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	Advances in optimizing enzyme electrostatic preorganization. Current Opinion in Structural Biology, 2022, 72, 1-8.	5.7	24
2	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
3	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
4	Histidineâ€Mediated Ion Specific Effects Enable Salt Tolerance of a Poreâ€Forming Marine Antimicrobial Peptide. Angewandte Chemie - International Edition, 2022, , .	13.8	6
5	High-temperature phonon-mediated superconductivity in monolayer Mg2B4C2. Npj Quantum Materials, 2022, 7, .	5.2	11
6	Oxidation Dynamics of Supported Catalytic Cu Clusters: Coupling to Fluxionality. ACS Catalysis, 2022, 12, 818-827.	11.2	7
7	Theoretical Perspective on Operando Spectroscopy of Fluxional Nanocatalysts. Journal of Physical Chemistry Letters, 2022, 13, 4321-4334.	4.6	7
8	Ensemble representation of catalytic interfaces: soloists, orchestras, and everything in-between. Chemical Science, 2022, 13, 8003-8016.	7.4	9
9	Fluxionality of Subnano Clusters Reshapes the Activity Volcano of Electrocatalysis. ChemCatChem, 2022, 14, .	3.7	10
10	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
11	Surface chemical trapping of optical cycling centers. Physical Chemistry Chemical Physics, 2021, 23, 211-218.	2.8	5
12	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
13	Heterogeneous Intramolecular Electric Field as a Descriptor of Dielsâ€“Alder Reactivity. Journal of Physical Chemistry A, 2021, 125, 1289-1298.	2.5	9
14	Franck-Condon Tuning of Optical Cycling Centers by Organic Functionalization. Physical Review Letters, 2021, 126, 123002.	7.8	26
15	When Fluxionality Beats Size Selection: Acceleration of Ostwald Ripening of Subâ€Nano Clusters. Angewandte Chemie, 2021, 133, 12080-12089.	2.0	3
16	Optical Cycling Functionalization of Arenes. Journal of Physical Chemistry Letters, 2021, 12, 3989-3995.	4.6	20
17	Understanding the Hardness of Doped WB4.2. Journal of Physical Chemistry C, 2021, 125, 9486-9496.	3.1	5
18	When Fluxionality Beats Size Selection: Acceleration of Ostwald Ripening of Subâ€Nano Clusters. Angewandte Chemie - International Edition, 2021, 60, 11973-11982.	13.8	13

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19	Local Electric Fields As a Natural Switch of Heme-Iron Protein Reactivity. ACS Catalysis, 2021, 11, 6534-6546.	11.2	40
20	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
21	Regularization of least squares problems in CHARMM parameter optimization by truncated singular value decompositions. Journal of Chemical Physics, 2021, 154, 184101.	3.0	2
22	Suggesting Reviewers to Improve Your Manuscript. Journal of Physical Chemistry A, 2021, 125, 5861-5862.	2.5	0
23	Suggesting Reviewers to Improve Your Manuscript. Journal of Physical Chemistry B, 2021, 125, 7333-7334.	2.6	0
24	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
25	Suggesting Reviewers to Improve Your Manuscript. Journal of Physical Chemistry C, 2021, 125, 14493-14494.	3.1	1
26	The Art of Reviewing Manuscripts. Journal of Physical Chemistry A, 2021, 125, 6512-6513.	2.5	0
27	The Art of Reviewing Manuscripts. Journal of Physical Chemistry B, 2021, 125, 8268-8269.	2.6	0
28	The Art of Reviewing Manuscripts. Journal of Physical Chemistry C, 2021, 125, 16369-16370.	3.1	0
29	Contrasting Effects of Inhibitors Li+ and Be2+ on Catalytic Cycle of Glycogen Synthase Kinase-3Î². Journal of Physical Chemistry B, 2021, 125, 9480-9489.	2.6	0
30	Revising Manuscripts: Trying to Make Everyone Happy. Journal of Physical Chemistry B, 2021, 125, 9387-9388.	2.6	0
31	Revising Manuscripts: Trying to Make Everyone Happy. Journal of Physical Chemistry C, 2021, 125, 18087-18088.	3.1	1
32	Revising Manuscripts: Trying to Make Everyone Happy. Journal of Physical Chemistry A, 2021, 125, 7123-7124.	2.5	0
33	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
34	Electrostatic regulation of blue copper sites. Chemical Science, 2021, 12, 11406-11413.	7.4	15
35	Electrocatalytic Methane Functionalization with d⁰ Early Transition Metals Under Ambient Conditions. Angewandte Chemie - International Edition, 2021, 60, 26630-26638.	13.8	5
36	Electrocatalytic Methane Functionalization with d⁰ Early Transition Metals Under Ambient Conditions. Angewandte Chemie, 2021, 133, 26834-26842.	2.0	1

