS Catalysis*, **2015**, 5, 5719-5727	13.1	35
121	Cu,Zn-superoxide dismutase without Zn is folded but catalytically inactive. *Journal of Molecular Biology*, **2014**, 426, 4112-4124	6.5	35
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	Lithium cluster anions: photoelectron spectroscopy and ab initio calculations. *Journal of Chemical Physics*, **2011**, 134, 044322	3.9	34
118	Prediction of Two-Dimensional Phase of Boron with Anisotropic Electric Conductivity. *Journal of Physical Chemistry Letters*, **2017**, 8, 1224-1228	6.4	32
117	Quantified electrostatic preorganization in enzymes using the geometry of the electron charge density. *Chemical Science*, **2017**, 8, 5010-5018	9.4	31
116	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
115	Persistent Covalency and Planarity in the BnAl6□2□and LiBnAl6□□(n = 0□6) Cluster Ions. *Journal of Physical Chemistry Letters*, **2011**, 2, 2046-2051	6.4	31
114	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
113	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
112	Installation of internal electric fields by non-redox active cations in transition metal complexes. *Chemical Science*, **2019**, 10, 10135-10142	9.4	29
111	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
110	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
109	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
108	Rutile-Deposited Pt-Pd clusters: A Hypothesis Regarding the Stability at 50/50 Ratio. *ACS Catalysis*, **2014**, 4, 3570-3580	13.1	27

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100	Structural Rearrangements of Subnanometer Cu Oxide Clusters Govern Catalytic Oxidation. *ACS Catalysis*, **2020**, 10, 5309-5317	13.1	24
99	Surface-supported cluster catalysis: Ensembles of metastable states run the show. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2019**, 9, e1420	7.9	22
98	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
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96	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
95	How metal substitution affects the enzymatic activity of catechol-o-methyltransferase. *PLoS ONE*, **2012**, 7, e47172	3.7	21
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93	Nanoalloying MgO-Deposited Pt Clusters with Si To Control the Selectivity of Alkane Dehydrogenation. *ACS Catalysis*, **2018**, 8, 8346-8356	13.1	20
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91	Photoelectron spectroscopic and theoretical study of the [HPd(2)-H2)](-) cluster anion. *Journal of Chemical Physics*, **2015**, 143, 094307	3.9	20
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88	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
87	On the mechanism and rate of spontaneous decomposition of amino acids. *Journal of Physical Chemistry B*, **2011**, 115, 13624-32	3.4	19
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85	Reagent-Triggered Isomerization of Fluxional Cluster Catalyst via Dynamic Coupling. *Journal of Physical Chemistry Letters*, **2020**, 11, 3089-3094	6.4	16
84	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
83	Histone Deacetylase 8: Characterization of Physiological Divalent Metal Catalysis. *Journal of Physical Chemistry B*, **2016**, 120, 5884-95	3.4	16
82	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
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76	Oxidative Dehydrogenation of Cyclohexane by Cu vs Pd Clusters: Selectivity Control by Specific Cluster Dynamics. *ChemCatChem*, **2020**, 12, 1307-1315	5.2	14
75	Direct Look at the Electric Field in Ketosteroid Isomerase and Its Variants. *ACS Catalysis*, **2020**, 10, 9915-9924	13.1	14
74	Geometry Change in a Series of Zirconium Compounds during Lactide Ring-Opening Polymerization. *Organometallics*, **2018**, 37, 4040-4047	3.8	14
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72	Pure and Zn-doped Pt clusters go flat and upright on MgO(100). *Physical Chemistry Chemical Physics* , **2014**, 16, 26436-42	3.6	13

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61	Metallic and Magnetic 2D Materials Containing Planar Tetracoordinated C and N. *Journal of Physical Chemistry C*, **2016**, 120, 21685-21690	3.8	10
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58	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
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45	Stoichiometry-controllable optical defects in CuxIn2□Sy quantum dots for energy harvesting. *Journal of Materials Chemistry A*, **2020**, 8, 12556-12565	13	6
44	Photoelectron spectroscopic and computational study of the PtMgH3,5(-) cluster anions. *Physical Chemistry Chemical Physics*, **2016**, 18, 19345-9	3.6	6
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41	The Case for Enzymatic Competitive Metal Affinity Methods. *ACS Catalysis*, **2020**, 10, 2298-2307	13.1	5
40	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
39	Optical Cycling Functionalization of Arenes. *Journal of Physical Chemistry Letters*, **2021**, 12, 3989-3995	6.4	5
38	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
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28	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
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15	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
14	Suggesting Reviewers to Improve Your Manuscript. *Journal of Physical Chemistry C*, **2021**, 125, 14493-14494	3.8	1
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11	Revising Manuscripts: Trying to Make Everyone Happy. *Journal of Physical Chemistry C*, **2021**, 125, 18087-18088	3.8	1
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9	Electrocatalytic Methane Functionalization with d Early Transition Metals Under Ambient Conditions. *Angewandte Chemie - International Edition*, **2021**, 60, 26630-26638	16.4	0
8	Regularization of least squares problems in CHARMM parameter optimization by truncated singular value decompositions. *Journal of Chemical Physics*, **2021**, 154, 184101	3.9	0
7	Theoretical Perspective on Spectroscopy of Fluxional Nanocatalysts.. *Journal of Physical Chemistry Letters*, **2022**, 13, 4321-4334	6.4	0
6	Electrocatalytic Methane Functionalization with d0 Early Transition Metals Under Ambient Conditions. *Angewandte Chemie*, **2021**, 133, 26834	3.6	
5	Tribute to Alexander I. Boldyrev. *Journal of Physical Chemistry A*, **2021**, 125, 9261-9263	2.8	
4	Towards a Single Chemical Model for Understanding Lanthanide Hexaborides. *Angewandte Chemie - International Edition*, **2020**, 59, 22684-22689	16.4	
3	When Fluxionality Beats Size Selection: Acceleration of Ostwald Ripening of Sub-Nano Clusters. *Angewandte Chemie*, **2021**, 133, 12080-12089	3.6	
2	The Art of Reviewing Manuscripts. *Journal of Physical Chemistry C*, **2021**, 125, 16369-16370	3.8	
1	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	