

Anastassia N Alexandrova

List of Publications by Year in descending order

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papers

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#	ARTICLE	IF	CITATIONS
1	All-boron aromatic clusters as potential new inorganic ligands and building blocks in chemistry. <i>Coordination Chemistry Reviews</i> , 2006, 250, 2811-2866.	9.5	588
2	Structure of the $\text{Na}_x\text{Cl}_x+1^{-}$ ($x=1-4$) clusters via ab initio genetic algorithm and photoelectron spectroscopy. <i>Journal of Chemical Physics</i> , 2004, 121, 5709-5719.	1.2	261
3	Electronic structure and chemical bonding of B_5^{+} and B_5 by photoelectron spectroscopy and ab initio calculations. <i>Journal of Chemical Physics</i> , 2002, 117, 7917-7924.	1.2	222
4	Search for the $\text{Li}_n^{0/+1/-1}$ ($n = 5-7$) Lowest-Energy Structures Using the ab Initio Gradient Embedded Genetic Algorithm (GEGA). Elucidation of the Chemical Bonding in the Lithium Clusters. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 566-580.	2.3	198
5	Structure and Bonding in B_6 - and B_6^{-} : Planarity and Antiaromaticity. <i>Journal of Physical Chemistry A</i> , 2003, 107, 1359-1369.	1.1	193
6	π -Aromaticity and π -Antiaromaticity in Alkali Metal and Alkaline Earth Metal Small Clusters. <i>Journal of Physical Chemistry A</i> , 2003, 107, 554-560.	1.1	193
7	Photoelectron Spectroscopy and ab Initio Study of B_3 - and B_4 -Anions and Their Neutrals. <i>Journal of Physical Chemistry A</i> , 2003, 107, 9319-9328.	1.1	183
8	Molecular Wheel B_8^{2-} as a New Inorganic Ligand. Photoelectron Spectroscopy and ab Initio Characterization of LiB_8 . <i>Inorganic Chemistry</i> , 2004, 43, 3552-3554.	1.9	150
9	Fluxionality of Catalytic Clusters: When It Matters and How to Address It. <i>ACS Catalysis</i> , 2017, 7, 1905-1911.	5.5	150
10	Ensembles of Metastable States Govern Heterogeneous Catalysis on Dynamic Interfaces. <i>Accounts of Chemical Research</i> , 2020, 53, 447-458.	7.6	134
11	Ethylene Dehydrogenation on $\text{Pt}_{4,7,8}$ Clusters on Al_2O_3 : Strong Cluster Size Dependence Linked to Preferred Catalyst Morphologies. <i>ACS Catalysis</i> , 2017, 7, 3322-3335.	5.5	124
12	Mysteries of Metals in Metalloenzymes. <i>Accounts of Chemical Research</i> , 2014, 47, 3110-3117.	7.6	114
13	Ensemble-Average Representation of Pt Clusters in Conditions of Catalysis Accessed through GPU Accelerated Deep Neural Network Fitting Global Optimization. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 6213-6226.	2.3	106
14	Photoelectron spectroscopy and ab initio study of the doubly antiaromatic B_6^{2-} dianion in the LiB_6 cluster. <i>Journal of Chemical Physics</i> , 2005, 122, 054313.	1.2	103
15	Boron Switch for Selectivity of Catalytic Dehydrogenation on Size-Selected Pt Clusters on Al_2O_3 . <i>Journal of the American Chemical Society</i> , 2017, 139, 11568-11575.	6.6	103
16	Visible-Light-Induced Olefin Activation Using 3D Aromatic Boron-Rich Cluster Photooxidants. <i>Journal of the American Chemical Society</i> , 2016, 138, 6952-6955.	6.6	95
17	Dodecaborane-Based Dopants Designed to Shield Anion Electrostatics Lead to Increased Carrier Mobility in a Doped Conjugated Polymer. <i>Advanced Materials</i> , 2019, 31, e1805647.	11.1	90
18	Artificial Photosynthesis on TiO_2 -Passivated InP Nanopillars. <i>Nano Letters</i> , 2015, 15, 6177-6181.	4.5	86