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37	Tribute to Alexander I. Boldyrev. Journal of Physical Chemistry A, 2021, 125, 9261-9263.	2.5	0
38	Recent Innovations in Solid-State and Molecular Qubits for Quantum Information Applications. Journal of Physical Chemistry C, 2021, 125, 24285-24288.	3.1	0
39	Recent Innovations in Solid-State and Molecular Qubits for Quantum Information Applications. Journal of Physical Chemistry Letters, 2021, 12, 10742-10745.	4.6	5
40	Recent Innovations in Solid-State and Molecular Qubits for Quantum Information Applications. Journal of Physical Chemistry A, 2021, 125, 9567-9570.	2.5	0
41	Recent Innovations in Solid-State and Molecular Qubits for Quantum Information Applications. Journal of Physical Chemistry B, 2021, 125, 12111-12114.	2.6	7
42	Electron Density Geometry and the Quantum Theory of Atoms in Molecules. Journal of Physical Chemistry A, 2021, 125, 10622-10631.	2.5	6
43	Global Optimization of Adsorbate Covered Supported Cluster Catalysts: The Case of Pt₇H₁₀CH₃ on Î±â€Al₂O₃. ChemCatChem, 2020, 12, 762-770.	3.7	11
44	Oxidative Dehydrogenation of Cyclohexane by Cu vs Pd Clusters: Selectivity Control by Specific Cluster Dynamics. ChemCatChem, 2020, 12, 1307-1315.	3.7	21
45	Towards a Single Chemical Model for Understanding Lanthanide Hexaborides. Angewandte Chemie, 2020, 132, 22873-22878.	2.0	2
46	Towards a Single Chemical Model for Understanding Lanthanide Hexaborides. Angewandte Chemie - International Edition, 2020, 59, 22684-22689.	13.8	0
47	Hydrogen Evolution on Restructured B-Rich WB: Metastable Surface States and Isolated Active Sites. ACS Catalysis, 2020, 10, 13867-13877.	11.2	20
48	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
49	Direct Look at the Electric Field in Ketosteroid Isomerase and Its Variants. ACS Catalysis, 2020, 10, 9915-9924.	11.2	26
50	Ambient methane functionalization initiated by electrochemical oxidation of a vanadium (V)-oxo dimer. Nature Communications, 2020, 11, 3686.	12.8	36
51	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
52	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
53	Fjord-Edge Graphene Nanoribbons with Site-Specific Nitrogen Substitution. Journal of the American Chemical Society, 2020, 142, 18093-18102.	13.7	24
54	Toxic and Physiological Metal Uptake and Release by Human Serum Transferrin. Biophysical Journal, 2020, 118, 2979-2988.	0.5	8

