

Jun Li

List of Publications by Year in descending order

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479
papers

52,832
citations

2832

97
h-index

1964

213
g-index

517
all docs

517
docs citations

517
times ranked

35247
citing authors

#	ARTICLE	IF	CITATIONS
1	CO oxidation on MXene (Mo ₂ CS ₂) supported single-atom catalyst: A termolecular Eley-Rideal mechanism. Chinese Chemical Letters, 2023, 34, 107412.	4.8	13
2	In situ encapsulated subnanometric CoO clusters within silicalite-1 zeolite for efficient propane dehydrogenation. AIChE Journal, 2022, 68, e17451.	1.8	29
3	Scalable two-step annealing method for preparing ultra-high-density single-atom catalyst libraries. Nature Nanotechnology, 2022, 17, 174-181.	15.6	279
4	Size sensitivity of supported Ru catalysts for ammonia synthesis: From nanoparticles to subnanometric clusters and atomic clusters. Chem, 2022, 8, 749-768.	5.8	59
5	A polyoxometalate cluster-based single-atom catalyst for NH ₃ synthesis via an enzymatic mechanism. Journal of Materials Chemistry A, 2022, 10, 6165-6177.	5.2	23
6	Ladder Oxygenation of Group VIII Metal Clusters and the Formation of Metalloxocubes M ₁₃ O ₈ ⁺ . Journal of Physical Chemistry Letters, 2022, 13, 733-739.	2.1	5
7	Theoretical investigation on hydrogenation of dinitrogen triggered by singly dispersed bimetallic sites. Journal of Materials Chemistry A, 2022, 10, 6146-6152.	5.2	10
8	Uncovering mechanisms of RT-LAMP colorimetric SARS-CoV-2 detection to improve assay reliability. Analytical Methods, 2022, 14, 378-382.	1.3	6
9	Infrared spectroscopic signature of the structural diversity of the water heptamer. Cell Reports Physical Science, 2022, 3, 100748.	2.8	9
10	Few-Atom Pt Ensembles Enable Efficient Catalytic Cyclohexane Dehydrogenation for Hydrogen Production. Journal of the American Chemical Society, 2022, 144, 3535-3542.	6.6	72
11	Au ₈ ⁺ : an Au ⁺ borozene complex. Chemical Communications, 2022, 58, 3134-3137.	2.2	6
12	Integrating Dissociative and Associative Routes for Efficient Ammonia Synthesis over a TiCN-Promoted Ru-Based Catalyst. ACS Catalysis, 2022, 12, 2651-2660.	5.5	18
13	Modification of Palladium Nanocrystals with Single Atom Platinum via an Electrochemical Self-Catalysis Strategy for Efficient Formic Acid Electrooxidation. ACS Applied Materials & Interfaces, 2022, 14, 8001-8009.	4.0	10
14	Recent progress and perspectives on single-atom catalysis. Journal of Materials Chemistry A, 2022, 10, 5670-5672.	5.2	15
15	Ultra-Efficient Americium/Lanthanide Separation through Oxidation State Control. Journal of the American Chemical Society, 2022, 144, 6383-6389.	6.6	33
16	Doping Ruthenium into Metal Matrix for Promoted pH-Universal Hydrogen Evolution. Advanced Science, 2022, 9, e2200010.	5.6	29
17	Quantum chemical studies of the electronic structures of anti-tumor agents: Au ^{III} + (L=porphine, Tj ETQq1 1 0.784314 rgBT /Over	1.1	1
18	Leaching of palladium atoms from small cluster models during Heck reactions – An experimental and theoretical study. Catalysis Communications, 2022, 165, 106441.	1.6	4

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19	Theoretical studies of MXene-supported single-atom catalysts: Os1/Ti2CS2 for low-temperature CO oxidation. <i>Science China Materials</i> , 2022, 65, 1303-1312.	3.5	10
20	On the highest oxidation states of the actinoids in AnO_4 molecules ($\text{An} = \text{Ac}, \text{Th}, \text{Pa}, \text{U}, \text{Np}, \text{Pu}, \text{Am}, \text{Cm}, \text{Bk}, \text{Cf}, \text{Es}, \text{Fm}, \text{Md}, \text{No}, \text{Lr}$). <i>Overlook</i> 1.5	1.5	0
21	An ultrastable Ti-based metallocalixarene nanocage cluster with photocatalytic amine oxidation activity. <i>Chemical Communications</i> , 2022, 58, 6028-6031.	2.2	12
22	Exploring Stability of Transition-Metal Single Atoms on Cu_2O Surfaces. <i>Journal of Physical Chemistry C</i> , 2022, 126, 8065-8078.	1.5	5
23	Non-noble metal single-atom catalyst with MXene support: Fe1/Ti2CO2 for CO oxidation. <i>Chinese Journal of Catalysis</i> , 2022, 43, 1830-1841.	6.9	16
24	Ruthenium/titanium oxide interface promoted electrochemical nitrogen reduction reaction. <i>Chem Catalysis</i> , 2022, 2, 1764-1774.	2.9	6
25	The Key Role of Competition between Orbital and Electrostatic Interactions in the Adsorption on Transition Metal Single-Atom Catalysts Anchored by N-doped Graphene. <i>ChemCatChem</i> , 2022, 14, .	1.8	12
26	Rational design of copper-based single-atom alloy catalysts for electrochemical CO2 reduction. <i>Nano Research</i> , 2022, 15, 7116-7123.	5.8	43
27	Identifying the Real Chemistry of the Synthesis and Reversible Transformation of AuCd Bimetallic Clusters. <i>Journal of the American Chemical Society</i> , 2022, 144, 14248-14257.	6.6	23
28	Breaking the scaling relations for efficient N2-to-NH3 conversion by a bowl active site design: Insight from LaRuSi and isostructural electrides. <i>Chinese Journal of Catalysis</i> , 2022, 43, 2183-2192.	6.9	9
29	Biomass-Derived Fe_2N @NCNTs from Bioaccumulation as an Efficient Electrocatalyst for Oxygen Reduction and Zn-Air Battery. <i>ACS Sustainable Chemistry and Engineering</i> , 2022, 10, 9105-9112.	3.2	12
30	A highly efficient Fenton-like catalyst based on isolated diatomic Fe-Co anchored on N-doped porous carbon. <i>Chemical Engineering Journal</i> , 2021, 404, 126376.	6.6	143
31	Distinct electronic structures and bonding interactions in inverse-sandwich samarium and ytterbium biphenyl complexes. <i>Chemical Science</i> , 2021, 12, 227-238.	3.7	12
32	Phosphorene Supported Single-Atom Catalysts for CO Oxidation: A Computational Study. <i>ChemPhysChem</i> , 2021, 22, 378-385.	1.0	12
33	Co13O8 metalloxocubes: a new class of perovskite-like neutral clusters with cubic aromaticity. <i>National Science Review</i> , 2021, 8, nwaa201.	4.6	21
34	Non-noble metal single-atom catalyst of Co1/MXene (Mo_2CS_2) for CO oxidation. <i>Science China Materials</i> , 2021, 64, 651-663.	3.5	44
35	Highly efficient ammonia synthesis at low temperature over a Ru-Co catalyst with dual atomically dispersed active centers. <i>Chemical Science</i> , 2021, 12, 7125-7137.	3.7	35
36	Coordination Sphere of Lanthanide Aqua Ions Resolved with Ab Initio Molecular Dynamics and X-ray Absorption Spectroscopy. <i>Inorganic Chemistry</i> , 2021, 60, 3117-3130.	1.9	33

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37	Formation and Characterization of BeFe(CO) ₄ ⁻ Anion with Beryllium-Iron Bonding. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 9334-9338.	7.2	16
38	Formation and Characterization of BeFe(CO) ₄ ⁻ Anion with Beryllium-Iron Bonding. <i>Angewandte Chemie</i> , 2021, 133, 9420-9424.	1.6	3
39	Expanded Inverse-Sandwich Complexes of Lanthanum Borides: La ₂ B ₁₀ ⁴⁻ and La ₂ B ₁₁ ⁴⁻ . <i>Journal of Physical Chemistry A</i> , 2021, 125, 2622-2630.		15
40	Understanding the Electronic Structure and Stability of B_nX_n ($n = 4, 6, 8, 10$)	1.7	0
41	Double π -Aromaticity in a Planar Zinc-Doped Gold Cluster: Au ₉ Zn ⁺ . <i>Journal of Physical Chemistry A</i> , 2021, 125, 4606-4613.	1.1	14
42	Norm-Conserving Pseudopotentials and Basis Sets to Explore Actinide Chemistry in Complex Environments. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3360-3371.	2.3	19
43	Metal Oxo-Fluoride Molecules OnMF ₂ (M = Mn and Fe; n = 1-4) and O ₂ MnF: Matrix Infrared Spectra and Quantum Chemistry. <i>Inorganic Chemistry</i> , 2021, 60, 7687-7696.	1.9	3
44	Screening silica-confined single-atom catalysts for nonoxidative conversion of methane. <i>Journal of Chemical Physics</i> , 2021, 154, 174706.	1.2	6
45	Triazine COF-supported single-atom catalyst (Pd1/trzn-COF) for CO oxidation. <i>Science China Materials</i> , 2021, 64, 1939-1951.	3.5	28
46	Unveiling the In Situ Generation of a Monovalent Fe(I) Site in the Single-Fe-Atom Catalyst for Electrochemical CO ₂ Reduction. <i>ACS Catalysis</i> , 2021, 11, 7292-7301.	5.5	51
47	Orientational Alignment of Oxygen Vacancies: Electric-Field-Inducing Conductive Channels in TiO ₂ Film to Boost Photocatalytic Conversion of CO ₂ into CO. <i>Nano Letters</i> , 2021, 21, 5060-5067.	4.5	19
48	Electronic Structure and Spectroscopic Properties of Group-7 Tri-Oxo-Halides MO ₃ X (M = Tj ETQqO 0,0rgBT /Oyerlock 10	1.9	3
49	Underpotential-deposition synthesis and in-line electrochemical analysis of single-atom copper electrocatalysts. <i>Applied Catalysis B: Environmental</i> , 2021, 289, 120028.	10.8	38
50	Rod-Shaped Silver Supercluster Unveiling Strong Electron Coupling between Substituent Icosahedral Units. <i>Journal of the American Chemical Society</i> , 2021, 143, 12261-12267.	6.6	46
51	Theoretical Inspection of M ₁ /PMA Single-Atom Electrocatalyst: Ultra-High Performance for Water Splitting (HER/OER) and Oxygen Reduction Reactions (OER). <i>ACS Catalysis</i> , 2021, 11, 8929-8941.	5.5	121
52	Single Iridium Atom Doped Ni ₂ P Catalyst for Optimal Oxygen Evolution. <i>Journal of the American Chemical Society</i> , 2021, 143, 13605-13615.	6.6	162
53	Using general computational chemistry strategy to unravel the reactivity of emerging pollutants: An example of sulfonamide chlorination. <i>Water Research</i> , 2021, 202, 117391.	5.3	13
54	Heterogeneous Two-Atom Single-Cluster Catalysts for the Nitrogen Electroreduction Reaction. <i>Journal of Physical Chemistry C</i> , 2021, 125, 19821-19830.	1.5	27