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19	Why Urea Eliminates Ammonia Rather than Hydrolyzes in Aqueous Solution. <i>Journal of Physical Chemistry B</i> , 2007, 111, 720-730.	1.2	85
20	Catalytic Mechanism and Performance of Computationally Designed Enzymes for Kemp Elimination. <i>Journal of the American Chemical Society</i> , 2008, 130, 15907-15915.	6.6	83
21	CO ₂ Hydrogenation to Formate and Formic Acid by Bimetallic Palladium-Copper Hydride Clusters. <i>Journal of the American Chemical Society</i> , 2020, 142, 7930-7936.	6.6	79
22	Why Boron Nitride is such a Selective Catalyst for the Oxidative Dehydrogenation of Propane. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 16527-16535.	7.2	75
23	B ₁₃ ⁺ : A Photodriven Molecular Wankel Engine. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 8512-8515.	7.2	72
24	Dynamics of Subnanometer Pt Clusters Can Break the Scaling Relationships in Catalysis. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 460-467.	2.1	72
25	Local Fluxionality of Surface-Deposited Cluster Catalysts: The Case of Pt ₇ on Al ₂ O ₃ . <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 1696-1702.	2.1	69
26	Origin of Extraordinary Stability of Square-Planar Carbon Atoms in Surface Carbides of Cobalt and Nickel. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 5312-5316.	7.2	67
27	H ₂ O _n Clusters: Microsolvation of the Hydrogen Atom via Molecular ab Initio Gradient Embedded Genetic Algorithm (GEGA). <i>Journal of Physical Chemistry A</i> , 2010, 114, 12591-12599.	1.1	66
28	Flattening the B ₆ H ₆ -Octahedron. Ab Initio Prediction of a New Family of Planar All-Boron Aromatic Molecules. <i>Journal of the American Chemical Society</i> , 2003, 125, 10786-10787.	6.6	64
29	Molecular Basis for Nanoscopic Membrane Curvature Generation from Quantum Mechanical Models and Synthetic Transporter Sequences. <i>Journal of the American Chemical Society</i> , 2012, 134, 19207-19216.	6.6	64
30	Computational Design of Clusters for Catalysis. <i>Annual Review of Physical Chemistry</i> , 2018, 69, 377-400.	4.8	59
31	Mechanism of CO ₂ Photocatalytic Reduction to Methane and Methanol on Defected Anatase TiO ₂ (101): A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2019, 123, 3505-3511.	1.5	57
32	Installation of internal electric fields by non-redox active cations in transition metal complexes. <i>Chemical Science</i> , 2019, 10, 10135-10142.	3.7	55
33	Photochemistry of DNA Fragments via Semiclassical Nonadiabatic Dynamics. <i>Journal of Physical Chemistry B</i> , 2010, 114, 12116-12128.	1.2	53
34	PtZnH ₅ ⁺ , A η^5 -Aromatic Cluster. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 1596-1601.	2.1	52
35	Theoretical study of hydrogenation of the doubly aromatic B ₇ η^7 cluster. <i>Journal of Molecular Modeling</i> , 2006, 12, 569-576.	0.8	49
36	Dynamic Phase Diagram of Catalytic Surface of Hexagonal Boron Nitride under Conditions of Oxidative Dehydrogenation of Propane. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 20-25.	2.1	49

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37	Cu,Zn-Superoxide Dismutase without Zn Is Folded but Catalytically Inactive. <i>Journal of Molecular Biology</i> , 2014, 426, 4112-4124.	2.0	47
