Anastassia N Alexandrova

List of Publications by Year
in descending order

174 papers	6,546 citations	71102 41 h-index	76900 74 g-index
189 all docs	189 docs citations	189 times ranked	5182 citing authors

#	Article	IF	Citations
1	All-boron aromatic clusters as potential new inorganic ligands and building blocks in chemistry. Coordination Chemistry Reviews, 2006, 250, 2811-2866.	18.8	588
2	Structure of the NaxClx+1â^'â€Š(x=1â€“4) clusters viaab initiogenetic algorithm and photoelectron spectroscopy. Journal of Chemical Physics, 2004, 121, 5709-5719.	3.0	261
3	Electronic structure and chemical bonding of B5â^' and B5 by photoelectron spectroscopy andab initiocalculations. Journal of Chemical Physics, 2002, 117, 7917-7924.	3.0	222
4	Search for the Lin0/+1/-1 (n = 5â^'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, 566-580.	5.3	198
5	Structure and Bonding in B6-and B6:Â Planarity and Antiaromaticity. Journal of Physical Chemistry A, 2003, 107, 1359-1369.	2.5	193
6	Ïƒ-Aromaticity and Ïƒ-Antiaromaticity in Alkali Metal and Alkaline Earth Metal Small Clusters. Journal of Physical Chemistry A, 2003, 107, 554-560.	2.5	193
7	Photoelectron Spectroscopy and ab Initio Study of B3-and B4-Anions and Their Neutrals. Journal of Physical Chemistry A, 2003, 107, 9319-9328.	2.5	183
8	Molecular Wheel B82- as a New Inorganic Ligand. Photoelectron Spectroscopy and ab Initio Characterization of LiB8-. Inorganic Chemistry, 2004, 43, 3552-3554.	4.0	150
9	Fluxionality of Catalytic Clusters: When It Matters and How to Address It. ACS Catalysis, 2017, 7, 1905-1911.	11.2	150
10	Ensembles of Metastable States Govern Heterogeneous Catalysis on Dynamic Interfaces. Accounts of Chemical Research, 2020, 53, 447-458.	15.6	134
11	Ethylene Dehydrogenation on Pt_{4,7,8} Clusters on Al₂O₃: Strong Cluster Size Dependence Linked to Preferred Catalyst Morphologies. ACS Catalysis, 2017, 7, 3322-3335.	11.2	124
12	Mysteries of Metals in Metalloenzymes. Accounts of Chemical Research, 2014, 47, 3110-3117.	15.6	114
13	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.	5.3	106
14	Photoelectron spectroscopy andab initiostudy of the doubly antiaromatic B62â^' dianion in the LiB6â^' cluster. Journal of Chemical Physics, 2005, 122, 054313.	3.0	103
15	Boron Switch for Selectivity of Catalytic Dehydrogenation on Size-Selected Pt Clusters on Al₂O₃. Journal of the American Chemical Society, 2017, 139, 11568-11575.	13.7	103
16	Visible-Light-Induced Olefin Activation Using 3D Aromatic Boron-Rich Cluster Photooxidants. Journal of the American Chemical Society, 2016, 138, 6952-6955.	13.7	95
17	Dodecaboraneâ€Based Dopants Designed to Shield Anion Electrostatics Lead to Increased Carrier Mobility in a Doped Conjugated Polymer. Advanced Materials, 2019, 31, e1805647.	21.0	90
18	Artificial Photosynthesis on TiO₂-Passivated InP Nanopillars. Nano Letters, 2015, 15, 6177-6181.	9.1	86

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19	Why Urea Eliminates Ammonia Rather than Hydrolyzes in Aqueous Solution. Journal of Physical Chemistry B, 2007, 111, 720-730.	2.6	85
20	Catalytic Mechanism and Performance of Computationally Designed Enzymes for Kemp Elimination. Journal of the American Chemical Society, 2008, 130, 15907-15915.	13.7	83
21	CO₂ Hydrogenation to Formate and Formic Acid by Bimetallic Palladiumâ€“Copper Hydride Clusters. Journal of the American Chemical Society, 2020, 142, 7930-7936.	13.7	79