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55	Anchoring single platinum atoms onto nickel nanoparticles affords highly selective catalysts for lignin conversion. <i>Cell Reports Physical Science</i> , 2021, 2, 100567.	2.8	13
56	Diketopyrrolopyrrole-based supramolecular nano-leveler for the enhancement of conformal copper electrodeposition. <i>Applied Surface Science</i> , 2021, 569, 150982.	3.1	6
57	Tandem catalyzing the hydrodeoxygenation of 5-hydroxymethylfurfural over a Ni ₃ Fe intermetallic supported Pt single-atom site catalyst. <i>Chemical Science</i> , 2021, 12, 4139-4146.	3.7	33
58	Adsorption energy as a promising single-parameter descriptor for single atom catalysis in the oxygen evolution reaction. <i>Journal of Materials Chemistry A</i> , 2021, 9, 6442-6450.	5.2	18
59	Theoretical Insights into Dual-Metal-Site Catalysts for the Nonoxidative Coupling of Methane. <i>ACS Catalysis</i> , 2021, 11, 13149-13159.	5.5	16
60	Monovalent lanthanide(I) in borozene complexes. <i>Nature Communications</i> , 2021, 12, 6467.	5.8	18
61	Singly Dispersed Bimetallic Sites as Stable and Efficient Single-Cluster Catalysts for Activating N ₂ and CO ₂ . <i>Journal of Physical Chemistry C</i> , 2021, 125, 27192-27198.	1.5	8
62	A general strategy for preparing pyrrolic-N ₄ type single-atom catalysts via pre-located isolated atoms. <i>Nature Communications</i> , 2021, 12, 6806.	5.8	81
63	Fundamental insights into heterogeneous single-atom catalysis. <i>Journal of Chemical Physics</i> , 2021, 155, 210401.	1.2	6
64	Efficient Gold-Palladium Nanoparticles Stabilized by Poly(amic acid) Salt: Synthesis and Application in Catalytic Oxidation of Amines to Imines. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2020, 30, 1384-1392.	1.9	4
65	Tuning radical interactions in triradical tricationic complexes by varying host-cavity sizes. <i>Chemical Science</i> , 2020, 11, 107-112.	3.7	14
66	On the mechanism of H ₂ activation over single-atom catalyst: An understanding of Pt ₁ /WO ₃ in the hydrogenolysis reaction. <i>Chinese Journal of Catalysis</i> , 2020, 41, 524-532.	6.9	50
67	Multiple Bonding Between Group 3 Metals and Fe(CO) ₃ ⁺ . <i>Angewandte Chemie - International Edition</i> , 2020, 59, 2344-2348.	7.2	17
68	A milestone in single-atom catalysis for direct formic acid fuel cell. <i>National Science Review</i> , 2020, 7, 1762-1762.	4.6	3
69	Carbon Monoxide Gas Induced 4H-to-fcc Phase Transformation of Gold As Revealed by In-Situ Transmission Electron Microscopy. <i>Inorganic Chemistry</i> , 2020, 59, 14415-14423.	1.9	4
70	Understanding the Uniqueness of 2p Elements in Periodic Tables. <i>Chemistry - A European Journal</i> , 2020, 26, 15558-15564.	1.7	31
71	Identification of the Electronic and Structural Dynamics of Catalytic Centers in Single-Fe-Atom Material. <i>CheM</i> , 2020, 6, 3440-3454.	5.8	231
72	From S ₂ to S ₄ : experimental and theoretical insights into the atmospheric degradation mechanism of dithiophosphinic acids. <i>RSC Advances</i> , 2020, 10, 40035-40042.	1.7	1

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73	Introduction: Heterogeneous Single-Atom Catalysis. <i>Chemical Reviews</i> , 2020, 120, 11699-11702.	23.0	99
74	Wet carbonate-promoted radical arylation of vinyl pinacolboronates with diaryliodonium salts yields substituted olefins. <i>Communications Chemistry</i> , 2020, 3, .	2.0	8
75	Revisiting the Intriguing Electronic Features of the BeOBeC Carbyne and Some Isomers: A Quantum-Chemical Assessment. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 17261-17265.	7.2	2
76	High-Valent Nickel Promoted by Atomically Embedded Copper for Efficient Water Oxidation. <i>ACS Catalysis</i> , 2020, 10, 9725-9734.	5.5	100
77	Selective hydrogenation of acetylene on graphene-supported non-noble metal single-atom catalysts. <i>Science China Materials</i> , 2020, 63, 1741-1749.	3.5	28
78	Insights into the electronic origin of enhancing the catalytic activity of Co ₃ O ₄ for oxygen evolution by single atom ruthenium. <i>Nano Today</i> , 2020, 34, 100955.	6.2	29
79	Theoretical Understandings of Graphene-based Metal Single-Atom Catalysts: Stability and Catalytic Performance. <i>Chemical Reviews</i> , 2020, 120, 12315-12341.	23.0	354
80	Infrared spectroscopic study of hydrogen bonding topologies in the smallest ice cube. <i>Nature Communications</i> , 2020, 11, 5449.	5.8	35
81	Exploring the difference of bonding strength between silver (ⁱ) and chalcogenides in block copolymer systems. <i>Polymer Chemistry</i> , 2020, 11, 7087-7093.	1.9	23
82	Atomically-precise dopant-controlled single cluster catalysis for electrochemical nitrogen reduction. <i>Nature Communications</i> , 2020, 11, 4389.	5.8	110
83	Coordination engineering of iridium nanocluster bifunctional electrocatalyst for highly efficient and pH-universal overall water splitting. <i>Nature Communications</i> , 2020, 11, 4246.	5.8	221
84	Chromium Single-Atom Catalyst with Graphyne Support: A Theoretical Study of NO Oxidation and Reduction. <i>ACS Catalysis</i> , 2020, 10, 11951-11961.	5.5	49
85	Cooperative Catalysis by Multiple Active Centers in Nonoxidative Conversion of Methane. <i>Journal of Physical Chemistry C</i> , 2020, 124, 13656-13663.	1.5	18
86	Efficient electrically powered CO ₂ -to-ethanol via suppression of deoxygenation. <i>Nature Energy</i> , 2020, 5, 478-486.	19.8	363
87	Non-noble metal single-atom catalysts with phosphotungstic acid (PTA) support: A theoretical study of ethylene epoxidation. <i>Science China Materials</i> , 2020, 63, 1003-1014.	3.5	41
88	2-Butene Tetraanion Bridged Dinuclear Samarium(III) Complexes via Sm(II)-Mediated Reduction of Electron-Rich Olefins. <i>Journal of the American Chemical Society</i> , 2020, 142, 10705-10714.	6.6	25
89	Recent progresses in the research of single-atom catalysts. <i>Science China Materials</i> , 2020, 63, 889-891.	3.5	52
90	Iridium single-atom catalyst on nitrogen-doped carbon for formic acid oxidation synthesized using a general host-guest strategy. <i>Nature Chemistry</i> , 2020, 12, 764-772.	6.6	452

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91	Infrared spectroscopy of neutral water clusters at finite temperature: Evidence for a noncyclic pentamer. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 15423-15428.	3.3	55
92	A Single-Atom Manipulation Approach for Synthesis of Atomically Mixed Nanoalloys as Efficient Catalysts. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 13568-13574.	7.2	23
93	Spherical trihedral metallo-borospherenes. <i>Nature Communications</i> , 2020, 11, 2766.	5.8	43
94	A Single-Atom Manipulation Approach for Synthesis of Atomically Mixed Nanoalloys as Efficient Catalysts. <i>Angewandte Chemie</i> , 2020, 132, 13670-13676.	1.6	8
95	High-loading and thermally stable Pt ₁ /MgAl _{1.2} Fe _{0.8} O ₄ single-atom catalysts for high-temperature applications. <i>Science China Materials</i> , 2020, 63, 949-958.	3.5	31
96	Surface Modification Strategy for Promoting the Performance of Non-noble Metal Single-Atom Catalysts in Low-Temperature CO Oxidation. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 19457-19466.	4.0	12
97	Catalytic mechanism and bonding analyses of Au-Pd single atom alloy (SAA): CO oxidation reaction. <i>Science China Materials</i> , 2020, 63, 993-1002.	3.5	23
98	Ultrahigh-Loading of Ir Single Atoms on NiO Matrix to Dramatically Enhance Oxygen Evolution Reaction. <i>Journal of the American Chemical Society</i> , 2020, 142, 7425-7433.	6.6	430
99	Multiple Bonding Between Group 3 Metals and Fe(CO) ₃ . <i>Angewandte Chemie</i> , 2020, 132, 2364-2368.	1.6	3
100	Revisiting the Intriguing Electronic Features of the BeOBeC Carbyne and Some Isomers: A Quantum-Chemical Assessment. <i>Angewandte Chemie</i> , 2020, 132, 17414-17418.	1.6	0
101	On the theoretical construction of Nb ₂ N ₂ -based superatoms by external field strategies. <i>Chemical Physics Letters</i> , 2020, 754, 137709.	1.2	6
102	Unravelling the Enigma of Nonoxidative Conversion of Methane on Iron Single-Atom Catalysts. <i>Angewandte Chemie</i> , 2020, 132, 18745-18749.	1.6	12
103	Unravelling the Enigma of Nonoxidative Conversion of Methane on Iron Single-Atom Catalysts. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 18586-18590.	7.2	44
104	Formation and Characterization of a BeOBeC Multiple Radical Featuring a Quartet Carbyne Moiety. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 6923-6928.	7.2	13
105	Formation and Characterization of a BeOBeC Multiple Radical Featuring a Quartet Carbyne Moiety. <i>Angewandte Chemie</i> , 2020, 132, 6990-6995.	1.6	9
106	Single-Atom Au ₁ -N ₃ Site for Acetylene Hydrochlorination Reaction. <i>ACS Catalysis</i> , 2020, 10, 1865-1870.	5.5	76
107	Infrared Spectroscopy of Neutral Water Dimer Based on a Tunable Vacuum Ultraviolet Free Electron Laser. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 851-855.	2.1	50
108	Constructing High-Loading Single-Atom/Cluster Catalysts via an Electrochemical Potential Window Strategy. <i>Journal of the American Chemical Society</i> , 2020, 142, 3375-3383.	6.6	147

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109	Development of novel highly stable synergistic quaternary photocatalyst for the efficient hydrogen evolution reaction. <i>Applied Surface Science</i> , 2020, 510, 145498.	3.1	16
110	Tuning the Electronic Properties and Performance of Low-Temperature CO Oxidation of the Gold Cluster by Oriented External Electronic Field. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 1093-1099.	2.1	23
111	Giant Emission Enhancement of Solid-State Gold Nanoclusters by Surface Engineering. <i>Angewandte Chemie</i> , 2020, 132, 8347-8353.	1.6	15
112	Gas-assisted transformation of gold from fcc to the metastable 4H phase. <i>Nature Communications</i> , 2020, 11, 552.	5.8	17
113	3D hierarchical heterostructure assembled by NiFe LDH/(NiFe) _x on biomass-derived hollow carbon microtubes as bifunctional electrocatalysts for overall water splitting. <i>Electrochimica Acta</i> , 2020, 348, 136339.	2.6	83
114	Dual Metal Active Sites in an Ir ₁ /FeO _x Single-Atom Catalyst: A Redox Mechanism for the Water-Gas Shift Reaction. <i>Angewandte Chemie</i> , 2020, 132, 12968-12975.	1.6	19
115	Excited-State Chemistry: Photocatalytic Methanol Oxidation by Uranyl@Zeolite through Oxygen-Centered Radicals. <i>Inorganic Chemistry</i> , 2020, 59, 6287-6300.	1.9	11
116	Isolated Ni Atoms Dispersed on Ru Nanosheets: High-Performance Electrocatalysts toward Hydrogen Oxidation Reaction. <i>Nano Letters</i> , 2020, 20, 3442-3448.	4.5	172
117	Dual Metal Active Sites in an Ir ₁ /FeO _x Single-Atom Catalyst: A Redox Mechanism for the Water-Gas Shift Reaction. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 12868-12875.	7.2	102
118	Rational design of an efficient descriptor for single-atom catalysts in the hydrogen evolution reaction. <i>Journal of Materials Chemistry A</i> , 2020, 8, 9202-9208.	5.2	41
119	Understanding Periodic and Non-periodic Chemistry in Periodic Tables. <i>Frontiers in Chemistry</i> , 2020, 8, 813.	1.8	22
120	Giant Emission Enhancement of Solid-State Gold Nanoclusters by Surface Engineering. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 8270-8276.	7.2	63
121	Cooperative CO ₂ -to-ethanol conversion via enriched intermediates at molecule-metal catalyst interfaces. <i>Nature Catalysis</i> , 2020, 3, 75-82.	16.1	390
122	Gas-Phase Mechanism Study of Methane Nonoxidative Conversion by ReaxFF Method. <i>Wuli Huaxue Xuebao/ Acta Physico-Chimica Sinica</i> , 2020, .	2.2	3
123	TGMin: An efficient global minimum searching program for free and surface-supported clusters. <i>Journal of Computational Chemistry</i> , 2019, 40, 1105-1112.	1.5	43
124	An Ultrastable Matryoshka [Hf ₁₃] Nanocluster as a Luminescent Sensor for Concentrated Alkali and Acid. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 16610-16616.	7.2	39
125	An Ultrastable Matryoshka [Hf ₁₃] Nanocluster as a Luminescent Sensor for Concentrated Alkali and Acid. <i>Angewandte Chemie</i> , 2019, 131, 16763-16769.	1.6	7
126	The Key Role of Support Surface Hydrogenation in the CH ₄ to CH ₃ OH Selective Oxidation by a ZrO ₂ -Supported Single-Atom Catalyst. <i>ACS Catalysis</i> , 2019, 9, 8903-8909.	5.5	65