38	Oxygen Vacancies of Anatase(101): Extreme Sensitivity to the Density Functional Theory Method. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2889-2895.	2.3	47
39	Mystery of Three Borides: Differential Metal-Boron Bonding Governing Superhard Structures. <i>Chemistry of Materials</i> , 2017, 29, 9892-9896.	3.2	45
40	The Golden Crown: A Single Au Atom that Boosts the CO Oxidation Catalyzed by a Palladium Cluster on Titania Surfaces. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 2250-2255.	2.1	42
41	(Photo)Electrocatalytic CO ₂ Reduction at the Defective Anatase TiO ₂ (101) Surface. <i>ACS Catalysis</i> , 2020, 10, 4048-4058.	5.5	42
42	AFFCK: Adaptive Force-Field-Assisted <i>ab Initio</i> Coalescence Kick Method for Global Minimum Search. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2385-2393.	2.3	41
43	Alloying Pt Sub-nano-clusters with Boron: Sintering Preventative and Coke Antagonist?. <i>ACS Catalysis</i> , 2015, 5, 5719-5727.	5.5	41
44	Prediction of Two-Dimensional Phase of Boron with Anisotropic Electric Conductivity. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 1224-1228.	2.1	41
45	SmB ₆ Cluster Anion: Covalency Involving f Orbitals. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1849-1854.	1.1	40
46	Quantified electrostatic preorganization in enzymes using the geometry of the electron charge density. <i>Chemical Science</i> , 2017, 8, 5010-5018.	3.7	40
47	Coking-Resistant Sub-Nano Dehydrogenation Catalysts: Pt _n Sn _x /SiO ₂ (<i>n</i> = 4, 7). <i>ACS Catalysis</i> , 2020, 10, 4543-4558.	5.5	40
48	Local Electric Fields As a Natural Switch of Heme-Iron Protein Reactivity. <i>ACS Catalysis</i> , 2021, 11, 6534-6546.	5.5	40
49	Lithium cluster anions: Photoelectron spectroscopy and <i>ab initio</i> calculations. <i>Journal of Chemical Physics</i> , 2011, 134, 044322.	1.2	38
50	Surface-supported cluster catalysis: Ensembles of metastable states run the show. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2019, 9, e1420.	6.2	36
51	Ambient methane functionalization initiated by electrochemical oxidation of a vanadium (V)-oxo dimer. <i>Nature Communications</i> , 2020, 11, 3686.	5.8	36
52	Structural Rearrangements of Subnanometer Cu Oxide Clusters Govern Catalytic Oxidation. <i>ACS Catalysis</i> , 2020, 10, 5309-5317.	5.5	36
53	Germanium as key dopant to boost the catalytic performance of small platinum clusters for alkane dehydrogenation. <i>Journal of Catalysis</i> , 2019, 374, 93-100.	3.1	35
54	Metal-Dependent Activity of Fe and Ni Acireductone Dioxygenases: How Two Electrons Reroute the Catalytic Pathway. <i>Journal of Molecular Biology</i> , 2013, 425, 3007-3018.	2.0	34

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55	Pt ₈ cluster on alumina under a pressure of hydrogen: Support-dependent reconstruction from first-principles global optimization. <i>Journal of Chemical Physics</i> , 2019, 151, 194703.	1.2	34
56	Persistent Covalency and Planarity in the B _n Al ₆ ²⁺ and LiB _n Al ₆ ⁺ (n = 0-6) Cluster Ions. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 2046-2051.	2.1	33
57	Selected AB ₄ ⁺ (A = C, Si, Ge; B = Al, Ga, In) ions: a battle between covalency and aromaticity, and prediction of square planar Si in SiIn ₄ ⁺ . <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 14815.	1.3	33
58	Cu ₃ C ₄ : A New Sandwich Molecule with Two Revolving C ₂₂ -Units. <i>Journal of Physical Chemistry A</i> , 2005, 109, 562-570.	1.1	32