22	Why Boron Nitride is such a Selective Catalyst for the Oxidative Dehydrogenation of Propane. Angewandte Chemie - International Edition, 2020, 59, 16527-16535.	13.8	75
23	B₁₃⁺: A Photodriven Molecular Wankel Engine. Angewandte Chemie - International Edition, 2012, 51, 8512-8515.	13.8	72
24	Dynamics of Subnanometer Pt Clusters Can Break the Scaling Relationships in Catalysis. Journal of Physical Chemistry Letters, 2019, 10, 460-467.	4.6	72
25	Local Fluxionality of Surface-Deposited Cluster Catalysts: The Case of Pt₇ on Al₂O₃. Journal of Physical Chemistry Letters, 2018, 9, 1696-1702.	4.6	69
26	Origin of Extraordinary Stability of Squareâ€Planar Carbon Atoms in Surface Carbides of Cobalt and Nickel. Angewandte Chemie - International Edition, 2015, 54, 5312-5316.	13.8	67
27	HÂ·(H₂O)_n Clusters: Microsolvation of the Hydrogen Atom via Molecular ab Initio Gradient Embedded Genetic Algorithm (GEGA). Journal of Physical Chemistry A, 2010, 114, 12591-12599.	2.5	66
28	Flattening the B6H62-Octahedron. Ab Initio Prediction of a New Family of Planar All-Boron Aromatic Molecules. Journal of the American Chemical Society, 2003, 125, 10786-10787.	13.7	64
29	Molecular Basis for Nanoscopic Membrane Curvature Generation from Quantum Mechanical Models and Synthetic Transporter Sequences. Journal of the American Chemical Society, 2012, 134, 19207-19216.	13.7	64
30	Computational Design of Clusters for Catalysis. Annual Review of Physical Chemistry, 2018, 69, 377-400.	10.8	59
31	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.	3.1	57
32	Installation of internal electric fields by non-redox active cations in transition metal complexes. Chemical Science, 2019, 10, 10135-10142.	7.4	55
33	Photochemistry of DNA Fragments via Semiclassical Nonadiabatic Dynamics. Journal of Physical Chemistry B, 2010, 114, 12116-12128.	2.6	53
34	PtZnH₅^{â€“}, A Ïƒ-Aromatic Cluster. Journal of Physical Chemistry Letters, 2014, 5, 1596-1601.	4.6	52
35	Theoretical study of hydrogenation of the doubly aromatic B 7 â^’ cluster. Journal of Molecular Modeling, 2006, 12, 569-576.	1.8	49
36	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.	4.6	49

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37	Cu,Zn-Superoxide Dismutase without Zn Is Folded but Catalytically Inactive. Journal of Molecular Biology, 2014, 426, 4112-4124.	4.2	47
38	Oxygen Vacancies of Anatase(101): Extreme Sensitivity to the Density Functional Theory Method. Journal of Chemical Theory and Computation, 2016, 12, 2889-2895.	5.3	47
39	Mystery of Three Borides: Differential Metalâ€“Boron Bonding Governing Superhard Structures. Chemistry of Materials, 2017, 29, 9892-9896.	6.7	45
40	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.	4.6	42
41	(Photo)Electrocatalytic CO₂ Reduction at the Defective Anatase TiO₂ (101) Surface. ACS Catalysis, 2020, 10, 4048-4058.	11.2	42
42	AFFCK: Adaptive Force-Field-Assisted ab Initio Coalescence Kick Method for Global Minimum Search. Journal of Chemical Theory and Computation, 2015, 11, 2385-2393.	5.3	41
43	Alloying Pt Sub-nano-clusters with Boron: Sintering Preventative and Coke Antagonist?. ACS Catalysis, 2015, 5, 5719-5727.	11.2	41
44	Prediction of Two-Dimensional Phase of Boron with Anisotropic Electric Conductivity. Journal of Physical Chemistry Letters, 2017, 8, 1224-1228.	4.6	41
45	SmB₆^{â€“} Cluster Anion: Covalency Involving f Orbitals. Journal of Physical Chemistry A, 2017, 121, 1849-1854.	2.5	40
46	Quantified electrostatic preorganization in enzymes using the geometry of the electron charge density. Chemical Science, 2017, 8, 5010-5018.	7.4	40