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127	Fluorine substitution enabling pseudocapacitive intercalation of sodium ions in niobium oxyfluoride. <i>Journal of Materials Chemistry A</i> , 2019, 7, 20813-20823.	5.2	18
128	Understanding Heterolytic H ₂ Cleavage and Water-Assisted Hydrogen Spillover on Fe ₃ O ₄ (001)-Supported Single Palladium Atoms. <i>ACS Catalysis</i> , 2019, 9, 7876-7887.	5.5	63
129	Destruction of the Uranyl Moiety in a U(V) π -Cation π -Interaction. <i>Inorganic Chemistry</i> , 2019, 58, 10148-10159.	1.9	14
130	NMR studies of daidzein and puerarin: active anti-oxidants in traditional Chinese medicine. <i>Journal of Molecular Modeling</i> , 2019, 25, 202.	0.8	16
131	Self-Selective Catalyst Synthesis for CO ₂ Reduction. <i>Joule</i> , 2019, 3, 1927-1936.	11.7	63
132	Three-dimensional open nano-netcage electrocatalysts for efficient pH-universal overall water splitting. <i>Nature Communications</i> , 2019, 10, 4875.	5.8	253
133	PdAg bimetallic electrocatalyst for highly selective reduction of CO ₂ with low COOH* formation energy and facile CO desorption. <i>Nano Research</i> , 2019, 12, 2866-2871.	5.8	61
134	A Supramolecular Radical Dimer: High Efficiency NIR Photothermal Conversion and Therapy. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 15526-15531.	7.2	168
135	A Supramolecular Radical Dimer: High Efficiency NIR Photothermal Conversion and Therapy. <i>Angewandte Chemie</i> , 2019, 131, 15672-15677.	1.6	44
136	Quadruple bonding between iron and boron in the BFe(CO) ₃ ⁺ complex. <i>Nature Communications</i> , 2019, 10, 4713.	5.8	34
137	Ag ₂ S decorated nanocubes with enhanced near-infrared photothermal and photodynamic properties for rapid sterilization. <i>Colloids and Interface Science Communications</i> , 2019, 33, 100201.	2.0	44
138	Insight into the elastic anisotropy and thermodynamics properties of Tantalum borides. <i>Vacuum</i> , 2019, 169, 108883.	1.6	19
139	Remarkable active-site dependent H ₂ O promoting effect in CO oxidation. <i>Nature Communications</i> , 2019, 10, 3824.	5.8	96
140	Probing the electronic structure of the CoB ₁₆ ⁺ drum complex: Unusual oxidation state of Co ⁺¹ . <i>Chinese Journal of Chemical Physics</i> , 2019, 32, 241-247.	0.6	5
141	Regulating the coordination structure of single-atom Fe-NxCy catalytic sites for benzene oxidation. <i>Nature Communications</i> , 2019, 10, 4290.	5.8	326
142	Unravelling a general mechanism of converting ionic B/N complexes into neutral B/N analogues of alkanes: H ⁺ \cdots H ⁺ dihydrogen bonding assisted dehydrogenation. <i>Chemical Communications</i> , 2019, 55, 12239-12242.	2.2	20
143	Unraveling the coordination structure-performance relationship in Pt ₁ /Fe ₂ O ₃ single-atom catalyst. <i>Nature Communications</i> , 2019, 10, 4500.	5.8	279
144	Norm-Conserving Pseudopotentials and Basis Sets To Explore Lanthanide Chemistry in Complex Environments. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5987-5997.	2.3	46

#	ARTICLE	IF	CITATIONS
145	Copper atom-pair catalyst anchored on alloy nanowires for selective and efficient electrochemical reduction of CO ₂ . <i>Nature Chemistry</i> , 2019, 11, 222-228.	6.6	571
146	Synergy of the catalytic activation on Ni and the CeO ₂ /TiO ₂ /Ce ₂ Ti ₂ O ₇ stoichiometric redox cycle for dramatically enhanced solar fuel production. <i>Energy and Environmental Science</i> , 2019, 12, 767-779.	15.6	90
147	Breaking Long-Range Order in Iridium Oxide by Alkali Ion for Efficient Water Oxidation. <i>Journal of the American Chemical Society</i> , 2019, 141, 3014-3023.	6.6	337
148	[La(μ _x -B _x)La] ⁺ (x = 7, 9): a new class of inverse sandwich complexes. <i>Chemical Science</i> , 2019, 10, 2534-2542.	3.7	65
149	Structure and Bonding in [Sb@In ₈ Sb ₁₂] ³⁺ and [Sb@In ₈ Sb ₁₂] ⁵⁺ . <i>Angewandte Chemie</i> , 2019, 131, 8455-8459.	1.6	8
150	Highly active enzyme-metal nanohybrids synthesized in protein-polymer conjugates. <i>Nature Catalysis</i> , 2019, 2, 718-725.	16.1	115
151	The dative Bonding in a Uranium-Cobalt Heterobimetallic Complex for Efficient Nitrogen Fixation. <i>Inorganic Chemistry</i> , 2019, 58, 7433-7439.	1.9	19
152	Re ₈ B ⁺ and Re ₉ B ⁺ : New Members of the Transition-Metal-Centered Borometallic Molecular Wheel Family. <i>Journal of Physical Chemistry A</i> , 2019, 123, 5317-5324.	1.1	40
153	La ₃ B ₁₄ ⁺ : an inverse triple-decker lanthanide boron cluster. <i>Chemical Communications</i> , 2019, 55, 7864-7867.	2.2	36
154	Probing the structures and bonding of size-selected boron and doped-boron clusters. <i>Chemical Society Reviews</i> , 2019, 48, 3550-3591.	18.7	169
155	Dynamic Frustrated Lewis Pairs on Ceria for Direct Nonoxidative Coupling of Methane. <i>ACS Catalysis</i> , 2019, 9, 5523-5536.	5.5	54
156	Structure and Bonding in [Sb@In ₈ Sb ₁₂] ³⁺ and [Sb@In ₈ Sb ₁₂] ⁵⁺ . <i>Angewandte Chemie - International Edition</i> , 2019, 58, 8367-8371.	7.2	27
157	Mechanistic Investigations on Thermal Hydrogenation of CO ₂ to Methanol by Nanostructured CeO ₂ (100): The Crystal-Plane Effect on Catalytic Reactivity. <i>Journal of Physical Chemistry C</i> , 2019, 123, 11763-11771.	1.5	35
158	CeO ₂ (111) electronic reducibility tuned by ultra-small supported bimetallic Pt-Cu clusters. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 15286-15296.	1.3	20
159	Selective photoelectrochemical oxidation of glycerol to high value-added dihydroxyacetone. <i>Nature Communications</i> , 2019, 10, 1779.	5.8	185
160	Triple bonds between iron and heavier group-14 elements in the AFe(CO) ₃ ⁺ complexes (A = Ge, Sn, and Pb). <i>Chemical Communications</i> , 2019, 55, 5685-5688.	2.2	19
161	Structure regulation of noble-metal-based nanomaterials at an atomic level. <i>Nano Today</i> , 2019, 26, 164-175.	6.2	33
162	Quantifying the Bonding Strength of Gold-Chalcogen Bonds in Block Copolymer Systems. <i>Chemistry - an Asian Journal</i> , 2019, 14, 1481-1486.	1.7	22

#	ARTICLE	IF	CITATIONS
163	Heterogeneous Single-Cluster Catalysts for Selective Semihydrogenation of Acetylene with Graphdiyne-Supported Triatomic Clusters. <i>Journal of Physical Chemistry C</i> , 2019, 123, 10494-10500.	1.5	48
164	Structural exploration of Au _x M ⁿ (M = Si, Ge, Sn; $x = 9-12$) clusters with a revised genetic algorithm. <i>RSC Advances</i> , 2019, 9, 7432-7439.	1.7	5
165	High Uptake of ReO ₄ ⁻ and CO ₂ Conversion by a Radiation-Resistant Thorium-Nickel [Th ₄₈ Ni ₆] Nanocage-Based Metal-Organic Framework. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 6022-6027.		109
166	High Uptake of ReO ₄ ⁻ and CO ₂ Conversion by a Radiation-Resistant Thorium-Nickel [Th ₄₈ Ni ₆] Nanocage-Based Metal-Organic Framework. <i>Angewandte Chemie</i> , 2019, 131, 6083-6088.	1.6	15
167	Atomically Dispersed Ruthenium Species Inside Metal-Organic Frameworks: Combining the High Activity of Atomic Sites and the Molecular Sieving Effect of MOFs. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 4271-4275.	7.2	162
168	Atomically Dispersed Ruthenium Species Inside Metal-Organic Frameworks: Combining the High Activity of Atomic Sites and the Molecular Sieving Effect of MOFs. <i>Angewandte Chemie</i> , 2019, 131, 4315-4319.	1.6	25
169	A Ligand-Protected Golden Fullerene: The Dipyridylamido Au ₃₂ ⁸⁺ Nanocluster. <i>Angewandte Chemie</i> , 2019, 131, 5967-5970.	1.6	34
170	A Ligand-Protected Golden Fullerene: The Dipyridylamido Au ₃₂ ⁸⁺ Nanocluster. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 5906-5909.	7.2	82
171	Planar B ₄₁ ⁿ and B ₄₂ ⁿ clusters with double-hexagonal vacancies. <i>Nanoscale</i> , 2019, 11, 23286-23295.	2.8	44
172	Interfacial synergy of ultralong jagged Pt ₈₅ Mo ₁₅ -S nanowires with abundant active sites on enhanced hydrogen evolution in an alkaline solution. <i>Journal of Materials Chemistry A</i> , 2019, 7, 24328-24336.	5.2	35
173	Physical origin of chemical periodicities in the system of elements. <i>Pure and Applied Chemistry</i> , 2019, 91, 1969-1999.	0.9	17
174	Rh single atoms on TiO ₂ dynamically respond to reaction conditions by adapting their site. <i>Nature Communications</i> , 2019, 10, 4488.	5.8	191
175	Molecular nitrogen promotes catalytic hydrodeoxygenation. <i>Nature Catalysis</i> , 2019, 2, 1078-1087.	16.1	63
176	Hydrogen evolution reaction catalyzed by nickel/nickel phosphide nanospheres synthesized through electrochemical methods. <i>Electrochimica Acta</i> , 2019, 298, 229-236.	2.6	27
177	Non defect-stabilized thermally stable single-atom catalyst. <i>Nature Communications</i> , 2019, 10, 234.	5.8	452
178	N ₂ Reduction on Fe-Based Complexes with Different Supporting Main-Group Elements: Critical Roles of Anchor and Peripheral Ligands. <i>Small Methods</i> , 2019, 3, 1800340.	4.6	17
179	Multi-site electrocatalysts for hydrogen evolution in neutral media by destabilization of water molecules. <i>Nature Energy</i> , 2019, 4, 107-114.	19.8	470
180	Impact of a Single Hydrogen Substitution by Fluorine on the Molecular Interaction and Miscibility between Sorafenib and Polymers. <i>Molecular Pharmaceutics</i> , 2019, 16, 318-326.	2.3	15