59	Structure, stability, and mobility of small Pd clusters on the stoichiometric and defective TiO ₂ (110) surfaces. <i>Journal of Chemical Physics</i> , 2011, 135, 174702.	1.2	32
60	Nanoalloying MgO-Deposited Pt Clusters with Si To Control the Selectivity of Alkane Dehydrogenation. <i>ACS Catalysis</i> , 2018, 8, 8346-8356.	5.5	32
61	Rutile-Deposited Pt-Pd clusters: A Hypothesis Regarding the Stability at 50/50 Ratio. <i>ACS Catalysis</i> , 2014, 4, 3570-3580.	5.5	30
62	Arachno, Nido, and Closo Aromatic Isomers of the Li ₆ B ₆ H ₆ Molecule. <i>Inorganic Chemistry</i> , 2004, 43, 3588-3592.	1.9	28
63	On the structure and chemical bonding of Si ₆ ²⁺ and Si ₆ ⁺ in NaSi ₆ ⁺ upon Na ⁺ coordination. <i>Journal of Chemical Physics</i> , 2006, 124, 124305.	1.2	28
64	Rigid substructure search. <i>Bioinformatics</i> , 2011, 27, 1327-1329.	1.8	28
65	Why Urease Is a Di-Nickel Enzyme whereas the CcrA ⁺ -Lactamase Is a Di-Zinc Enzyme. <i>Journal of Physical Chemistry B</i> , 2012, 116, 10649-10656.	1.2	27
66	Microscopic Study of Atomic Layer Deposition of TiO ₂ on GaAs and Its Photocatalytic Application. <i>Chemistry of Materials</i> , 2015, 27, 7977-7981.	3.2	27
67	Charge Density in Enzyme Active Site as a Descriptor of Electrostatic Preorganization. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2367-2373.	2.5	27
68	Hybrid Dynamics Simulation Engine for Metalloproteins. <i>Biophysical Journal</i> , 2012, 103, 767-776.	0.2	26
69	Direct Look at the Electric Field in Ketosteroid Isomerase and Its Variants. <i>ACS Catalysis</i> , 2020, 10, 9915-9924.	5.5	26
70	Global Activity Search Uncovers Reaction Induced Concomitant Catalyst Restructuring for Alkane Dissociation on Model Pt Catalysts. <i>ACS Catalysis</i> , 2021, 11, 1877-1885.	5.5	26
71	Franck-Condon Tuning of Optical Cycling Centers by Organic Functionalization. <i>Physical Review Letters</i> , 2021, 126, 123002.	2.9	26
72	Preparation of Size- and Composition-Controlled Pt _n Sn _x /SiO ₂ (n = 4, 7, 24) Bimetallic Model Catalysts with Atomic Layer Deposition. <i>Journal of Physical Chemistry C</i> , 2019, 123, 16194-16209.	1.5	25

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73	Sn-modification of Pt7/alumina model catalysts: Suppression of carbon deposition and enhanced thermal stability. <i>Journal of Chemical Physics</i> , 2020, 152, 024702.	1.2	25
74	Fjord-Edge Graphene Nanoribbons with Site-Specific Nitrogen Substitution. <i>Journal of the American Chemical Society</i> , 2020, 142, 18093-18102.	6.6	24
75	Interpreting the Operando XANES of Surface-Supported Subnanometer Clusters: When Fluxionality, Oxidation State, and Size Effect Fight. <i>Journal of Physical Chemistry C</i> , 2020, 124, 10057-10066.	1.5	24
76	Advances in optimizing enzyme electrostatic preorganization. <i>Current Opinion in Structural Biology</i> , 2022, 72, 1-8.	2.6	24
77	Acid-Base Control of Valency within Carboranedithiol Self-Assembled Monolayers: Molecules Do the Can-Can. <i>ACS Nano</i> , 2018, 12, 2211-2221.	7.3	23
78	How Metal Substitution Affects the Enzymatic Activity of Catechol-O-Methyltransferase. <i>PLoS ONE</i> , 2012, 7, e47172.	1.1	23
79	Origin of the Activity Drop with the E50D Variant of Catalytic Antibody 34E4 for Kemp Elimination. <i>Journal of Physical Chemistry B</i> , 2009, 113, 497-504.	1.2	22