47	Coking-Resistant Sub-Nano Dehydrogenation Catalysts: Pt_nSn_x/SiO₂ (n = 4, 7). ACS Catalysis, 2020, 10, 4543-4558.	11.2	40
48	Local Electric Fields As a Natural Switch of Heme-Iron Protein Reactivity. ACS Catalysis, 2021, 11, 6534-6546.	11.2	40
49	Lithium cluster anions: Photoelectron spectroscopy and ab initio calculations. Journal of Chemical Physics, 2011, 134, 044322.	3.0	38
50	Surfaceâ€supported cluster catalysis: Ensembles of metastable states run the show. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1420.	14.6	36
51	Ambient methane functionalization initiated by electrochemical oxidation of a vanadium (V)-oxo dimer. Nature Communications, 2020, 11, 3686.	12.8	36
52	Structural Rearrangements of Subnanometer Cu Oxide Clusters Govern Catalytic Oxidation. ACS Catalysis, 2020, 10, 5309-5317.	11.2	36
53	Germanium as key dopant to boost the catalytic performance of small platinum clusters for alkane dehydrogenation. Journal of Catalysis, 2019, 374, 93-100.	6.2	35
54	Metal-Dependent Activity of Fe and Ni Acireductone Dioxygenases: How Two Electrons Reroute the Catalytic Pathway. Journal of Molecular Biology, 2013, 425, 3007-3018.	4.2	34

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55	Pt8 cluster on alumina under a pressure of hydrogen: Support-dependent reconstruction from first-principles global optimization. Journal of Chemical Physics, 2019, 151, 194703.	3.0	34
56	Persistent Covalency and Planarity in the B_nAl_{6â€“n}^{2â€“} and LiB_nAl_{6â€“n}^{â€“} (n = 0â€“6) Cluster Ions. Journal of Physical Chemistry Letters, 2011, 2, 2046-2051.	4.6	33
57	Selected AB42â^'/â^' (A = C, Si, Ge; B = Al, Ga, In) ions: a battle between covalency and aromaticity, and prediction of square planar Si in SiIn42â^'/â^'. Physical Chemistry Chemical Physics, 2012, 14, 14815.	2.8	33
58	Cu3C4-:Â A New Sandwich Molecule with Two Revolving C22-Units. Journal of Physical Chemistry A, 2005, 109, 562-570.	2.5	32
59	Structure, stability, and mobility of small Pd clusters on the stoichiometric and defective TiO2 (110) surfaces. Journal of Chemical Physics, 2011, 135, 174702.	3.0	32
60	Nanoalloying MgO-Deposited Pt Clusters with Si To Control the Selectivity of Alkane Dehydrogenation. ACS Catalysis, 2018, 8, 8346-8356.	11.2	32
61	Rutile-Deposited Ptâ€“Pd clusters: A Hypothesis Regarding the Stability at 50/50 Ratio. ACS Catalysis, 2014, 4, 3570-3580.	11.2	30
62	Arachno, Nido, and Closo Aromatic Isomers of the Li6B6H6 Molecule. Inorganic Chemistry, 2004, 43, 3588-3592.	4.0	28
63	On the structure and chemical bonding of Si62â^' and Si62â^' in NaSi6â^' upon Na+ coordination. Journal of Chemical Physics, 2006, 124, 124305.	3.0	28
64	Rigid substructure search. Bioinformatics, 2011, 27, 1327-1329.	4.1	28
65	Why Urease Is a Di-Nickel Enzyme whereas the CcrA Î²-Lactamase Is a Di-Zinc Enzyme. Journal of Physical Chemistry B, 2012, 116, 10649-10656.	2.6	27
66	Microscopic Study of Atomic Layer Deposition of TiO₂ on GaAs and Its Photocatalytic Application. Chemistry of Materials, 2015, 27, 7977-7981.	6.7	27
67	Charge Density in Enzyme Active Site as a Descriptor of Electrostatic Preorganization. Journal of Chemical Information and Modeling, 2019, 59, 2367-2373.	5.4	27
68	Hybrid Dynamics Simulation Engine for Metalloproteins. Biophysical Journal, 2012, 103, 767-776.	0.5	26
69	Direct Look at the Electric Field in Ketosteroid Isomerase and Its Variants. ACS Catalysis, 2020, 10, 9915-9924.	11.2	26
