Jun Li

List of Publications by Year in Descending Order

469 papers	36,987 citations	85 h-index	179 g-index
517 ext. papers	44,868 ext. citations	9.9 avg, IF	7.74 L-index

#	Paper	IF	Citations
469	Ladder Oxygenation of Group VIII Metal Clusters and the Formation of Metalloxocubes MO.. *Journal of Physical Chemistry Letters*, **2022**, 733-739	6.4	1
468	Infrared spectroscopic signature of the structural diversity of the water heptamer. *Cell Reports Physical Science*, **2022**, 3, 100748	6.1	3
467	Few-Atom Pt Ensembles Enable Efficient Catalytic Cyclohexane Dehydrogenation for Hydrogen Production.. *Journal of the American Chemical Society*, **2022**,	16.4	10
466	AuB: an Au-borozene complex.. *Chemical Communications*, **2022**,	5.8	1
465	Modification of Palladium Nanocrystals with Single Atom Platinum via an Electrochemical Self-Catalysis Strategy for Efficient Formic Acid Electrooxidation.. *ACS Applied Materials & Interfaces*, **2022**,	9.5	1
464	Doping Ruthenium into Metal Matrix for Promoted pH-Universal Hydrogen Evolution.. *Advanced Science*, **2022**, e2200010	13.6	5
463	Quantum chemical studies of the electronic structures of anti-tumor agents: AuIIIL+ (L□=□porphine, tetraphenylporphyrin). *Computational and Theoretical Chemistry*, **2022**, 1211, 113685	2	
462	Leaching of palladium atoms from small cluster models during Heck reactions □An experimental and theoretical study. *Catalysis Communications*, **2022**, 165, 106441	3.2	0
461	Theoretical studies of MXene-supported single-atom catalysts: Os1/Ti2CS2 for low-temperature CO oxidation. *Science China Materials*, **2022**, 65, 1303-1312	7.1	0
460	Exploring Stability of Transition-Metal Single Atoms on Cu2O Surfaces. *Journal of Physical Chemistry C*, **2022**, 126, 8065-8078	3.8	0
459	Non-noble metal single-atom catalyst with MXene support: Fe1/Ti2CO2 for CO oxidation. *Chinese Journal of Catalysis*, **2022**, 43, 1830-1841	11.3	0
458	Monovalent lanthanide(I) in borozene complexes. *Nature Communications*, **2021**, 12, 6467	17.4	3
457	Scalable two-step annealing method for preparing ultra-high-density single-atom catalyst libraries. *Nature Nanotechnology*, **2021**,	28.7	40
456	A general strategy for preparing pyrrolic-N type single-atom catalysts via pre-located isolated atoms. *Nature Communications*, **2021**, 12, 6806	17.4	18
455	Size sensitivity of supported Ru catalysts for ammonia synthesis: From nanoparticles to subnanometric clusters and atomic clusters. *CheM*, **2021**,	16.2	4
454	Formation and Characterization of BeFe(CO) Anion with Beryllium-Iron Bonding. *Angewandte Chemie - International Edition*, **2021**, 60, 9334-9338	16.4	4
453	Formation and Characterization of BeFe(CO)4□Anion with Beryllium□Iron Bonding. *Angewandte Chemie*, **2021**, 133, 9420-9424	3.6	0