80	Visualizing the Dynamic Metalation State of New Delhi Metallo- β -lactamase-1 in Bacteria Using a Reversible Fluorescent Probe. <i>Journal of the American Chemical Society</i> , 2021, 143, 8314-8323.	6.6	22
81	On the Mechanism and Rate of Spontaneous Decomposition of Amino Acids. <i>Journal of Physical Chemistry B</i> , 2011, 115, 13624-13632.	1.2	21
82	The Role of the Flexible L43-S54 Protein Loop in the CcrA Metallo- β -lactamase in Binding Structurally Dissimilar β -Lactam Antibiotics. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 730-737.	2.3	21
83	Photoelectron spectroscopic and theoretical study of the $[\text{HPd}(\beta\text{-H}_2)]^{\ominus}$ cluster anion. <i>Journal of Chemical Physics</i> , 2015, 143, 094307.	1.2	21
84	Oxidative Dehydrogenation of Cyclohexane by Cu vs Pd Clusters: Selectivity Control by Specific Cluster Dynamics. <i>ChemCatChem</i> , 2020, 12, 1307-1315.	1.8	21
85	Double π -Aromaticity in a Surface-Deposited Cluster: Pd ₄ on TiO ₂ (110). <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 751-754.	2.1	20
86	Hydrogen Evolution on Restructured B-Rich WB: Metastable Surface States and Isolated Active Sites. <i>ACS Catalysis</i> , 2020, 10, 13867-13877.	5.5	20
87	Optical Cycling Functionalization of Arenes. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 3989-3995.	2.1	20
88	Alloying with Sn Suppresses Sintering of Size-Selected Subnano Pt Clusters on SiO ₂ with and without Adsorbates. <i>Chemistry of Materials</i> , 2020, 32, 8595-8605.	3.2	19
89	Reagent-Triggered Isomerization of Fluxional Cluster Catalyst via Dynamic Coupling. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 3089-3094.	2.1	19
90	Computational Treatment of Metalloproteins. <i>Journal of Physical Chemistry B</i> , 2015, 119, 5945-5956.	1.2	18

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91	Pt ⁺ Zn Clusters on Stoichiometric MgO(100) and TiO ₂ (110): Dramatically Different Sintering Behavior. <i>Journal of Physical Chemistry C</i> , 2015, 119, 6047-6055.	1.5	17
92	Diborane Interactions with Pt ₇ /Alumina: Preparation of Size-Controlled Borated Pt Model Catalysts. <i>Journal of Physical Chemistry C</i> , 2018, 122, 1631-1644.	1.5	17
93	Geometry Change in a Series of Zirconium Compounds during Lactide Ring-Opening Polymerization. <i>Organometallics</i> , 2018, 37, 4040-4047.	1.1	17
94	Histone Deacetylase 8: Characterization of Physiological Divalent Metal Catalysis. <i>Journal of Physical Chemistry B</i> , 2016, 120, 5884-5895.	1.2	16
95	Machine Learning to Predict Diels-Alder Reaction Barriers from the Reactant State Electron Density. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6203-6213.	2.3	16
96	Pure and Zn-doped Pt clusters go flat and upright on MgO(100). <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 26436-26442.	1.3	15
97	Electrostatic regulation of blue copper sites. <i>Chemical Science</i> , 2021, 12, 11406-11413.	3.7	15
98	Tug of war between AO-hybridization and aromaticity in dictating structures of Li-doped alkali clusters. <i>Chemical Physics Letters</i> , 2012, 533, 1-5.	1.2	14
99	Assessing the Bonding Properties of Individual Molecular Orbitals. <i>Journal of Physical Chemistry A</i> , 2015, 119, 12862-12867.	1.1	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. <i>Biochemistry</i> , 2015, 54, 6490-6500.	1.2	13