70	Global Activity Search Uncovers Reaction Induced Concomitant Catalyst Restructuring for Alkane Dissociation on Model Pt Catalysts. ACS Catalysis, 2021, 11, 1877-1885.	11.2	26
71	Franck-Condon Tuning of Optical Cycling Centers by Organic Functionalization. Physical Review Letters, 2021, 126, 123002.	7.8	26
72	Preparation of Size- and Composition-Controlled Pt_nSn_x/SiO₂ (n = 4, 7, 24) Bimetallic Model Catalysts with Atomic Layer Deposition. Journal of Physical Chemistry C, 2019, 123, 16194-16209.	3.1	25

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73	Sn-modification of Pt7/alumina model catalysts: Suppression of carbon deposition and enhanced thermal stability. Journal of Chemical Physics, 2020, 152, 024702.	3.0	25
74	Fjord-Edge Graphene Nanoribbons with Site-Specific Nitrogen Substitution. Journal of the American Chemical Society, 2020, 142, 18093-18102.	13.7	24
75	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.	3.1	24
76	Advances in optimizing enzyme electrostatic preorganization. Current Opinion in Structural Biology, 2022, 72, 1-8.	5.7	24
77	Acidâ€“Base Control of Valency within Carboranedithiol Self-Assembled Monolayers: Molecules Do the Can-Can. ACS Nano, 2018, 12, 2211-2221.	14.6	23
78	How Metal Substitution Affects the Enzymatic Activity of Catechol-O-Methyltransferase. PLoS ONE, 2012, 7, e47172.	2.5	23
79	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.	2.6	22
80	Visualizing the Dynamic Metalation State of New Delhi Metallo-Î²-lactamase-1 in Bacteria Using a Reversible Fluorescent Probe. Journal of the American Chemical Society, 2021, 143, 8314-8323.	13.7	22
81	On the Mechanism and Rate of Spontaneous Decomposition of Amino Acids. Journal of Physical Chemistry B, 2011, 115, 13624-13632.	2.6	21
82	The Role of the Flexible L43-S54 Protein Loop in the CcrA Metallo-Î²-lactamase in Binding Structurally Dissimilar Î²-Lactam Antibiotics. Journal of Chemical Theory and Computation, 2013, 9, 730-737.	5.3	21
83	Photoelectron spectroscopic and theoretical study of the [HPd(Î·2-H2)]â^' cluster anion. Journal of Chemical Physics, 2015, 143, 094307.	3.0	21
84	Oxidative Dehydrogenation of Cyclohexane by Cu vs Pd Clusters: Selectivity Control by Specific Cluster Dynamics. ChemCatChem, 2020, 12, 1307-1315.	3.7	21
85	Double Ïƒ-Aromaticity in a Surface-Deposited Cluster: Pd₄ on TiO₂ (110). Journal of Physical Chemistry Letters, 2012, 3, 751-754.	4.6	20
86	Hydrogen Evolution on Restructured B-Rich WB: Metastable Surface States and Isolated Active Sites. ACS Catalysis, 2020, 10, 13867-13877.	11.2	20
87	Optical Cycling Functionalization of Arenes. Journal of Physical Chemistry Letters, 2021, 12, 3989-3995.	4.6	20
88	Alloying with Sn Suppresses Sintering of Size-Selected Subnano Pt Clusters on SiO₂ with and without Adsorbates. Chemistry of Materials, 2020, 32, 8595-8605.	6.7	19
89	Reagent-Triggered Isomerization of Fluxional Cluster Catalyst via Dynamic Coupling. Journal of Physical Chemistry Letters, 2020, 11, 3089-3094.	4.6	19
90	Computational Treatment of Metalloproteins. Journal of Physical Chemistry B, 2015, 119, 5945-5956.	2.6	18

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91	Ptâ€“Zn Clusters on Stoichiometric MgO(100) and TiO₂(110): Dramatically Different Sintering Behavior. Journal of Physical Chemistry C, 2015, 119, 6047-6055.	3.1	17
92	Diborane Interactions with Pt₇/Alumina: Preparation of Size-Controlled Borated Pt Model Catalysts. Journal of Physical Chemistry C, 2018, 122, 1631-1644.	3.1	17