452	Expanded Inverse-Sandwich Complexes of Lanthanum Borides: LaB and LaB. *Journal of Physical Chemistry A*, **2021**, 125, 2622-2630	2.8	10
451	Understanding the Electronic Structure and Stability of BnXn0/2 (n = 4, 6; X = H, F, Cl, Br, I, At, Ts) Clusters *Chinese Journal of Chemistry*, **2021**, 39, 1811-1818	4.9	
450	Double Aromaticity in a Planar Zinc-Doped Gold Cluster: AuZn. *Journal of Physical Chemistry A*, **2021**, 125, 4606-4613	2.8	9
449	Norm-Conserving Pseudopotentials and Basis Sets to Explore Actinide Chemistry in Complex Environments. *Journal of Chemical Theory and Computation*, **2021**, 17, 3360-3371	6.4	4
448	Metal Oxo-Fluoride Molecules OMF (M = Mn and Fe; = 1-4) and OMnF: Matrix Infrared Spectra and Quantum Chemistry. *Inorganic Chemistry*, **2021**, 60, 7687-7696	5.1	1
447	Screening silica-confined single-atom catalysts for nonoxidative conversion of methane. *Journal of Chemical Physics*, **2021**, 154, 174706	3.9	2
446	Triazine COF-supported single-atom catalyst (Pd1/trzn-COF) for CO oxidation. *Science China Materials*, **2021**, 64, 1939-1951	7.1	6
445	Unveiling the In Situ Generation of a Monovalent Fe(I) Site in the Single-Fe-Atom Catalyst for Electrochemical CO2 Reduction. *ACS Catalysis*, **2021**, 11, 7292-7301	13.1	14
444	Orientational Alignment of Oxygen Vacancies: Electric-Field-Inducing Conductive Channels in TiO Film to Boost Photocatalytic Conversion of CO into CO. *Nano Letters*, **2021**, 21, 5060-5067	11.5	3
443	Electronic Structure and Spectroscopic Properties of Group-7 Tri-Oxo-Halides MOX (M = Mn-Bh, X = F-Ts). *Inorganic Chemistry*, **2021**, 60, 9504-9515	5.1	1
442	Underpotential-deposition synthesis and in-line electrochemical analysis of single-atom copper electrocatalysts. *Applied Catalysis B: Environmental*, **2021**, 289, 120028	21.8	15
441	A highly efficient Fenton-like catalyst based on isolated diatomic Fe-Co anchored on N-doped porous carbon. *Chemical Engineering Journal*, **2021**, 404, 126376	14.7	52
440	Phosphorene Supported Single-Atom Catalysts for CO Oxidation: A Computational Study. *ChemPhysChem*, **2021**, 22, 378-385	3.2	2
439	CoO-metalloxocubes: a new class of perovskite-like neutral clusters with cubic aromaticity. *National Science Review*, **2021**, 8, nwaa201	10.8	13
438	Non-noble metal single-atom catalyst of Co1/MXene (Mo2CS2) for CO oxidation. *Science China Materials*, **2021**, 64, 651-663	7.1	19
437	Highly efficient ammonia synthesis at low temperature over a Ru-Co catalyst with dual atomically dispersed active centers. *Chemical Science*, **2021**, 12, 7125-7137	9.4	12
436	Coordination Sphere of Lanthanide Aqua Ions Resolved with Ab Initio Molecular Dynamics and X-ray Absorption Spectroscopy. *Inorganic Chemistry*, **2021**, 60, 3117-3130	5.1	16
435	Rod-Shaped Silver Supercluster Unveiling Strong Electron Coupling between Substituent Icosahedral Units. *Journal of the American Chemical Society*, **2021**, 143, 12261-12267	16.4	11