#	ARTICLE	IF	CITATIONS
181	Lanthanides with Unusually Low Oxidation States in the PrB ₃ and PrB ₄ Boride Clusters. <i>Inorganic Chemistry</i> , 2019, 58, 411-418.	1.9	39
182	Implanting Mo Atoms into Surface Lattice of Pt ₃ Mn Alloys Enclosed by High-Indexed Facets: Promoting Highly Active Sites for Ethylene Glycol Oxidation. <i>ACS Catalysis</i> , 2019, 9, 442-455.	5.5	79
183	Design of Single-Atom Co ^{N5} Catalytic Site: A Robust Electrocatalyst for CO ₂ Reduction with Nearly 100% CO Selectivity and Remarkable Stability. <i>Journal of the American Chemical Society</i> , 2018, 140, 4218-4221.	6.6	945
184	Electronic Structure and Bonding Situation in M ₂ O ₂ (M = Be, Mg, Ca) Rhombic Clusters. <i>Journal of Physical Chemistry A</i> , 2018, 122, 2816-2822.	1.1	34
185	A Durable Nickel Single-Atom Catalyst for Hydrogenation Reactions and Cellulose Valorization under Harsh Conditions. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 7071-7075.	7.2	243
186	Heterogeneous Fe ₃ single-cluster catalyst for ammonia synthesis via an associative mechanism. <i>Nature Communications</i> , 2018, 9, 1610.	5.8	409
187	Relativity-Induced Bonding Pattern Change in Coinage Metal Dimers M ₂ (M = Cu, Ag, Au, Rg). <i>Inorganic Chemistry</i> , 2018, 57, 5499-5506.	1.9	12
188	NMR measurements and DFT studies of nuclear magnetic shielding in emodin and chuanxiongzine molecules. <i>Journal of Molecular Structure</i> , 2018, 1166, 304-310.	1.8	9
189	Tuning defects in oxides at room temperature by lithium reduction. <i>Nature Communications</i> , 2018, 9, 1302.	5.8	428
190	Synergistic effect between undercoordinated platinum atoms and defective nickel hydroxide on enhanced hydrogen evolution reaction in alkaline solution. <i>Nano Energy</i> , 2018, 48, 590-599.	8.2	76
191	Tracking the energy flow in the hydrogen exchange reaction OH + H ₂ O → H ₂ O + OH. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 12543-12556.	1.3	19
192	Efficient Nitrogen Fixation via a Redox-Flexible Single-Iron Site with Reverse-Dative Iron → Boron ÿf Bonding. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4530-4537.	1.1	23
193	Periodic Trends in Actinyl Thio-Crown Ether Complexes. <i>Inorganic Chemistry</i> , 2018, 57, 2899-2907.	1.9	23
194	Äœber Oxidationszahl-Öbergrenzen in der Chemie. <i>Angewandte Chemie</i> , 2018, 130, 3297-3300.	1.6	15
195	Triple Bonds Between Iron and Heavier Group 15 Elements in AFe(CO) ₃ (A=As, Sb, Bi). <i>Journal of Physical Chemistry A</i> , 2018, 122, 10784-10791.	1.6	16
196	Theoretical studies on copper-catalyzed arylation of nitrogen heterocycles from benzenediazonium acetate under ligand-free conditions. <i>Journal of Organometallic Chemistry</i> , 2018, 864, 50-57.	0.8	10
197	On the Upper Limits of Oxidation States in Chemistry. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 3242-3245.	7.2	46
198	A Durable Nickel Single-Atom Catalyst for Hydrogenation Reactions and Cellulose Valorization under Harsh Conditions. <i>Angewandte Chemie</i> , 2018, 130, 7189-7193.	1.6	64

#	ARTICLE	IF	CITATIONS
199	Fe Isolated Single Atoms on S, N Codoped Carbon by Copolymer Pyrolysis Strategy for Highly Efficient Oxygen Reduction Reaction. <i>Advanced Materials</i> , 2018, 30, e1800588.	11.1	511
200	Maximizing the Number of Interfacial Sites in Single-Atom Catalysts for the Highly Selective, Solvent-Free Oxidation of Primary Alcohols. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 7795-7799.	7.2	151
201	Maximizing the Number of Interfacial Sites in Single-Atom Catalysts for the Highly Selective, Solvent-Free Oxidation of Primary Alcohols. <i>Angewandte Chemie</i> , 2018, 130, 7921-7925.	1.6	18
202	Uranyl/12-crown-4 Ether Complexes and Derivatives: Structural Characterization and Isomeric Differentiation. <i>Inorganic Chemistry</i> , 2018, 57, 4125-4134.	1.9	6
203	Spin-Orbit Splittings and Low-Lying Electronic States of AuSi and AuGe: Anion Photoelectron Spectroscopy and <i>ab Initio</i> Calculations. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3374-3382.	1.1	13
204	Catalysis on Singly Dispersed Rh Atoms Anchored on an Inert Support. <i>ACS Catalysis</i> , 2018, 8, 110-121.	5.5	81
205	A binding-block ion selective mechanism revealed by a Na/K selective channel. <i>Protein and Cell</i> , 2018, 9, 629-639.	4.8	14
206	A systematic theoretical study on FeOx-supported single-atom catalysts: M1/FeOx for CO oxidation. <i>Nano Research</i> , 2018, 11, 1599-1611.	5.8	75
207	Triple Bonds Between Iron and Heavier Group 15 Elements in $AFe(CO)_3$ ($A=As, Sb, Bi$). <i>Journal of Physical Chemistry A</i> , 2018, 122, 7123-7131.	1.1	14
208	Surface Single-Cluster Catalyst for N_2 -to- NH_3 Thermal Conversion. <i>Journal of the American Chemical Society</i> , 2018, 140, 46-49.	6.6	233
209	Probing Ligand-Induced Cooperative Orbital Redistribution That Dominates Nanoscale Molecule-Surface Interactions with One-Unit-Thin TiO_2 Nanosheets. <i>Nano Letters</i> , 2018, 18, 7809-7815.	4.5	30
210	Chemical Bonding of Crystalline LnB_6 ($Ln = La-Lu$) and Its Relationship with Ln_2B_8 Gas-Phase Complexes. <i>Inorganic Chemistry</i> , 2018, 57, 12999-13008.	1.9	57
211	Symmetry Reduction upon Size Mismatch: The Nonicosahedral Intermetallic Cluster $[Co@Ge_{12}]^{3+}$. <i>Chinese Journal of Chemistry</i> , 2018, 36, 1165-1168.	2.6	25
212	Polarizable force field parameterization and theoretical simulations of $ThCl_4 \cdot LiCl$ molten salts. <i>Journal of Computational Chemistry</i> , 2018, 39, 2432-2438.	1.5	11
213	Constructing NiCo/Fe ₃ O ₄ Heteroparticles within MOF-74 for Efficient Oxygen Evolution Reactions. <i>Journal of the American Chemical Society</i> , 2018, 140, 15336-15341.	6.6	310
214	Exceptional Antisintering Gold Nanocatalyst for Diesel Exhaust Oxidation. <i>Nano Letters</i> , 2018, 18, 6489-6493.	4.5	19
215	Theoretical understanding of the stability of single-atom catalysts. <i>National Science Review</i> , 2018, 5, 638-641.	4.6	194
216	Atomic Energies from a Convolutional Neural Network. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3933-3942.	2.3	54

#	ARTICLE	IF	CITATIONS
217	A supramolecular radical cation: folding-enhanced electrostatic effect for promoting radical-mediated oxidation. <i>Chemical Science</i> , 2018, 9, 5015-5020.	3.7	21
218	Structural basis of ubiquitin modification by the Legionella effector SdeA. <i>Nature</i> , 2018, 557, 674-678.	13.7	69
219	Heterogeneous single-atom catalysis. <i>Nature Reviews Chemistry</i> , 2018, 2, 65-81.	13.8	2,728
220	Mechanistic investigations of Co(II)-Catalyzed C-N coupling reactions. <i>Journal of Organometallic Chemistry</i> , 2018, 868, 144-153.	0.8	16
221	An Isolable Diphosphene Radical Cation Stabilized by Threeâ€Center Threeâ€Electron Î€â€Bonding with Chromium: Endâ€On versus Sideâ€On Coordination. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 9419-9424.	7.2	24
222	MOFâ€Confined Subâ€2 nm Atomically Ordered Intermetallic PdZn Nanoparticles as Highâ€Performance Catalysts for Selective Hydrogenation of Acetylene. <i>Advanced Materials</i> , 2018, 30, e1801878.	11.1	133
223	A diuranium carbide cluster stabilized inside a C80 fullerene cage. <i>Nature Communications</i> , 2018, 9, 2753.	5.8	63
224	Observation of highly stable and symmetric lanthanide octa-boron inverse sandwich complexes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E6972-E6977.	3.3	72
225	Direct observation of noble metal nanoparticles transforming to thermally stable single atoms. <i>Nature Nanotechnology</i> , 2018, 13, 856-861.	15.6	741
226	Size-dependent dynamic structures of supported gold nanoparticles in CO oxidation reaction condition. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 7700-7705.	3.3	183
227	An Isolable Diphosphene Radical Cation Stabilized by Threeâ€Center Threeâ€Electron Î€â€Bonding with Chromium: Endâ€On versus Sideâ€On Coordination. <i>Angewandte Chemie</i> , 2018, 130, 9563-9568.	1.6	9
228	Recent Progress on the investigations of boron clusters and boron-based materials (I): borophene. <i>Scientia Sinica Chimica</i> , 2018, 48, 98-107.	0.2	12
229	B26â€: The smallest planar boron cluster with a hexagonal vacancy and a complicated potential landscape. <i>Chemical Physics Letters</i> , 2017, 683, 336-341.	1.2	48
230	Bonding trends across the series of tricarbonato-actinyl anions [(AnO ₂)(CO ₃) ₃] ⁴⁻ (An = Uâ€Cm): the plutonium turn. <i>Dalton Transactions</i> , 2017, 46, 2542-2550.	1.6	34
231	Structural Rearrangement of Auâ€Pd Nanoparticles under Reaction Conditions: An <i>ab Initio</i> Molecular Dynamics Study. <i>ACS Nano</i> , 2017, 11, 1649-1658.	7.3	47
232	Manipulating Stabilities and Catalytic Properties of Trinuclear Metal Clusters through Tuning the Chemical Bonding: H ₂ Adsorption and Activation. <i>Journal of Physical Chemistry C</i> , 2017, 121, 10992-11001.	1.5	10
233	Hittorf's phosphorus: the missing link during transformation of red phosphorus to black phosphorus. <i>CrystEngComm</i> , 2017, 19, 905-909.	1.3	36
234	Toward Rational Design of Oxide-Supported Single-Atom Catalysts: Atomic Dispersion of Gold on Ceria. <i>Journal of the American Chemical Society</i> , 2017, 139, 6190-6199.	6.6	333

#	ARTICLE	IF	CITATIONS
235	Isolated Single-Atom Pd Sites in Intermetallic Nanostructures: High Catalytic Selectivity for Semihydrogenation of Alkynes. <i>Journal of the American Chemical Society</i> , 2017, 139, 7294-7301.	6.6	354
236	PrB ₇ ⁺ : A Praseodymium-Doped Boron Cluster with a Pr ^{II} Center Coordinated by a Doubly Aromatic Planar I ₇ B ₇ ³⁺ Ligand. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 6916-6920.	7.2	63
237	Preparation and Characterization of Uranium-Iron Triple-Bonded UFe(CO) ₃ ⁺ and OUFe(CO) ₃ ⁺ Complexes. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 6932-6936.	7.2	53
238	Preparation and Characterization of Uranium-Iron Triple-Bonded UFe(CO) ₃ ⁺ and OUFe(CO) ₃ ⁺ Complexes. <i>Angewandte Chemie</i> , 2017, 129, 7036-7040.	1.6	10
239	PrB ₇ ⁺ : A Praseodymium-Doped Boron Cluster with a Pr ^{II} Center Coordinated by a Doubly Aromatic Planar I ₇ B ₇ ³⁺ Ligand. <i>Angewandte Chemie</i> , 2017, 129, 7020-7024.	1.6	13
240	Theoretical Investigations of Pt ₁ @CeO ₂ Single-Atom Catalyst for CO Oxidation. <i>Journal of Physical Chemistry C</i> , 2017, 121, 11281-11289.	1.5	138
241	Diversity of Chemical Bonding and Oxidation States in MS ₄ Molecules of Group...8 Elements. <i>Chemistry - A European Journal</i> , 2017, 23, 10580-10589.	1.7	7
242	Quasi-classical trajectory studies on the full-dimensional accurate potential energy surface for the OH + H ₂ O = H ₂ O + OH reaction. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 17718-17725.	1.3	30
243	High-Performance Rh ₂ P Electrocatalyst for Efficient Water Splitting. <i>Journal of the American Chemical Society</i> , 2017, 139, 5494-5502.	6.6	343
244	Pentavalent lanthanide nitride-oxides: NPrO and NPrO ⁺ complexes with Ni, Pr triple bonds. <i>Chemical Science</i> , 2017, 8, 4035-4043.	3.7	40
245	A Very Short Be-Be Distance but No Bond: Synthesis and Bonding Analysis of NgBe ₂ O ₂ Ng (Ng, Ng = Ne, Ar, Kr, Xe). <i>Chemistry - A European Journal</i> , 2017, 23, 2035-2039.	1.23	46
246	Recent progresses of global minimum searches of nanoclusters with a constrained Basin-Hopping algorithm in the TGMIn program. <i>Computational and Theoretical Chemistry</i> , 2017, 1107, 57-65.	1.1	80
247	Observation of a metal-centered B ₂ -Ta@B ₁₈ ⁺ tubular molecular rotor and a perfect Ta@B ₂₀ ⁺ boron drum with the record coordination number of twenty. <i>Chemical Communications</i> , 2017, 53, 1587-1590.	2.2	114
248	From planar boron clusters to borophenes and metalloborophenes. <i>Nature Reviews Chemistry</i> , 2017, 1, .	13.8	169
249	Identification of activity trends for CO oxidation on supported transition-metal single-atom catalysts. <i>Catalysis Science and Technology</i> , 2017, 7, 5860-5871.	2.1	69
250	Catalytic activities of single-atom catalysts for CO oxidation: Pt ₁ /FeO _x vs. Fe ₁ /FeO _x . <i>Chinese Journal of Catalysis</i> , 2017, 38, 1566-1573.	6.9	22
251	Investigation of water adsorption and dissociation on Au ₁ /CeO ₂ single-atom catalysts using density functional theory. <i>Chinese Journal of Catalysis</i> , 2017, 38, 1558-1565.	6.9	16
252	Crown ether complexes of actinyls: a computational assessment of AnO ₂ (15-crown-5) ²⁺ (An = U, Np, Pu, Am, Cm). <i>Dalton Transactions</i> , 2017, 46, 12354-12363.	1.6	28