101	When Fluxionality Beats Size Selection: Acceleration of Ostwald Ripening of Sub-Nano Clusters. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 11973-11982.	7.2	13
102	The PtAl ⁺ and PtAl ₂ ⁺ anions: Theoretical and photoelectron spectroscopic characterization. <i>Journal of Chemical Physics</i> , 2014, 140, 164316.	1.2	12
103	Metallic and Magnetic 2D Materials Containing Planar Tetracoordinated C and N. <i>Journal of Physical Chemistry C</i> , 2016, 120, 21685-21690.	1.5	12
104	Multicenter Bonding Effects in Oxygen Vacancy in the Bulk and on the Surface of MgO. <i>Journal of Physical Chemistry C</i> , 2018, 122, 11933-11937.	1.5	12
105	Heterogeneity in Local Chemical Bonding Explains Spectral Broadening in Quantum Dots with Cu Impurities. <i>Journal of Physical Chemistry C</i> , 2019, 123, 5705-5713.	1.5	12
106	Vibrational predissociation spectra of the , n=3-10, 12 clusters: Even-odd alternation in the core ion. <i>International Journal of Mass Spectrometry</i> , 2009, 283, 94-99.	0.7	11
107	Predictive methods for computational metalloenzyme redesign - a test case with carboxypeptidase A. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 31744-31756.	1.3	11
108	Designing clusters for heterogeneous catalysis. <i>Physics Today</i> , 2019, 72, 38-43.	0.3	11

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109	Global Optimization of Adsorbate Covered Supported Cluster Catalysts: The Case of Pt ₇ H ₁₀ CH ₃ on Î±-Al ₂ O ₃ . ChemCatChem, 2020, 12, 762-770.	1.8	11
110	High-temperature phonon-mediated superconductivity in monolayer Mg ₂ B ₄ C ₂ . Npj Quantum Materials, 2022, 7, .	1.8	11
111	Hydrogen Trioxide Anion: A Possible Atmospheric Intermediate and Path to Oxygen-Rich Molecules. Journal of Physical Chemistry A, 2003, 107, 1203-1206.	1.1	10
112	Co ²⁺ acireductone dioxygenase: Fe ²⁺ mechanism, Ni ²⁺ mechanism, or something else?. Chemical Physics Letters, 2014, 604, 77-82.	1.2	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.	1.5	10
114	Fluxionality of Subnano Clusters Reshapes the Activity Volcano of Electrocatalysis. ChemCatChem, 2022, 14, .	1.8	10
115	Promiscuous DNA alkyladenine glycosylase dramatically favors a bound lesion over undamaged adenine. Biophysical Chemistry, 2010, 152, 118-127.	1.5	9
116	The mechanism of the Pd-catalyzed formation of coumarins: a theoretical study. Physical Chemistry Chemical Physics, 2015, 17, 1347-1353.	1.3	9
117	Strain to alter the covalency and superconductivity in transition metal diborides. Journal of Materials Chemistry C, 2019, 7, 10700-10707.	2.7	9
118	Heterogeneous Intramolecular Electric Field as a Descriptor of Diels-Alder Reactivity. Journal of Physical Chemistry A, 2021, 125, 1289-1298.	1.1	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.	1.2	9
120	Ensemble representation of catalytic interfaces: soloists, orchestras, and everything in-between. Chemical Science, 2022, 13, 8003-8016.	3.7	9
121	Photoinduced Carrier Generation and Distribution in Solution-Deposited Titanyl Phthalocyanine Monolayers. Chemistry of Materials, 2019, 31, 10109-10116.	3.2	8
122	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.	5.5	8
123	Can Fluxionality of Subnanometer Cluster Catalysts Solely Cause Non-Arrhenius Behavior in Catalysis?. Journal of Physical Chemistry C, 2020, 124, 19556-19562.	1.5	8