93	Geometry Change in a Series of Zirconium Compounds during Lactide Ring-Opening Polymerization. Organometallics, 2018, 37, 4040-4047.	2.3	17
94	Histone Deacetylase 8: Characterization of Physiological Divalent Metal Catalysis. Journal of Physical Chemistry B, 2016, 120, 5884-5895.	2.6	16
95	Machine Learning to Predict Dielsâ€“Alder Reaction Barriers from the Reactant State Electron Density. Journal of Chemical Theory and Computation, 2021, 17, 6203-6213.	5.3	16
96	Pure and Zn-doped Pt clusters go flat and upright on MgO(100). Physical Chemistry Chemical Physics, 2014, 16, 26436-26442.	2.8	15
97	Electrostatic regulation of blue copper sites. Chemical Science, 2021, 12, 11406-11413.	7.4	15
98	Tug of war between AO-hybridization and aromaticity in dictating structures of Li-doped alkali clusters. Chemical Physics Letters, 2012, 533, 1-5.	2.6	14
99	Assessing the Bonding Properties of Individual Molecular Orbitals. Journal of Physical Chemistry A, 2015, 119, 12862-12867.	2.5	14
100	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, 6490-6500.	2.5	13
101	When Fluxionality Beats Size Selection: Acceleration of Ostwald Ripening of Subâ€Nano Clusters. Angewandte Chemie - International Edition, 2021, 60, 11973-11982.	13.8	13
102	The PtAlâ¯and PtAl2â¯anions: Theoretical and photoelectron spectroscopic characterization. Journal of Chemical Physics, 2014, 140, 164316.	3.0	12
103	Metallic and Magnetic 2D Materials Containing Planar Tetracoordinated C and N. Journal of Physical Chemistry C, 2016, 120, 21685-21690.	3.1	12
104	Multicenter Bonding Effects in Oxygen Vacancy in the Bulk and on the Surface of MgO. Journal of Physical Chemistry C, 2018, 122, 11933-11937.	3.1	12
105	Heterogeneity in Local Chemical Bonding Explains Spectral Broadening in Quantum Dots with Cu Impurities. Journal of Physical Chemistry C, 2019, 123, 5705-5713.	3.1	12
106	Vibrational predissociation spectra of the , n=3â€“10, 12 clusters: Evenâ€“odd alternation in the core ion. International Journal of Mass Spectrometry, 2009, 283, 94-99.	1.5	11
107	Predictive methods for computational metalloenzyme redesign â€“ a test case with carboxypeptidase A. Physical Chemistry Chemical Physics, 2016, 18, 31744-31756.	2.8	11
108	Designing clusters for heterogeneous catalysis. Physics Today, 2019, 72, 38-43.	0.3	11

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109	Global Optimization of Adsorbate Covered Supported Cluster Catalysts: The Case of Pt₇H₁₀CH₃ on Î±â€Al₂O₃. ChemCatChem, 2020, 12, 762-770.	3.7	11
110	High-temperature phonon-mediated superconductivity in monolayer Mg2B4C2. Npj Quantum Materials, 2022, 7, .	5.2	11
111	Hydrogen Trioxide Anion:â€‰ A Possible Atmospheric Intermediate and Path to Oxygen-Rich Molecules. Journal of Physical Chemistry A, 2003, 107, 1203-1206.	2.5	10
112	Co2+ acireductone dioxygenase: Fe2+ mechanism, Ni2+ mechanism, or something else?. Chemical Physics Letters, 2014, 604, 77-82.	2.6	10
113	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.	3.1	10
114	Fluxionality of Subnano Clusters Reshapes the Activity Volcano of Electrocatalysis. ChemCatChem, 2022, 14, .	3.7	10
115	Promiscuous DNA alkyladenine glycosylase dramatically favors a bound lesion over undamaged adenine. Biophysical Chemistry, 2010, 152, 118-127.	2.8	9
116	The mechanism of the Pd-catalyzed formation of coumarins: a theoretical study. Physical Chemistry Chemical Physics, 2015, 17, 1347-1353.	2.8	9