#	ARTICLE	IF	CITATIONS
253	Structural transition in metal-centered boron clusters: from tubular molecular rotors Ta@B ₂₁ and Ta@B ₂₂ ⁺ to cage-like endohedral metalloborospherene Ta@B ₂₂ ⁺ . <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 27025-27030.	1.3	38
254	TGMin: A global-minimum structure search program based on a constrained basin-hopping algorithm. <i>Nano Research</i> , 2017, 10, 3407-3420.	5.8	97
255	Pentavalent Lanthanide Compounds: Formation and Characterization of Praseodymium(V) Oxides. <i>Angewandte Chemie</i> , 2016, 128, 7010-7014.	1.6	10
256	Frontispiz: The Planar CoB ₁₈ ⁺ Cluster as a Motif for Metallo-Borophenes. <i>Angewandte Chemie</i> , 2016, 128, .	1.6	1
257	The Planar CoB ₁₈ ⁺ Cluster as a Motif for Metallo-Borophenes. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 7358-7363.	7.2	90
258	A Supramolecularly Activated Radical Cation for Accelerated Catalytic Oxidation. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 8933-8937.	7.2	69
259	The promotional role of water in heterogeneous catalysis: mechanism insights from computational modeling. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2016, 6, 679-693.	6.2	58
260	A Supramolecularly Activated Radical Cation for Accelerated Catalytic Oxidation. <i>Angewandte Chemie</i> , 2016, 128, 9079-9083.	1.6	19
261	Frontispiece: The Planar CoB ₁₈ ⁺ Cluster as a Motif for Metallo-Borophenes. <i>Angewandte Chemie - International Edition</i> , 2016, 55, .	7.2	0
262	Pentavalent Lanthanide Compounds: Formation and Characterization of Praseodymium(V) Oxides. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 6896-6900.	7.2	66
263	Periodicity and Covalency of [MX ₂] ⁺ (M = Cu, Ag, Au, Rg; X = H, Cl, CN) Complexes. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 1395-1404.	1.0	9
264	The Planar CoB ₁₈ ⁺ Cluster as a Motif for Metallo-Borophenes. <i>Angewandte Chemie</i> , 2016, 128, 7484-7489.	1.6	30
265	A combined photoelectron spectroscopy and relativistic <i>ab initio</i> studies of the electronic structures of UFO and UFO ⁺ . <i>Journal of Chemical Physics</i> , 2016, 144, 084309.	1.2	4
266	Observation and characterization of the smallest borospherene, B ₂₈ ⁺ and B ₂₈ . <i>Journal of Chemical Physics</i> , 2016, 144, 064307.	1.2	141
267	Manganese-centered tubular boron cluster MnB ₁₆ ⁺ : A new class of transition-metal molecules. <i>Journal of Chemical Physics</i> , 2016, 144, 154310.	1.2	107
268	How Much Can Density Functional Approximations (DFA) Fail? The Extreme Case of the FeO ₄ Species. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1525-1533.	2.3	33
269	On the oxidation states of metal elements in MO ₃ (M=V, Nb, Ta, Db, Pr, Gd, Pa) anions. <i>Science China Chemistry</i> , 2016, 59, 442-451.	4.2	28
270	On the Highest Oxidation States of Metal Elements in MO ₄ Molecules (M = Fe, Ru, Os, Hs, Tj) <i>Journal of Chemical Theory and Computation</i> , 2016, 16, 1525-1533.	1.9	37

#	ARTICLE	IF	CITATIONS
271	Design of Efficient Catalysts with Double Transition Metal Atoms on C ₂ N Layer. Journal of Physical Chemistry Letters, 2016, 7, 1750-1755.	2.1	196
272	Electronic structure and characterization of a uranyl di-15-crown-5 complex with an unprecedented sandwich structure. Chemical Communications, 2016, 52, 12761-12764.	2.2	21
273	New mechanistic pathways for CO oxidation catalyzed by single-atom catalysts: Supported and doped Au ₁ /ThO ₂ . Nano Research, 2016, 9, 3868-3880.	5.8	68
274	Theoretical Studies on Reactions of OH with H ₂ SO ₄ ⁺ ⋅NH ₃ Complex and NH ₂ with H ₂ SO ₄ in the Presence of Water. ChemistrySelect, 2016, 1, 1421-1430.	0.7	18
275	CO Oxidation on Au/TiO ₂ : Condition-Dependent Active Sites and Mechanistic Pathways. Journal of the American Chemical Society, 2016, 138, 10467-10476.	6.6	159
276	Competition between drum and quasi-planar structures in RhB ₁₈ ⁺ : motifs for metallo-boronanotubes and metallo-borophenes. Chemical Science, 2016, 7, 7020-7027.	3.7	97
277	Pd ₃ cluster catalysis: Compelling evidence from in operando spectroscopic, kinetic, and density functional theory studies. Nano Research, 2016, 9, 2544-2550.	5.8	22
278	On the Nature of Support Effects of Metal Dioxides MO ₂ (M = Ti, Zr, Hf, Ce, Th) in Single-Atom Gold Catalysts: Importance of Quantum Primogenic Effect. Journal of Physical Chemistry C, 2016, 120, 17514-17526.	1.5	120
279	Experimental and theoretical identification of the Fe(^{vii}) oxidation state in FeO ₄ ⁺ . Physical Chemistry Chemical Physics, 2016, 18, 31125-31131.	1.3	18
280	Unraveling the Origin of Visible Light Capture by Core-Shell TiO ₂ Nanotubes. Chemistry of Materials, 2016, 28, 4467-4475.	3.2	42
281	Theoretical investigations of non-noble metal single-atom catalysis: Ni ₁ /FeO _x for CO oxidation. Catalysis Science and Technology, 2016, 6, 6886-6892.	2.1	79
282	A niobium-necked cluster [As ₃ Nb(As ₃ Sn ₃)] ³⁺ with aromatic Sn ₃ ²⁺ . Dalton Transactions, 2016, 45, 3874-3879.	1.6	14
283	Theoretical studies of CO oxidation with lattice oxygen on Co ₃ O ₄ surfaces. Chinese Journal of Catalysis, 2016, 37, 193-198.	6.9	21
284	Relativistic Effects Break Periodicity in Group 6 Diatomic Molecules. Journal of the American Chemical Society, 2016, 138, 1126-1129.	6.6	38
285	Theoretical studies of the global minima and polarizabilities of small lithium clusters. Chemical Physics Letters, 2016, 644, 235-242.	1.2	13
286	Mechanistic Insights into Propene Epoxidation with O ₂ ⋅H ₂ O Mixture on Au ₇ /Al ₂ O ₃ : A Hydroperoxyl Pathway from ab Initio Molecular Dynamics Simulations. ACS Catalysis, 2016, 6, 2525-2535.	5.5	70
287	Synergetic Integration of Cu _{1.94} ⋅Zn _x Cd ₁ ⋅S Heteronanorods for Enhanced Visible-Light-Driven Photocatalytic Hydrogen Production. Journal of the American Chemical Society, 2016, 138, 4286-4289.	6.6	257
288	Probing the Electronic Structure and Chemical Bonding of Mono-Uranium Oxides with Different Oxidation States: UO _x ⁺ and UO _x (x = 3-5). Journal of Physical Chemistry A, 2016, 120, 1084-1096.	1.1	29

#	ARTICLE	IF	CITATIONS
289	Theoretical studies on the bonding and electron structures of a $[Au_3Sb_6]^{3+}$ complex and its oligomers. Dalton Transactions, 2016, 45, 11657-11667.	1.6	8
290	PdZn Intermetallic Nanostructure with Pd–Zn Ensembles for Highly Active and Chemoselective Semi-Hydrogenation of Acetylene. ACS Catalysis, 2016, 6, 1054-1061.	5.5	334
291	Bond-bending isomerism of Au_2I_3 : competition between covalent bonding and aurophilicity. Chemical Science, 2016, 7, 475-481.	3.7	16
292	Metal–Organic Frameworks (MOFs) of a Cubic Metal Cluster with Multicentered Mn–Mn Bonds. Angewandte Chemie - International Edition, 2015, 54, 11681-11685.	7.2	50
293	Structure Evolution and Associated Catalytic Properties of Pt–Sn Bimetallic Nanoparticles. Chemistry - A European Journal, 2015, 21, 12034-12041.	1.7	53
294	Formation and Characterization of the Boron Dicarbonyl Complex $[B(CO)_2]^-$. Angewandte Chemie - International Edition, 2015, 54, 11078-11083.	7.2	107
295	Catalysis on singly dispersed bimetallic sites. Nature Communications, 2015, 6, 7938.	5.8	235
296	Microemulsion-Controlled Synthesis of One-Dimensional Ir Nanowires and Their Catalytic Activity in Selective Hydrogenation of <i>o</i> -Chloronitrobenzene. Langmuir, 2015, 31, 90-95.	1.6	22
297	Experimental and Theoretical Evidence of an Axially Chiral Borospherene. ACS Nano, 2015, 9, 754-760.	7.3	228
298	An efficient molybdenum disulfide/cobalt diselenide hybrid catalyst for electrochemical hydrogen generation. Nature Communications, 2015, 6, 5982.	5.8	897
299	A multicentre-bonded $[Zn]_8$ cluster with cubic aromaticity. Nature Communications, 2015, 6, 6331.	5.8	94
300	On the gold–ligand covalency in linear $[AuX_2]^-$ complexes. Dalton Transactions, 2015, 44, 5535-5546.	1.6	27
301	Infrared spectroscopic and theoretical study of the reactions of cerium atoms with methanol in solid argon. Journal of Molecular Spectroscopy, 2015, 310, 50-56.	0.4	10
302	Dynamic formation of single-atom catalytic active sites on ceria-supported gold nanoparticles. Nature Communications, 2015, 6, 6511.	5.8	370
303	Photoelectron spectroscopy and theoretical studies of gaseous uranium hexachlorides in different oxidation states: UCl_6^{q-} ($q = 0-2$). Journal of Chemical Physics, 2015, 142, 134308.	1.2	30
304	Theoretical Studies on the Synergetic Effects of Au–Pd Bimetallic Catalysts in the Selective Oxidation of Methanol. Journal of Physical Chemistry C, 2015, 119, 16072-16081.	1.5	45
305	Ultrastable single-atom gold catalysts with strong covalent metal-support interaction (CMSI). Nano Research, 2015, 8, 2913-2924.	5.8	422
306	Conversion of PtNi alloy from disordered to ordered for enhanced activity and durability in methanol-tolerant oxygen reduction reactions. Nano Research, 2015, 8, 2777-2788.	5.8	124