124	Toxic and Physiological Metal Uptake and Release by Human Serum Transferrin. Biophysical Journal, 2020, 118, 2979-2988.	0.2	8
125	Stoichiometry-controllable optical defects in Cu _x In _{2-x} S _y quantum dots for energy harvesting. Journal of Materials Chemistry A, 2020, 8, 12556-12565.	5.2	8
126	Influence of Terminal Carboxyl Groups on the Structure and Reactivity of Functionalized <i>m</i> -Carboranethiolate Self-Assembled Monolayers. Chemistry of Materials, 2020, 32, 6800-6809.	3.2	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, .	3.3	8
128	Photoelectron spectroscopic and computational study of the PtMgH _{3,5} ⁺ cluster anions. Physical Chemistry Chemical Physics, 2016, 18, 19345-19349.	1.3	7
129	Photooxidative Generation of Dodecaborate-Based Weakly Coordinating Anions. Inorganic Chemistry, 2019, 58, 10516-10526.	1.9	7
130	Uncovered Dynamic Coupling Resolves the Ambiguous Mechanism of Phenylalanine Hydroxylase Oxygen Binding. Journal of Physical Chemistry B, 2019, 123, 4534-4539.	1.2	7
131	Why Boron Nitride is such a Selective Catalyst for the Oxidative Dehydrogenation of Propane. Angewandte Chemie, 2020, 132, 16670-16678.	1.6	7
132	Recent Innovations in Solid-State and Molecular Qubits for Quantum Information Applications. Journal of Physical Chemistry B, 2021, 125, 12111-12114.	1.2	7
133	Oxidation Dynamics of Supported Catalytic Cu Clusters: Coupling to Fluxionality. ACS Catalysis, 2022, 12, 818-827.	5.5	7
134	Theoretical Perspective on <i>Operando</i> Spectroscopy of Fluxional Nanocatalysts. Journal of Physical Chemistry Letters, 2022, 13, 4321-4334.	2.1	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.	3.2	6
136	The Case for Enzymatic Competitive Metal Affinity Methods. ACS Catalysis, 2020, 10, 2298-2307.	5.5	6
137	Titration of a Rapid, Coarse-Grained Quasi-All-Atom Constant pH Molecular Dynamics Framework. Journal of Chemical Theory and Computation, 2021, 17, 4538-4549.	2.3	6
138	Histidine-Mediated Ion Specific Effects Enable Salt Tolerance of a Pore-Forming Marine Antimicrobial Peptide. Angewandte Chemie - International Edition, 2022, , .	7.2	6
139	Electron Density Geometry and the Quantum Theory of Atoms in Molecules. Journal of Physical Chemistry A, 2021, 125, 10622-10631.	1.1	6
140	Computational design and characterisation of artificial enzymes for Kemp elimination. Molecular Simulation, 2011, 37, 557-571.	0.9	5
141	The same in the bulk but different as clusters: X ₃ Y ₃ (X=B, Al, Ga; Y=P, As). Chemical Physics Letters, 2013, 588, 37-42.	1.2	5
142	π-Aromaticity in polyhydride complexes of Ru, Ir, Os, and Pt. Physical Chemistry Chemical Physics, 2016, 18, 11644-11652.	1.3	5
143	Dynamical Bonding Driving Mixed Valency in a Metal Boride. Angewandte Chemie - International Edition, 2020, 59, 10996-11002.	7.2	5
144	Surface chemical trapping of optical cycling centers. Physical Chemistry Chemical Physics, 2021, 23, 211-218.	1.3	5

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145	Understanding the Hardness of Doped WB4.2. <i>Journal of Physical Chemistry C</i> , 2021, 125, 9486-9496.	1.5	5
146	Electrocatalytic Methane Functionalization with d^{0} Early Transition Metals Under Ambient Conditions. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 26630-26638.	7.2	5
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