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55	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
56	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
57	Coking-Resistant Sub-Nano Dehydrogenation Catalysts: Pt_nSn_x/SiO₂ (n = 4, 7). ACS Catalysis, 2020, 10, 4543-4558.	11.2	40
58	Dynamical Bonding Driving Mixed Valency in a Metal Boride. Angewandte Chemie - International Edition, 2020, 59, 10996-11002.	13.8	5
59	Reagent-Triggered Isomerization of Fluxional Cluster Catalyst via Dynamic Coupling. Journal of Physical Chemistry Letters, 2020, 11, 3089-3094.	4.6	19
60	(Photo)Electrocatalytic CO₂ Reduction at the Defective Anatase TiO₂ (101) Surface. ACS Catalysis, 2020, 10, 4048-4058.	11.2	42
61	Why Boron Nitride is such a Selective Catalyst for the Oxidative Dehydrogenation of Propane. Angewandte Chemie, 2020, 132, 16670-16678.	2.0	7
62	Characteristics of Impactful Computational Contributions to The Journal of Physical Chemistry C. Journal of Physical Chemistry C, 2020, 124, 13509-13510.	3.1	3
63	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
64	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
65	Ensembles of Metastable States Govern Heterogeneous Catalysis on Dynamic Interfaces. Accounts of Chemical Research, 2020, 53, 447-458.	15.6	134
66	The Case for Enzymatic Competitive Metal Affinity Methods. ACS Catalysis, 2020, 10, 2298-2307.	11.2	6
67	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
68	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
69	Dynamical Bonding Driving Mixed Valency in a Metal Boride. Angewandte Chemie, 2020, 132, 11089-11095.	2.0	4
70	Structural Rearrangements of Subnanometer Cu Oxide Clusters Govern Catalytic Oxidation. ACS Catalysis, 2020, 10, 5309-5317.	11.2	36
71	Designing clusters for heterogeneous catalysis. Physics Today, 2019, 72, 38-43.	0.3	11
72	Strain to alter the covalency and superconductivity in transition metal diborides. Journal of Materials Chemistry C, 2019, 7, 10700-10707.	5.5	9

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73	Installation of internal electric fields by non-redox active cations in transition metal complexes. Chemical Science, 2019, 10, 10135-10142.	7.4	55
74	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
75	Photooxidative Generation of Dodecaborate-Based Weakly Coordinating Anions. Inorganic Chemistry, 2019, 58, 10516-10526.	4.0	7
76	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
77	Surfaceâ€supported cluster catalysis: Ensembles of metastable states run the show. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1420.	14.6	36
78	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
79	Uncovered Dynamic Coupling Resolves the Ambiguous Mechanism of Phenylalanine Hydroxylase Oxygen Binding. Journal of Physical Chemistry B, 2019, 123, 4534-4539.	2.6	7
80	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
81	Resonant and Selective Excitation of Photocatalytically Active Defect Sites in TiO₂. ACS Applied Materials & Interfaces, 2019, 11, 10351-10355.	8.0	1
82	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
83	Photoinduced Carrier Generation and Distribution in Solution-Deposited Titanyl Phthalocyanine Monolayers. Chemistry of Materials, 2019, 31, 10109-10116.	6.7	8
84	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
85	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
86	Dynamics of Subnanometer Pt Clusters Can Break the Scaling Relationships in Catalysis. Journal of Physical Chemistry Letters, 2019, 10, 460-467.	4.6	72
87	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
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.	3.1	10
89	Computational Design of Clusters for Catalysis. Annual Review of Physical Chemistry, 2018, 69, 377-400.	10.8	59
90	Acidâ€“Base Control of Valency within Carboranedithiol Self-Assembled Monolayers: Molecules Do the Can-Can. ACS Nano, 2018, 12, 2211-2221.	14.6	23