#	ARTICLE	IF	CITATIONS
307	Theoretical Studies on Hexanuclear Oxometalates $[M_6L_{19}]^{+q}$ (M = Cr, Mo, W, Sg, Nd, U). Electronic Structures, Oxidation States, Aromaticity, and Stability. <i>Inorganic Chemistry</i> , 2015, 54, 7171-7180.	1.9	24
308	An 18-Electron System Containing a Superheavy Element: Theoretical Studies of $Sg@Au_{12}$. <i>Inorganic Chemistry</i> , 2015, 54, 3695-3701.	1.9	42
309	Copper Nanocrystal Plane Effect on Stereoselectivity of Catalytic Deoxygenation of Aromatic Epoxides. <i>Journal of the American Chemical Society</i> , 2015, 137, 3791-3794.	6.6	50
310	Infrared Multiphoton Dissociation Spectroscopy of a Gas-Phase Complex of Uranyl and 3-Oxa-Glutaramide: An Extreme Red-Shift of the $[O=U=O]^{2+}$ Asymmetric Stretch. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3366-3374.	1.1	21
311	Highly Efficient Catalysis of Preferential Oxidation of CO in H_2 -Rich Stream by Gold Single-Atom Catalysts. <i>ACS Catalysis</i> , 2015, 5, 6249-6254.	5.5	380
312	Is Octavalent Pu(VIII) Possible? Mapping the Plutonium Oxyfluoride Series PuO_nF_{8-2n} ($n = 0-4$). <i>Inorganic Chemistry</i> , 2015, 54, 8825-8831.	1.9	26
313	Actinide (An = Th-Pu) dimetalloenes: promising candidates for metal-metal multiple bonds. <i>Dalton Transactions</i> , 2015, 44, 17045-17053.	1.6	41
314	Hydrogenation of molecular oxygen to hydroperoxyl: An alternative pathway for O_2 activation on nanogold catalysts. <i>Nano Research</i> , 2015, 8, 3737-3748.	5.8	34
315	Periodicity, Electronic Structures, and Bonding of Gold Tetrahalides $[AuX_4]^+$ (X = F, Cl, Br, I, At, Uus). <i>Inorganic Chemistry</i> , 2015, 54, 11157-11167.	1.9	18
316	Planar substrate-binding site dictates the specificity of ECF-type nickel/cobalt transporters. <i>Cell Research</i> , 2014, 24, 267-277.	5.7	39
317	Theoretical Studies of Structure and Dynamics of Molten Salts: The $LiF-ThF_4$ System. <i>Journal of Physical Chemistry B</i> , 2014, 118, 13954-13962.	1.2	25
318	Advances in computational actinide chemistry in China. <i>Radiochimica Acta</i> , 2014, 102, 13-25.	0.5	7
319	Quadruple bonding of carbon in terminal carbides. <i>Science China Chemistry</i> , 2014, 57, 426-434.	4.2	14
320	$[B_{30}]^+$: A Quasiplanar Chiral Boron Cluster. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 5540-5545.	7.2	144
321	Strong electron correlation in UO_2^+ : A photoelectron spectroscopy and relativistic quantum chemistry study. <i>Journal of Chemical Physics</i> , 2014, 140, 094306.	1.2	29
322	Planar hexagonal B36 as a potential basis for extended single-atom layer boron sheets. <i>Nature Communications</i> , 2014, 5, 3113.	5.8	645
323	Characterization of Fe Substitution into La-Hexaaluminate Systems and the Effect on N_2O Catalytic Decomposition. <i>Journal of Physical Chemistry C</i> , 2014, 118, 1999-2010.	1.5	21
324	Actinide-Silicon Multiradical Bonding: Infrared Spectra and Electronic Structures of the $Si(1/4-X)AnF_3$ (An = Th, U; X = H, F) Molecules. <i>Journal of the American Chemical Society</i> , 2014, 136, 1427-1437.	6.6	40

#	ARTICLE	IF	CITATIONS
325	Excited States and Luminescent Properties of UO_2F_2 and Its Solvated Complexes in Aqueous Solution. <i>Inorganic Chemistry</i> , 2014, 53, 7340-7350.	1.9	20
326	Identification of an iridium-containing compound with a formal oxidation state of IX. <i>Nature</i> , 2014, 514, 475-477.	13.7	171
327	Theoretical and experimental studies of the interactions between Au^{2+} and nucleobases. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 2928.	1.3	15
328	The B_{35} Cluster with a Double-Hexagonal Vacancy: A New and More Flexible Structural Motif for Borophene. <i>Journal of the American Chemical Society</i> , 2014, 136, 12257-12260.	6.6	298
329	$[\text{B}_{30}]^+$: A Quasiplanar Chiral Boron Cluster. <i>Angewandte Chemie</i> , 2014, 126, 5646-5651.	1.6	33
330	Observation of an all-boron fullerene. <i>Nature Chemistry</i> , 2014, 6, 727-731.	6.6	724
331	Theoretical and Experimental Investigations on Single-Atom Catalysis: Ir_1/FeO_x for CO Oxidation. <i>Journal of Physical Chemistry C</i> , 2014, 118, 21945-21951.	1.5	145
332	Ultrathin rhodium nanosheets. <i>Nature Communications</i> , 2014, 5, 3093.	5.8	428
333	Theoretical study of the crystal plane effect and ion-pair active center for C-H bond activation by Co_3O_4 nanocrystals. <i>Chinese Journal of Catalysis</i> , 2014, 35, 462-467.	6.9	28
334	A Water-Promoted Mechanism of Alcohol Oxidation on a $\text{Au}(111)$ Surface: Understanding the Catalytic Behavior of Bulk Gold. <i>ACS Catalysis</i> , 2013, 3, 1693-1699.	5.5	118
335	Probing the nature of gold-carbon bonding in gold-alkynyl complexes. <i>Nature Communications</i> , 2013, 4, 2223.	5.8	52
336	Theoretical Studies on the Photoelectron and Absorption Spectra of MnO_4^+ and TcO_4^+ . <i>Inorganic Chemistry</i> , 2013, 52, 9867-9874.	1.9	23
337	B_{30}H_8 , $\text{B}_{39}\text{H}_9^{2+}$, $\text{B}_{42}\text{H}_{10}$, $\text{B}_{48}\text{H}_{10}$, and $\text{B}_{72}\text{H}_{12}$: polycyclic aromatic nido hydroboron clusters analogous to polycyclic aromatic hydrocarbons. <i>Journal of Molecular Modeling</i> , 2013, 19, 1195-1204.	0.8	15
338	Aspects of bonding in small gold clusters. <i>International Journal of Mass Spectrometry</i> , 2013, 354-355, 15-18.	0.7	15
339	Remarkable Performance of Ir_1/FeO_x Single-Atom Catalyst in Water Gas Shift Reaction. <i>Journal of the American Chemical Society</i> , 2013, 135, 15314-15317.	6.6	811
340	DFT+U Study on the Localized Electronic States and Their Potential Role During H_2O Dissociation and CO Oxidation Processes on $\text{CeO}_2(111)$ Surface. <i>Journal of Physical Chemistry C</i> , 2013, 117, 23082-23089.	1.5	85
341	Oxidation States, Geometries, and Electronic Structures of Plutonium Tetroxide PuO_4 Isomers: Is Octavalent Pu Viable?. <i>Inorganic Chemistry</i> , 2013, 52, 14237-14245.	1.9	38
342	Theoretical studies on the complexation of uranyl with typical carboxylate and amidoximate ligands. <i>Science China Chemistry</i> , 2013, 56, 1525-1532.	4.2	16

#	ARTICLE	IF	CITATIONS
343	Surface-specific interaction by structure-match confined pure high-energy facet of unstable TiO ₂ (B) polymorph. <i>Scientific Reports</i> , 2013, 3, 1411.	1.6	51
344	The Role of Reducible Oxide-Metal Cluster Charge Transfer in Catalytic Processes: New Insights on the Catalytic Mechanism of CO Oxidation on Au/TiO ₂ from ab Initio Molecular Dynamics. <i>Journal of the American Chemical Society</i> , 2013, 135, 10673-10683.	6.6	308
345	Single-Atom Catalysts: A New Frontier in Heterogeneous Catalysis. <i>Accounts of Chemical Research</i> , 2013, 46, 1740-1748.	7.6	3,405
346	A Tetrapositive Metal Ion in the Gas Phase: Thorium(IV) Coordinated by Neutral Tridentate Ligands. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 6885-6888.	7.2	34
347	Photocatalysis with visible-light-active uranyl complexes. <i>Science China Chemistry</i> , 2013, 56, 1671-1681.	4.2	51
348	Experimental and Theoretical Studies on the Fragmentation of Gas-Phase Uranyl ⁺ , Neptunyl ⁺ , and Plutonyl ⁺ Diglycolamide Complexes. <i>Journal of Physical Chemistry A</i> , 2013, 117, 10544-10550.	1.1	33
349	Probing the Electronic Structure and Chemical Bonding in Tricoordinate Uranyl Complexes UO ₂ X ₃ ⁺ (X = F, Cl, Br, I): Competition between Coulomb Repulsion and U-X Bonding. <i>Inorganic Chemistry</i> , 2013, 52, 6617-6626.	1.9	53
350	Probing the electronic structures of low oxidation-state uranium fluoride molecules UF _x ⁺ (x = 2-4). <i>Journal of Chemical Physics</i> , 2013, 139, 244303.	1.2	15
351	A Joint Photoelectron Spectroscopy and Theoretical Study on the Electronic Structure of UCl ₅ ⁺ and UCl ₅ . <i>Chemistry - an Asian Journal</i> , 2013, 8, 2489-2496.	1.7	18
352	On Two Different Objectives of the Concepts of Ionic Radii. <i>Chemistry - A European Journal</i> , 2013, 19, 14758-14767.	1.7	11
353	Photoelectron spectroscopy and the electronic structure of the uranyl tetrachloride dianion: UO ₂ Cl ₄ ²⁻ . <i>Journal of Chemical Physics</i> , 2012, 137, 064315.	1.2	47
354	Photoelectron spectroscopy and theoretical studies of UF ₅ ⁺ and UF ₆ ⁺ . <i>Journal of Chemical Physics</i> , 2012, 136, 194304.	1.2	19
355	The electronic structure and chemical bonding in gold dihydride: AuH ₂ ⁺ and AuH ₂ . <i>Chemical Science</i> , 2012, 3, 3286.	3.7	49
356	Deduction of Bond Length Changes of Symmetric Molecules from Experimental Vibrational Progressions, Including a Topological Mass Factor. <i>Journal of Physical Chemistry A</i> , 2012, 116, 12299-12304.	1.1	9
357	3-Fold-Interpenetrated Uranium-Organic Frameworks: New Strategy for Rationally Constructing Three-Dimensional Uranyl Organic Materials. <i>Inorganic Chemistry</i> , 2012, 51, 3103-3107.	1.9	74
358	Theoretical study on the leaching of palladium in a CO atmosphere. <i>Catalysis Science and Technology</i> , 2012, 2, 2238.	2.1	18
359	Observation and investigation of the uranyl tetrafluoride dianion (UO ₂ F ₄ ²⁻) and its solvation complexes with water and acetonitrile. <i>Chemical Science</i> , 2012, 3, 1137.	3.7	46
360	Theoretical Study of Syngas Hydrogenation to Methanol on the Polar Zn-Terminated ZnO(0001) Surface. <i>Journal of Physical Chemistry C</i> , 2012, 116, 15952-15961.	1.5	45