117	Strain to alter the covalency and superconductivity in transition metal diborides. Journal of Materials Chemistry C, 2019, 7, 10700-10707.	5.5	9
118	Heterogeneous Intramolecular Electric Field as a Descriptor of Dielsâ€“Alder Reactivity. Journal of Physical Chemistry A, 2021, 125, 1289-1298.	2.5	9
119	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, 126, 132-143.	2.6	9
120	Ensemble representation of catalytic interfaces: soloists, orchestras, and everything in-between. Chemical Science, 2022, 13, 8003-8016.	7.4	9
121	Photoinduced Carrier Generation and Distribution in Solution-Deposited Titanyl Phthalocyanine Monolayers. Chemistry of Materials, 2019, 31, 10109-10116.	6.7	8
122	Promoting the Cleavage of Câ€“O Bonds at the Interface between a Metal Oxide Cluster and a Co(0001) Support. ACS Catalysis, 2020, 10, 14722-14731.	11.2	8
123	Can Fluxionality of Subnanometer Cluster Catalysts Solely Cause Non-Arrhenius Behavior in Catalysis?. Journal of Physical Chemistry C, 2020, 124, 19556-19562.	3.1	8
124	Toxic and Physiological Metal Uptake and Release by Human Serum Transferrin. Biophysical Journal, 2020, 118, 2979-2988.	0.5	8
125	Stoichiometry-controllable optical defects in Cu_xIn_{2â^'x}S_y quantum dots for energy harvesting. Journal of Materials Chemistry A, 2020, 8, 12556-12565.	10.3	8
126	Influence of Terminal Carboxyl Groups on the Structure and Reactivity of Functionalized m-Carboranethiolate Self-Assembled Monolayers. Chemistry of Materials, 2020, 32, 6800-6809.	6.7	8

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127	Inverse molecular design of alkoxides and phenoxides for aqueous direct air capture of CO ₂. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	7.1	8
128	Photoelectron spectroscopic and computational study of the PtMgH_{3,5}^{â˜’} cluster anions. Physical Chemistry Chemical Physics, 2016, 18, 19345-19349.	2.8	7
129	Photooxidative Generation of Dodecaborate-Based Weakly Coordinating Anions. Inorganic Chemistry, 2019, 58, 10516-10526.	4.0	7
130	Uncovered Dynamic Coupling Resolves the Ambiguous Mechanism of Phenylalanine Hydroxylase Oxygen Binding. Journal of Physical Chemistry B, 2019, 123, 4534-4539.	2.6	7
131	Why Boron Nitride is such a Selective Catalyst for the Oxidative Dehydrogenation of Propane. Angewandte Chemie, 2020, 132, 16670-16678.	2.0	7
132	Recent Innovations in Solid-State and Molecular Qubits for Quantum Information Applications. Journal of Physical Chemistry B, 2021, 125, 12111-12114.	2.6	7
133	Oxidation Dynamics of Supported Catalytic Cu Clusters: Coupling to Fluxionality. ACS Catalysis, 2022, 12, 818-827.	11.2	7
134	Theoretical Perspective on Operando Spectroscopy of Fluxional Nanocatalysts. Journal of Physical Chemistry Letters, 2022, 13, 4321-4334.	4.6	7
135	Divide-and-Conquer Chemical Bonding Models for Materials: A Tool for Materials Design at the Electronic Level. Chemistry of Materials, 2017, 29, 8555-8565.	6.7	6
136	The Case for Enzymatic Competitive Metal Affinity Methods. ACS Catalysis, 2020, 10, 2298-2307.	11.2	6
137	Titr-DMDâ€”A Rapid, Coarse-Grained Quasi-All-Atom Constant pH Molecular Dynamics Framework. Journal of Chemical Theory and Computation, 2021, 17, 4538-4549.	5.3	6
138	Histidineâ€Mediated Ion Specific Effects Enable Salt Tolerance of a Poreâ€Forming Marine Antimicrobial Peptide. Angewandte Chemie - International Edition, 2022, , .	13.8	6
139	Electron Density Geometry and the Quantum Theory of Atoms in Molecules. Journal of Physical Chemistry A, 2021, 125, 10622-10631.	2.5	6