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91	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
92	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
93	Geometry Change in a Series of Zirconium Compounds during Lactide Ring-Opening Polymerization. Organometallics, 2018, 37, 4040-4047.	2.3	17
94	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
95	Nanoalloying MgO-Deposited Pt Clusters with Si To Control the Selectivity of Alkane Dehydrogenation. ACS Catalysis, 2018, 8, 8346-8356.	11.2	32
96	Fluxionality of Catalytic Clusters: When It Matters and How to Address It. ACS Catalysis, 2017, 7, 1905-1911.	11.2	150
97	Prediction of Two-Dimensional Phase of Boron with Anisotropic Electric Conductivity. Journal of Physical Chemistry Letters, 2017, 8, 1224-1228.	4.6	41
98	SmB₆^{â€“} Cluster Anion: Covalency Involving f Orbitals. Journal of Physical Chemistry A, 2017, 121, 1849-1854.	2.5	40
99	Quantified electrostatic preorganization in enzymes using the geometry of the electron charge density. Chemical Science, 2017, 8, 5010-5018.	7.4	40
100	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
101	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
102	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
103	Mystery of Three Borides: Differential Metalâ€“Boron Bonding Governing Superhard Structures. Chemistry of Materials, 2017, 29, 9892-9896.	6.7	45
104	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
105	Histone Deacetylase 8: Characterization of Physiological Divalent Metal Catalysis. Journal of Physical Chemistry B, 2016, 120, 5884-5895.	2.6	16
106	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
107	Metallic and Magnetic 2D Materials Containing Planar Tetracoordinated C and N. Journal of Physical Chemistry C, 2016, 120, 21685-21690.	3.1	12
108	Use of QM/DMD as a Multiscale Approach to Modeling Metalloenzymes. Methods in Enzymology, 2016, 577, 319-339.	1.0	1

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109	Photoelectron spectroscopic and computational study of the PtMgH_{3,5}^{â˜’} cluster anions. Physical Chemistry Chemical Physics, 2016, 18, 19345-19349.	2.8	7
110	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
111	4th International Conference on Chemical Bonding. Journal of Physical Chemistry A, 2016, 120, 9353-9356.	2.5	1
112	Predictive methods for computational metalloenzyme redesign â€“ a test case with carboxypeptidase A. Physical Chemistry Chemical Physics, 2016, 18, 31744-31756.	2.8	11
113	Ïƒ-Aromaticity in polyhydride complexes of Ru, Ir, Os, and Pt. Physical Chemistry Chemical Physics, 2016, 18, 11644-11652.	2.8	5
114	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
115	Photoelectron spectroscopic and theoretical study of the [HPd(Î·2-H2)]â˜’ cluster anion. Journal of Chemical Physics, 2015, 143, 094307.	3.0	21
116	Assessing the Bonding Properties of Individual Molecular Orbitals. Journal of Physical Chemistry A, 2015, 119, 12862-12867.	2.5	14
117	The mechanism of the Pd-catalyzed formation of coumarins: a theoretical study. Physical Chemistry Chemical Physics, 2015, 17, 1347-1353.	2.8	9
118	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
119	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
120	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
121	Computational Treatment of Metalloproteins. Journal of Physical Chemistry B, 2015, 119, 5945-5956.	2.6	18
122	Artificial Photosynthesis on TiO₂-Passivated InP Nanopillars. Nano Letters, 2015, 15, 6177-6181.	9.1	86
123	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
124	Alloying Pt Sub-nano-clusters with Boron: Sintering Preventative and Coke Antagonist?. ACS Catalysis, 2015, 5, 5719-5727.	11.2	41
125	Microscopic Study of Atomic Layer Deposition of TiO₂ on GaAs and Its Photocatalytic Application. Chemistry of Materials, 2015, 27, 7977-7981.	6.7	27
126	The PtAlâ˜’and PtAl2â˜’anions: Theoretical and photoelectron spectroscopic characterization. Journal of Chemical Physics, 2014, 140, 164316.	3.0	12