#	ARTICLE	IF	CITATIONS
361	Electronic Spectra and Excited States of Neptunyl and Its $[\text{NpO}_2\text{Cl}_4]^{2+}$ Complex. <i>Inorganic Chemistry</i> , 2012, 51, 3231-3238.	1.9	27
362	Rare-earth monocarbonyls MCO: comprehensive infrared observations and a transparent theoretical interpretation for M = Sc; Y; La–Lu. <i>Chemical Science</i> , 2012, 3, 1548.	3.7	31
363	Bimetallic Au–Pd Alloy Catalysts for N_2O Decomposition: Effects of Surface Structures on Catalytic Activity. <i>Journal of Physical Chemistry C</i> , 2012, 116, 6222-6232.	1.5	128
364	Probing the electronic structure and chemical bonding of the σ -motifs of thiolate gold nanoparticles: $\text{Au}(\text{SCH}_3)_2^+$ and $\text{Au}_2(\text{SCH}_3)_3^+$. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 9323.	1.3	43
365	Size-Dependent Surface Activity of Rutile and Anatase TiO_2 Nanocrystals: Facile Surface Modification and Enhanced Photocatalytic Performance. <i>Chemistry - A European Journal</i> , 2012, 18, 4759-4765.	1.7	30
366	On the maximum bond multiplicity of carbon: unusual C–C quadruple bonding in molecular C_{10}U . <i>Chemical Science</i> , 2012, 3, 2786.	3.7	49
367	Recent advances in computational modeling and simulations on the An(III)/Ln(III) separation process. <i>Coordination Chemistry Reviews</i> , 2012, 256, 1406-1417.	9.5	117
368	Aurophilic attractions between a closed-shell molecule and a gold cluster. <i>Faraday Discussions</i> , 2011, 152, 169.	1.6	38
369	The mixed cyanide halide Au(I) complexes, $[\text{XAuCN}]^+$ (X = F, Cl, Br, and I): evolution from ionic to covalent bonding. <i>Chemical Science</i> , 2011, 2, 2101.	3.7	41
370	Uranyl-Glycine-Water Complexes in Solution: Comprehensive Computational Modeling of Coordination Geometries, Stabilization Energies, and Luminescence Properties. <i>Inorganic Chemistry</i> , 2011, 50, 2082-2093.	1.9	68
371	Matrix Infrared Spectroscopic and Computational Investigations of the Lanthanide–Methylene Complexes CH_2LnF_2 with Single Ln–C Bonds. <i>Journal of Physical Chemistry A</i> , 2011, 115, 1913-1921.	1.1	31
372	Chemisorption-Induced 2D–3D Structural Transitions in Gold Heptamer: $(\text{CO})_n\text{Au}_7$ ($n = 1-4$). <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 2288-2293.	2.1	29
373	Trivalent Actinide and Lanthanide Separations by Tetradentate Nitrogen Ligands: A Quantum Chemistry Study. <i>Inorganic Chemistry</i> , 2011, 50, 9230-9237.	1.9	96
374	Single-atom catalysis of CO oxidation using Pt1/FeOx. <i>Nature Chemistry</i> , 2011, 3, 634-641.	6.6	5,149
375	Theoretical Study of the Luminescent States and Electronic Spectra of UO_2Cl_2 in an Argon Matrix. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3293-3303.	2.3	33
376	Excited States and Absorption Spectra of UF_6 : A RASPT2 Theoretical Study with Spin–Orbit Coupling. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3223-3231.	2.3	19
377	Insight into methanol synthesis from CO_2 hydrogenation on Cu(111): Complex reaction network and the effects of H_2O . <i>Journal of Catalysis</i> , 2011, 281, 199-211.	3.1	347
378	Geometries, electronic structures, and excited states of UN_2 , NUO^+ , and UO_2^{2+} : a combined CCSD(T), RAS/CASPT2 and TDDFT study. <i>Theoretical Chemistry Accounts</i> , 2011, 129, 467-481.	0.5	39

#	ARTICLE	IF	CITATIONS
379	Theoretical investigations of the catalytic role of water in propene epoxidation on gold nanoclusters: A hydroperoxyl-mediated pathway. <i>Nano Research</i> , 2011, 4, 131-142.	5.8	98
380	Density functional theory investigations on the catalytic mechanisms of hydrazine decompositions on Ir(111). <i>Catalysis Today</i> , 2011, 165, 80-88.	2.2	87
381	Shape control of CoO and LiCoO ₂ nanocrystals. <i>Nano Research</i> , 2010, 3, 1-7.	5.8	76
382	Chemistry on Single Atoms: Spontaneous Hydrogen Production from Reactions of Transition-Metal Atoms with Methanol at Cryogenic Temperatures. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 1302-1305.	7.2	21
383	Theoretical Studies of the Electronic Structure of Compounds of the Actinide Elements. , 2010, , 1893-2012.		8
384	Unusual Selectivity of Gold Catalysts for Hydrogenation of 1,3-Butadiene toward <i>cis</i> -2-Butene: A Joint Experimental and Theoretical Investigation. <i>Journal of Physical Chemistry C</i> , 2010, 114, 3131-3139.	1.5	65
385	Vibrationally Resolved Photoelectron Spectroscopy of Di-Gold Carbonyl Clusters Au ₂ (CO) _{<i>n</i>} ⁺ (<i>n</i> = 1-3): Experiment and Theory. <i>Journal of Physical Chemistry A</i> , 2010, 114, 1247-1254.	1.1	47
386	Photoelectron Imaging and Spectroscopy of M ₂ ⁺ (M = Cs, Cu, Au): Evolution from Ionic to Covalent Bonding. <i>Journal of Physical Chemistry A</i> , 2010, 114, 11244-11251.	1.1	51
387	Theoretical Investigations on the Formation and Dehydrogenation Reaction Pathways of H(NH ₂) ₂ BH ₂ _{<i>n</i>} H (<i>n</i> = 1-4) Oligomers: Importance of Dihydrogen Interactions. <i>Inorganic Chemistry</i> , 2010, 49, 7710-7720.	1.9	38
388	Theoretical Investigations of Geometry, Electronic Structure and Stability of UO ₆ : Octahedral Uranium Hexoxide and Its Isomers. <i>Journal of Physical Chemistry A</i> , 2010, 114, 8837-8844.	1.1	39
389	Adsorption-induced structural changes of gold cations from two- to three-dimensions. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 3038.	1.3	20
390	Diversity of Functionalized Germanium Zintl Clusters: Syntheses and Theoretical Studies of [Ge ₉ PdPPh ₃] ₃ ⁻ and [Ni@(Ge ₉ PdPPh ₃) ₂] ⁻ . <i>Journal of Cluster Science</i> , 2009, 20, 601-609.	1.7	34
391	Out-of-plane dimeric Mn(III) quadridentate Schiff-base complexes: Synthesis, structure and magnetic properties. <i>Inorganica Chimica Acta</i> , 2009, 362, 3563-3568.	1.2	22
392	Thermodynamic Studies and Hydride Transfer Reactions from a Rhodium Complex to BX ₃ Compounds. <i>Journal of the American Chemical Society</i> , 2009, 131, 14454-14465.	6.6	93
393	Evidence of Significant Covalent Bonding in Au(CN) ₂ ⁺ . <i>Journal of the American Chemical Society</i> , 2009, 131, 16368-16370.	6.6	161
394	Shape Control of CdSe Nanocrystals with Zinc Blende Structure. <i>Journal of the American Chemical Society</i> , 2009, 131, 16423-16429.	6.6	168
395	Synthesis of Thermally Stable and Highly Active Bimetallic Au-Ag Nanoparticles on Inert Supports. <i>Chemistry of Materials</i> , 2009, 21, 410-418.	3.2	262
396	Combined Experimental and Theoretical Investigation on the Selectivities of Ag, Au, and Pt Catalysts for Hydrogenation of Crotonaldehyde. <i>Journal of Physical Chemistry C</i> , 2009, 113, 20918-20926.	1.5	41

#	ARTICLE	IF	CITATIONS
397	Theoretical Studies of the Electronic Structure of Compounds of the Actinide Elements. , 2008, , 1893-2012.		31
398	Correlation of Calculated Excited-state Energies and Experimental Quantum Yields of Luminescent Tb(III) β^2 -diketonates. Journal of Physical Chemistry A, 2008, 112, 4527-4530.	1.1	41
399	Noble-Gas-Induced Disproportionation Reactions: Facile Superoxo-to-Peroxo Conversion on Chromium Dioxide. Journal of Physical Chemistry A, 2008, 112, 8606-8611.	1.1	22
400	Infrared Spectra and Electronic Structures of Agostic Uranium Methylidene Molecules. Inorganic Chemistry, 2008, 47, 1435-1442.	1.9	53
401	Chemisorption-induced Structural Changes and Transition from Chemisorption to Physisorption in Au ₆ (CO) _n (n = 4-9). Journal of Physical Chemistry C, 2008, 112, 11920-11928.	1.5	51
402	Low-lying isomers of the B ₉ boron cluster: The planar molecular wheel versus three-dimensional structures. Journal of Chemical Physics, 2008, 129, 024302.	1.2	82
403	Formation of unprecedented actinidecarbon triple bonds in uranium methylidyne molecules. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 18919-18924.	3.3	80
404	Au ₃₄ : A Fluxional Core-Shell Cluster. Journal of Physical Chemistry C, 2007, 111, 8228-8232.	1.5	103
405	On the Chemical Bonding of Gold in Auro-Boron Oxide Clusters Au _n BO-(n= 1-3). Journal of Physical Chemistry A, 2007, 111, 1648-1658.	1.1	44
406	Pd ₂ @Sn ₁₈ : Fusion of Two Endohedral Stannaspherenes. Journal of the American Chemical Society, 2007, 129, 9560-9561.	6.6	116
407	Isomers and Conformers of H(NH ₂ BH ₂) _n H Oligomers: Understanding the Geometries and Electronic Structure of Boron-Nitrogen-Hydrogen Compounds as Potential Hydrogen Storage Materials. Journal of Physical Chemistry C, 2007, 111, 3294-3299.	1.5	38
408	Infrared and DFT Investigations of the XC ₃ and HC ₃ Complexes: Jahn-Teller Distortion and the Methylidyne C-X(H) Stretching Absorptions. Inorganic Chemistry, 2007, 46, 8728-8738.	1.9	22
409	Endohedral Stannaspherenes M@Sn ₁₂ : A Rich Class of Stable Molecular Cage Clusters. Angewandte Chemie - International Edition, 2007, 46, 742-745.	7.2	106
410	Remarkable Dinitrogen Activation and Cleavage by the Gd Dimer: From Dinitrogen Complexes to Ring and Cage Nitrides. Angewandte Chemie - International Edition, 2007, 46, 2911-2914.	7.2	65
411	Chirality, Agostic Interactions, and Pyramidality in Actinide Methylidene Complexes. Angewandte Chemie - International Edition, 2007, 46, 9045-9049.	7.2	40
412	Basis Set Exchange: A Community Database for Computational Sciences. Journal of Chemical Information and Modeling, 2007, 47, 1045-1052.	2.5	2,685
413	Reactions of Cerium Atoms and Dicerium Molecules with CO: Formation of Cerium Carbonyls and Photoconversion to CO-Activated Insertion Molecules. Journal of Physical Chemistry A, 2006, 110, 10206-10211.	1.1	34
414	Experimental and Theoretical Investigations of IR Spectra and Electronic Structures of the U(OH) ₂ , UO ₂ (OH), and UO ₂ (OH) ₂ Molecules. Inorganic Chemistry, 2006, 45, 4157-4166.	1.9	23

#	ARTICLE	IF	CITATIONS
415	Formation and Characterization of the XeOO+Cation in Solid Argon. Journal of the American Chemical Society, 2006, 128, 2504-2505.	6.6	20
416	Sn122-:Â Stannaspherene. Journal of the American Chemical Society, 2006, 128, 8390-8391.	6.6	157
417	Pb122-:Â Plumbaspherene. Journal of Physical Chemistry A, 2006, 110, 10169-10172.	1.1	122
418	Theoretical Probing of Deltahedralcloso-AuroBoranes BxAux2-(x= 5â~12). Inorganic Chemistry, 2006, 45, 5269-5271.	1.9	30
419	On the Structure and Chemical Bonding of Tri-Tungsten Oxide Clusters W3On- and W3On (n = 7â~10):â€% W3O8 As A Potential Molecular Model for O-Deficient Defect Sites in Tungsten Oxides. Journal of Physical Chemistry A, 2006, 110, 85-92.	1.1	83
420	Free tetra- and hexa-coordinated platinum-cyanide dianions, and : A combined photodetachment photoelectron spectroscopic and theoretical study. Chemical Physics, 2006, 329, 230-238.	0.9	22
421	Potential Application of KIÃui Ligands in Actinide Separations. ACS Symposium Series, 2006, , 201-218.	0.5	2
422	Experimental and Theoretical Characterization of Superoxide Complexes [W2O6(O2â~)] and [W3O9(O2â~)]: Models for the Interaction of O2 with Reduced W Sites on Tungsten Oxide Surfaces. Angewandte Chemie - International Edition, 2006, 45, 657-660.	7.2	66
423	The OH radical-H2O molecular interaction potential. Journal of Chemical Physics, 2006, 124, 224318.	1.2	67
424	Experimental and Theoretical Investigation of the Electronic and Geometrical Structures of the Au32 Cluster. Angewandte Chemie - International Edition, 2005, 44, 7119-7123.	7.2	129
425	Photoelectron Spectroscopy of Free Polyoxoanions Mo6O2-19 and W6O2-19 in the Gas Phase.. ChemInform, 2005, 36, no.	0.1	0
426	Reactions of Laser-Ablated Uranium Atoms with H2O in Excess Argon: A Matrix Infrared and Relativistic DFT Investigation of Uranium Oxyhydrides.. ChemInform, 2005, 36, no.	0.1	0
427	Electronic Structure Differences in ZrO2vs HfO2â€. Journal of Physical Chemistry A, 2005, 109, 11521-11525.	1.1	114
428	Electronic and Structural Evolution and Chemical Bonding in Ditungsten Oxide Clusters:Â W2On-and W2On(n= 1â~6). Journal of Physical Chemistry A, 2005, 109, 6019-6030.	1.1	67
429	Unique CO Chemisorption Properties of Gold Hexamer:â€% Au6(CO)n- (n = 0â~3). Journal of the American Chemical Society, 2005, 127, 12098-12106.	6.6	102
430	157 nm Pellicles (Thin Films) for Photolithography:Â Mechanistic Investigation of the VUV and UV-C Photolysis of Fluorocarbons. Journal of the American Chemical Society, 2005, 127, 8320-8327.	6.6	12
431	Reactions of Laser-Ablated Uranium Atoms with H2O in Excess Argon:â€% A Matrix Infrared and Relativistic DFT Investigation of Uranium Oxyhydrides. Inorganic Chemistry, 2005, 44, 2159-2168.	1.9	51
432	Significant Interactions between Uranium and Noble-Gas Atoms: Coordination of the UO2+ Cation by Ne, Ar, Kr, and Xe Atoms. Angewandte Chemie - International Edition, 2004, 43, 2554-2557.	7.2	86