140	Computational design and characterisation of artificial enzymes for Kemp elimination. Molecular Simulation, 2011, 37, 557-571.	2.0	5
141	The same in the bulk but different as clusters: X3Y3 (X=B, Al, Ga; Y=P, As). Chemical Physics Letters, 2013, 588, 37-42.	2.6	5
142	Ï*f*-Aromaticity in polyhydride complexes of Ru, Ir, Os, and Pt. Physical Chemistry Chemical Physics, 2016, 18, 11644-11652.	2.8	5
143	Dynamical Bonding Driving Mixed Valency in a Metal Boride. Angewandte Chemie - International Edition, 2020, 59, 10996-11002.	13.8	5
144	Surface chemical trapping of optical cycling centers. Physical Chemistry Chemical Physics, 2021, 23, 211-218.	2.8	5

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145	Understanding the Hardness of Doped WB4.2. Journal of Physical Chemistry C, 2021, 125, 9486-9496.	3.1	5
146	Electrocatalytic Methane Functionalization with d⁰ Early Transition Metals Under Ambient Conditions. Angewandte Chemie - International Edition, 2021, 60, 26630-26638.	13.8	5
147	Recent Innovations in Solid-State and Molecular Qubits for Quantum Information Applications. Journal of Physical Chemistry Letters, 2021, 12, 10742-10745.	4.6	5
148	Dynamical Bonding Driving Mixed Valency in a Metal Boride. Angewandte Chemie, 2020, 132, 11089-11095.	2.0	4
149	Characteristics of Impactful Computational Contributions to The Journal of Physical Chemistry C. Journal of Physical Chemistry C, 2020, 124, 13509-13510.	3.1	3
150	When Fluxionality Beats Size Selection: Acceleration of Ostwald Ripening of Subâ€Nano Clusters. Angewandte Chemie, 2021, 133, 12080-12089.	2.0	3
151	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.	3.1	3
152	Guest Editorial: The 3rd Transatlantic Frontiers in Chemistry Symposium. Chemistry - A European Journal, 2013, 19, 15777-15783.	3.3	2
153	Towards a Single Chemical Model for Understanding Lanthanide Hexaborides. Angewandte Chemie, 2020, 132, 22873-22878.	2.0	2
154	Regularization of least squares problems in CHARMM parameter optimization by truncated singular value decompositions. Journal of Chemical Physics, 2021, 154, 184101.	3.0	2
155	Frontispiece: Origin of Extraordinary Stability of Squareâ€Planar Carbon Atoms in Surface Carbides of Cobalt and Nickel. Angewandte Chemie - International Edition, 2015, 54, .	13.8	1
156	Use of QM/DMD as a Multiscale Approach to Modeling Metalloenzymes. Methods in Enzymology, 2016, 577, 319-339.	1.0	1
157	4th International Conference on Chemical Bonding. Journal of Physical Chemistry A, 2016, 120, 9353-9356.	2.5	1
158	Resonant and Selective Excitation of Photocatalytically Active Defect Sites in TiO₂. ACS Applied Materials & Interfaces, 2019, 11, 10351-10355.	8.0	1
159	Suggesting Reviewers to Improve Your Manuscript. Journal of Physical Chemistry C, 2021, 125, 14493-14494.	3.1	1
160	Revising Manuscripts: Trying to Make Everyone Happy. Journal of Physical Chemistry C, 2021, 125, 18087-18088.	3.1	1
161	Electrocatalytic Methane Functionalization with d⁰ Early Transition Metals Under Ambient Conditions. Angewandte Chemie, 2021, 133, 26834-26842.	2.0	1
162	Towards a Single Chemical Model for Understanding Lanthanide Hexaborides. Angewandte Chemie - International Edition, 2020, 59, 22684-22689.	13.8	0

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163	Suggesting Reviewers to Improve Your Manuscript. Journal of Physical Chemistry A, 2021, 125, 5861-5862.	2.5	0
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