434	Theoretical Inspection of M1/PMA Single-Atom Electrocatalyst: Ultra-High Performance for Water Splitting (HER/OER) and Oxygen Reduction Reactions (OER). *ACS Catalysis*, **2021**, 11, 8929-8941	13.1	28
433	Single Iridium Atom Doped NiP Catalyst for Optimal Oxygen Evolution. *Journal of the American Chemical Society*, **2021**, 143, 13605-13615	16.4	32
432	Using general computational chemistry strategy to unravel the reactivity of emerging pollutants: An example of sulfonamide chlorination. *Water Research*, **2021**, 202, 117391	12.5	3
431	Heterogeneous Two-Atom Single-Cluster Catalysts for the Nitrogen Electroreduction Reaction. *Journal of Physical Chemistry C*, **2021**, 125, 19821-19830	3.8	5
430	Anchoring single platinum atoms onto nickel nanoparticles affords highly selective catalysts for lignin conversion. *Cell Reports Physical Science*, **2021**, 2, 100567	6.1	2
429	Diketopyrrolopyrrole-based supramolecular nano-leveler for the enhancement of conformal copper electrodeposition. *Applied Surface Science*, **2021**, 569, 150982	6.7	0
428	Tandem catalyzing the hydrodeoxygenation of 5-hydroxymethylfurfural over a NiFe intermetallic supported Pt single-atom site catalyst. *Chemical Science*, **2021**, 12, 4139-4146	9.4	11
427	Adsorption energy as a promising single-parameter descriptor for single atom catalysis in the oxygen evolution reaction. *Journal of Materials Chemistry A*, **2021**, 9, 6442-6450	13	7
426	Cooperative Catalysis by Multiple Active Centers in Nonoxidative Conversion of Methane. *Journal of Physical Chemistry C*, **2020**, 124, 13656-13663	3.8	12
425	Efficient electrically powered CO2-to-ethanol via suppression of deoxygenation. *Nature Energy*, **2020**, 5, 478-486	62.3	163
424	Non-noble metal single-atom catalysts with phosphotungstic acid (PTA) support: A theoretical study of ethylene epoxidation. *Science China Materials*, **2020**, 63, 1003-1014	7.1	21
423	2-Butene Tetraanion Bridged Dinuclear Samarium(III) Complexes via Sm(II)-Mediated Reduction of Electron-Rich Olefins. *Journal of the American Chemical Society*, **2020**, 142, 10705-10714	16.4	9
422	Iridium single-atom catalyst on nitrogen-doped carbon for formic acid oxidation synthesized using a general host-guest strategy. *Nature Chemistry*, **2020**, 12, 764-772	17.6	207
421	Infrared spectroscopy of neutral water clusters at finite temperature: Evidence for a noncyclic pentamer. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 15423-15428	11.5	24
420	A Single-Atom Manipulation Approach for Synthesis of Atomically Mixed Nanoalloys as Efficient Catalysts. *Angewandte Chemie - International Edition*, **2020**, 59, 13568-13574	16.4	10
419	Spherical trihedral metallo-borospherenes. *Nature Communications*, **2020**, 11, 2766	17.4	20
418	A Single-Atom Manipulation Approach for Synthesis of Atomically Mixed Nanoalloys as Efficient Catalysts. *Angewandte Chemie*, **2020**, 132, 13670-13676	3.6	6
417	High-loading and thermally stable Pt1/MgAl1.2Fe0.8O4 single-atom catalysts for high-temperature applications. *Science China Materials*, **2020**, 63, 949-958	7.1	21

416	Surface Modification Strategy for Promoting the Performance of Non-noble Metal Single-Atom Catalysts in Low-Temperature CO Oxidation. *ACS Applied Materials & Interfaces*, **2020**, 12, 19457-19466	8.5	8
415	Catalytic mechanism and bonding analyses of Au-Pd single atom alloy (SAA): CO oxidation reaction. *Science China Materials*, **2020**, 63, 993-1002	7.1	14
414	Ultrahigh-Loading of Ir Single Atoms on NiO Matrix to Dramatically Enhance Oxygen Evolution Reaction. *Journal of the American Chemical Society*, **2020**, 142, 7425-7433	16.4	186
413	Multiple Bonding Between Group 3 Metals and Fe(CO)3□*Angewandte Chemie*, **2020**, 132, 2364-2368	3.6	0
412	Revisiting the Intriguing Electronic Features of the BeOBeC Carbyne and Some Isomers: A Quantum-Chemical Assessment. *Angewandte Chemie*, **2020**, 132, 17414-17418	3.6	
411	On the theoretical construction of Nb2N2-based superatoms by external field strategies. *Chemical Physics Letters*, **2020**, 754, 137709	2.5	4
410	Unravelling the Enigma of Nonoxidative Conversion of Methane on Iron Single-Atom Catalysts. *Angewandte Chemie*, **2020**, 132, 18745-18749	3.6	6
409	Unravelling the Enigma of Nonoxidative Conversion of Methane on Iron Single-Atom Catalysts. *Angewandte Chemie - International Edition*, **2020**, 59, 18586-18590	16.4	20
408	Formation and Characterization of a BeOBeC Multiple Radical Featuring a Quartet Carbyne Moiety. *Angewandte Chemie - International Edition*, **2020**, 59, 6923-6928	16.4	9
407	Formation and Characterization of a BeOBeC Multiple Radical Featuring a Quartet Carbyne Moiety. *Angewandte Chemie*, **2020**, 132, 6990-6995	3.6	9
406	Single-Atom AuIN3 Site for Acetylene Hydrochlorination Reaction. *ACS Catalysis*, **2020**, 10, 1865-1870	13.1	41
405	Infrared Spectroscopy of Neutral Water Dimer Based on a Tunable Vacuum Ultraviolet Free Electron Laser. *Journal of Physical Chemistry Letters*, **2020**, 11, 851-855	6.4	22
404	Constructing High-Loading Single-Atom/Cluster Catalysts via an Electrochemical Potential Window Strategy. *Journal of the American Chemical Society*, **2020**, 142, 3375-3383	16.4	78
403	Development of novel highly stable synergistic quaternary photocatalyst for the efficient hydrogen evolution reaction. *Applied Surface Science*, **2020**, 510, 145498	6.7	11
402	Tuning the Electronic Properties and Performance of Low-Temperature CO Oxidation of the Gold Cluster by Oriented External Electronic Field. *Journal of Physical Chemistry Letters*, **2020**, 11, 1093-1099	6.4	12
401	Giant Emission Enhancement of Solid-State Gold Nanoclusters by Surface Engineering. *Angewandte Chemie*, **2020**, 132, 8347-8353	3.6	7
400	Gas-assisted transformation of gold from fcc to the metastable 4H phase. *Nature Communications*, **2020**, 11, 552	17.4	8
399	3D hierarchical heterostructure assembled by NiFe LDH/(NiFe)Sx on biomass-derived hollow carbon microtubes as bifunctional electrocatalysts for overall water splitting. *Electrochimica Acta*, **2020**, 348, 136339	6.7	33