#	ARTICLE	IF	CITATIONS
433	Remarkable second-order optical nonlinearity of nano-sized Au ₂₀ cluster: a TDDFT study. <i>Chemical Physics Letters</i> , 2004, 388, 353-357.	1.2	59
434	Noble gas-uranium coordination and intersystem crossing for the CUO(Ne) _x (Ng) _n (Ng=Ar, Kr, Xe) complexes in solid neon. <i>New Journal of Chemistry</i> , 2004, 28, 289-294.	1.4	17
435	On the Noble-Gas-Induced Intersystem Crossing for the CUO Molecule: Experimental and Theoretical Investigations of CUO(Ng) _n (Ng = Ar, Kr, Xe; n= 1, 2, 3, 4) Complexes in Solid Neon. <i>Inorganic Chemistry</i> , 2004, 43, 882-894.	1.9	54
436	On the Electronic Structure of Molecular UO ₂ in the Presence of Ar Atoms: Evidence for Direct U-Ar Bonding. <i>Journal of the American Chemical Society</i> , 2004, 126, 3424-3425.	6.6	76
437	Raman under nitrogen. The high-resolution Raman spectroscopy of crystalline uranocene, thorocene, and ferrocene. <i>Journal of Chemical Physics</i> , 2004, 120, 2708-2718.	1.2	32
438	Toward the Solution Synthesis of the Tetrahedral Au ₂₀ Cluster. <i>Journal of Physical Chemistry B</i> , 2004, 108, 12259-12263.	1.2	106
439	Photoelectron Spectroscopy of Free Polyoxoanions Mo ₆ O ₁₉ ²⁻ and W ₆ O ₁₉ ²⁻ in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2004, 108, 10089-10093.	1.1	54
440	Icosahedral gold cage clusters: M@Au ₁₂ (M=V, Nb, and Ta). <i>Journal of Chemical Physics</i> , 2004, 121, 8369.	1.2	137
441	Au ₂₀ : A Tetrahedral Cluster. <i>Science</i> , 2003, 299, 864-867.	6.0	1,091
442	Infrared absorption-edges of molecular nonlinear optical crystals: an ab initio calculation. <i>Applied Physics A: Materials Science and Processing</i> , 2003, 76, 427-431.	1.1	7
443	Experimental Observation and Confirmation of Icosahedral W@Au ₁₂ and Mo@Au ₁₂ Molecules. <i>ChemInform</i> , 2003, 34, no.	0.1	0
444	Au ₂₀ : A Tetrahedral Cluster. <i>ChemInform</i> , 2003, 34, no.	0.1	3
445	Bonding of Multiple Noble-Gas Atoms to CUO in Solid Neon: CUO(Ng) _n (Ng=Ar, Kr, Xe; n=1, 2, 3, 4) Complexes and the Singlet-Triplet Crossover Point. <i>Chemistry - A European Journal</i> , 2003, 9, 4781-4788.	1.7	22
446	Hydrocarbon analogues of boron clusters: planarity, aromaticity and antiaromaticity. <i>Nature Materials</i> , 2003, 2, 827-833.	13.3	650
447	Spiers Memorial Lecture. <i>Faraday Discussions</i> , 2003, 124, 1.	1.6	28
448	Noble Gas-Actinide Complexes of the CUO Molecule with Multiple Ar, Kr, and Xe Atoms in Noble-Gas Matrices. <i>Journal of the American Chemical Society</i> , 2003, 125, 3126-3139.	6.6	124
449	Noble Gas-Actinide Compounds: Evidence for the Formation of Distinct CUO(Ar) _{4-n} (Xe) _n and CUO(Ar) _{4-n} (Kr) _n (n= 1, 2, 3, 4) Complexes. <i>Journal of the American Chemical Society</i> , 2002, 124, 9016-9017.	6.6	62
450	Experimental and Theoretical Studies of the Products of Laser-Ablated Thorium Atom Reactions with H ₂ O in Excess Argon. <i>Journal of the American Chemical Society</i> , 2002, 124, 6723-6733.	6.6	42

#	ARTICLE	IF	CITATIONS
451	Noble Gas-Actinide Compounds: Complexation of the CUO Molecule by Ar, Kr, and Xe Atoms in Noble Gas Matrices. <i>Science</i> , 2002, 295, 2242-2245.	6.0	224
452	Experimental Observation and Confirmation of Icosahedral W@Au ₁₂ and Mo@Au ₁₂ Molecules. <i>Angewandte Chemie - International Edition</i> , 2002, 41, 4786-4789.	7.2	325
453	Title is missing!. <i>Journal of Cluster Science</i> , 2002, 13, 137-163.	1.7	42
454	Title is missing!. <i>Journal of Cluster Science</i> , 2002, 13, 119-136.	1.7	39
455	Electronic coupling between molybdenum and tungsten quadruple bonds in molecular squares and extended chains linked by oxalate, acetylenedicarboxylate, and perfluoroterephthalate bridges. <i>Israel Journal of Chemistry</i> , 2001, 41, 187-195.	1.0	7
456	M ₂ delta-to-oxalate pi* conjugation in oxalate-bridged complexes containing M-M quadruple bonds. <i>Chemical Communications</i> , 2001, , 2382-2383.	2.2	18
457	A Combined Theoretical and Experimental Study of the Reaction Products of Laser-Ablated Thorium Atoms with CO: A First Identification of the CThO, CThO-, OThCCO, OTh(Î-3-CCO), and Th(CO) _n (n= 1-6) Molecules. <i>Inorganic Chemistry</i> , 2001, 40, 5448-5460.	1.9	41
458	Ground-State Reversal by Matrix Interaction: Electronic States and Vibrational Frequencies of CUO in Solid Argon and Neon. <i>Angewandte Chemie - International Edition</i> , 2000, 39, 4565-4567.	7.2	42
459	Reactions of Laser-Ablated U and Th with CO ₂ : Neon Matrix Infrared Spectra and Density Functional Calculations of OUCO, OThCO, and Other Products. <i>Journal of the American Chemical Society</i> , 2000, 122, 11440-11449.	6.6	63
460	Electronic Structures and Properties of Eight-Coordinate Metal-Polyarsenic Complexes MAs ₈ n- (M = Tl, Bi, Pb, Sn, Te, Se, S). <i>Journal of the American Chemical Society</i> , 2000, 122, 11440-11449.	1.9	21
461	Ground-State Reversal by Matrix Interaction: Electronic States and Vibrational Frequencies of CUO in Solid Argon and Neon This work was supported by the National Science Foundation (CHE 97-00116), the US Department of Energy (DE-FG02-86ER13519), and the Los Alamos National Laboratory, and by grants of computer time from the Ohio Supercomputer Center and the Pacific Northwest National Laboratory. <i>Angewandte Chemie - International Edition</i> , 2000, 39, 4565-4567.	7.2	1
462	Infrared Absorption Cut-Off of Molecular Nonlinear Optical Crystals: Theoretical Studies on Vibrational Spectra of MDNB, Urea and MNA Molecules. <i>Chinese Physics Letters</i> , 1999, 16, 925-927.	1.3	1
463	Reactions of Th Atoms with CO: The First Thorium Carbonyl Complex and an Unprecedented Bent Triplet Insertion Product. <i>Journal of the American Chemical Society</i> , 1999, 121, 12188-12189.	6.6	54
464	Reaction of Laser-Ablated Uranium Atoms with CO: Infrared Spectra of the CUO, CUO-, OUCCO, (Î-2-C ₂)UO ₂ , and U(CO) _x (x = 1-6) Molecules in Solid Neon. <i>Journal of the American Chemical Society</i> , 1999, 121, 9712-9721.	6.6	125
465	Bis(arene) Actinide Sandwich Complexes, (Î-6-C ₆ H ₃ R ₃) ₂ An: Linear or Bent?. <i>Journal of the American Chemical Society</i> , 1999, 121, 10243-10244.	6.6	22
466	Relativistic Density Functional Study of the Geometry, Electronic Transitions, Ionization Energies, and Vibrational Frequencies of Protactinocene, Pa(Î-8-C ₈ H ₈) ₂ . <i>Journal of the American Chemical Society</i> , 1998, 120, 11456-11466.	6.6	60
467	Electronic Structure of Cycloheptatrienyl Sandwich Compounds of Actinides: An(Î-7-C ₇ H ₇) ₂ (An = Th, Pa). <i>Journal of the American Chemical Society</i> , 1998, 120, 11456-11466.	6.6	93
468	Electronic Structure and Properties of Trihalogen Cations X ₃ ⁺ and XY ₂ ⁺ (X, Y = F, Cl, Br, I). <i>Inorganic Chemistry</i> , 1996, 35, 100-109.	1.9	16

#	ARTICLE	IF	CITATIONS
469	Theoretical studies of (d-p) π bonding, electronic spectra, and reactivities in homo- and heterometallic clusters: $[Mo_{3-n}W_nX_4(H_2O)_9]^{4+}$ ($X = O, S, Se, Te; n = 0-3$). <i>Journal of Cluster Science</i> , 1996, 7, 469-500.	1.7	11
470	Localized Molecular Orbital Studies of Fullerenes: C ₆₀ and C ₇₀ . <i>Fullerenes, Nanotubes, and Carbon Nanostructures</i> , 1994, 2, 35-48.	0.6	2
471	Quantum chemical studies on the bonding characteristics of some M ₃ X ₄ transition-metal halogenide clusters. <i>Journal of Cluster Science</i> , 1994, 5, 505-521.	1.7	5
472	Electronic structures and d π -p π bonding of some M ₃ X ₄ cluster compounds. <i>Polyhedron</i> , 1994, 13, 1841-1851.	1.0	26
473	Ab initio studies of electronic structures and quasi-aromaticity in M ₃ S ₄ μ_4 -O ₄ +n (M = Mo, W; n = 0-4) clusters. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1994, 90, 39-45.	1.7	24
474	Symmetrical clusters of carbon and boron. <i>Chemical Physics Letters</i> , 1993, 201, 465-469.	1.2	70
475	Ab initio studies on the electronic structures of certain 10 π -electron six-membered ring compounds. <i>Computational and Theoretical Chemistry</i> , 1993, 280, 223-231.	1.5	26
476	Electronic structures of $[M_3(\mu_3-X)(\mu_2-S)_2]^{4+}$ (M = Mo, Ti) cluster compounds and the effects of the μ_3-X cap to the self-assembly in cluster synthesis. <i>Computational and Theoretical Chemistry</i> , 1991, 251, 165-171.	1.5	4
477	Quantum chemical calculations on buckminsterfullerene and related structures. II. The electronic structure and spectra of some C _n and C _n Ca ₂₊ cages. <i>International Journal of Quantum Chemistry</i> , 1991, 39, 331-344.	1.0	34
478	Quantum-chemical investigation of Buckminsterfullerene and related carbon clusters (I): The electronic structure and UV spectra of Buckminsterfullerene, and other C ₆₀ cages. <i>International Journal of Quantum Chemistry</i> , 1990, 37, 599-607.	1.0	56
479	Embedding Single Platinum Atoms Into Nickel Nanoparticles Affords Highly Selective Catalysts for Lignin Conversion. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0