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127	Cu,Zn-Superoxide Dismutase without Zn Is Folded but Catalytically Inactive. Journal of Molecular Biology, 2014, 426, 4112-4124.	4.2	47
128	Rutile-Deposited Ptâ€“Pd clusters: A Hypothesis Regarding the Stability at 50/50 Ratio. ACS Catalysis, 2014, 4, 3570-3580.	11.2	30
129	PtZnH₅^{â€“}, A Ïƒ-Aromatic Cluster. Journal of Physical Chemistry Letters, 2014, 5, 1596-1601.	4.6	52
130	Pure and Zn-doped Pt clusters go flat and upright on MgO(100). Physical Chemistry Chemical Physics, 2014, 16, 26436-26442.	2.8	15
131	Mysteries of Metals in Metalloenzymes. Accounts of Chemical Research, 2014, 47, 3110-3117.	15.6	114
132	Co2+ acireductone dioxygenase: Fe2+ mechanism, Ni2+ mechanism, or something else?. Chemical Physics Letters, 2014, 604, 77-82.	2.6	10
133	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
134	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
135	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
136	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
137	Guest Editorial: The 3rd Transatlantic Frontiers in Chemistry Symposium. Chemistry - A European Journal, 2013, 19, 15777-15783.	3.3	2
138	B₁₃⁺: A Photodriven Molecular Wankel Engine. Angewandte Chemie - International Edition, 2012, 51, 8512-8515.	13.8	72
139	Hybrid Dynamics Simulation Engine for Metalloproteins. Biophysical Journal, 2012, 103, 767-776.	0.5	26
140	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
141	Double Ïƒ-Aromaticity in a Surface-Deposited Cluster: Pd₄ on TiO₂ (110). Journal of Physical Chemistry Letters, 2012, 3, 751-754.	4.6	20
142	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
143	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
144	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

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145	How Metal Substitution Affects the Enzymatic Activity of Catechol-O-Methyltransferase. PLoS ONE, 2012, 7, e47172.	2.5	23
146	Lithium cluster anions: Photoelectron spectroscopy and ab initio calculations. Journal of Chemical Physics, 2011, 134, 044322.	3.0	38
147	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
148	On the Mechanism and Rate of Spontaneous Decomposition of Amino Acids. Journal of Physical Chemistry B, 2011, 115, 13624-13632.	2.6	21
149	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
150	Computational design and characterisation of artificial enzymes for Kemp elimination. Molecular Simulation, 2011, 37, 557-571.	2.0	5
151	Rigid substructure search. Bioinformatics, 2011, 27, 1327-1329.	4.1	28
152	Promiscuous DNA alkyladenine glycosylase dramatically favors a bound lesion over undamaged adenine. Biophysical Chemistry, 2010, 152, 118-127.	2.8	9
153	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
154	Photochemistry of DNA Fragments via Semiclassical Nonadiabatic Dynamics. Journal of Physical Chemistry B, 2010, 114, 12116-12128.	2.6	53
155	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
156	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
157	Catalytic Mechanism and Performance of Computationally Designed Enzymes for Kemp Elimination. Journal of the American Chemical Society, 2008, 130, 15907-15915.	13.7	83
158	Why Urea Eliminates Ammonia Rather than Hydrolyzes in Aqueous Solution. Journal of Physical Chemistry B, 2007, 111, 720-730.	2.6	85
159	All-boron aromatic clusters as potential new inorganic ligands and building blocks in chemistry. Coordination Chemistry Reviews, 2006, 250, 2811-2866.	18.8	588
160	Theoretical study of hydrogenation of the doubly aromatic B 7 â^’ cluster. Journal of Molecular Modeling, 2006, 12, 569-576.	1.8	49
161	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
162	Photoelectron spectroscopy andab initiostudy of the doubly antiaromatic B62â^’ dianion in the LiB6â^’ cluster. Journal of Chemical Physics, 2005, 122, 054313.	3.0	103

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163	Cu3C4-:Â A New Sandwich Molecule with Two Revolving C22-Units. Journal of Physical Chemistry A, 2005, 109, 562-570.	2.5	32
164	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
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