398	Cooperative CO2-to-ethanol conversion via enriched intermediates at molecule-metal catalyst interfaces. *Nature Catalysis*, **2020**, 3, 75-82	36.5	164
397	Tuning radical interactions in trisradical tricationic complexes by varying host-cavity sizes. *Chemical Science*, **2020**, 11, 107-112	9.4	9
396	On the mechanism of H2 activation over single-atom catalyst: An understanding of Pt1/WO in the hydrogenolysis reaction. *Chinese Journal of Catalysis*, **2020**, 41, 524-532	11.3	28
395	Multiple Bonding Between Group 3 Metals and Fe(CO). *Angewandte Chemie - International Edition*, **2020**, 59, 2344-2348	16.4	9
394	A milestone in single-atom catalysis for direct formic acid fuel cell. *National Science Review*, **2020**, 7, 1762	20.8	1
393	Carbon Monoxide Gas Induced 4H-to- Phase Transformation of Gold As Revealed by Transmission Electron Microscopy. *Inorganic Chemistry*, **2020**, 59, 14415-14423	5.1	1
392	Understanding the Uniqueness of 2p Elements in Periodic Tables. *Chemistry - A European Journal*, **2020**, 26, 15558-15564	4.8	17
391	Identification of the Electronic and Structural Dynamics of Catalytic Centers in Single-Fe-Atom Material. *CheM*, **2020**, 6, 3440-3454	16.2	79
390	From "S" to "O": experimental and theoretical insights into the atmospheric degradation mechanism of dithiophosphinic acids.. *RSC Advances*, **2020**, 10, 40035-40042	3.7	1
389	Wet carbonate-promoted radical arylation of vinyl pinacolboronates with diaryliodonium salts yields substituted olefins. *Communications Chemistry*, **2020**, 3,	6.3	4
388	Revisiting the Intriguing Electronic Features of the BeOBeC Carbyne and Some Isomers: A Quantum-Chemical Assessment. *Angewandte Chemie - International Edition*, **2020**, 59, 17261-17265	16.4	0
387	High-Valent Nickel Promoted by Atomically Embedded Copper for Efficient Water Oxidation. *ACS Catalysis*, **2020**, 10, 9725-9734	13.1	42
386	Selective hydrogenation of acetylene on graphene-supported non-noble metal single-atom catalysts. *Science China Materials*, **2020**, 63, 1741-1749	7.1	12
385	Insights into the electronic origin of enhancing the catalytic activity of Co3O4 for oxygen evolution by single atom ruthenium. *Nano Today*, **2020**, 34, 100955	17.9	12
384	Theoretical Understandings of Graphene-based Metal Single-Atom Catalysts: Stability and Catalytic Performance. *Chemical Reviews*, **2020**, 120, 12315-12341	68.1	125
383	Infrared spectroscopic study of hydrogen bonding topologies in the smallest ice cube. *Nature Communications*, **2020**, 11, 5449	17.4	15
382	Exploring the difference of bonding strength between silver(I) and chalcogenides in block copolymer systems. *Polymer Chemistry*, **2020**, 11, 7087-7093	4.9	12
381	Atomically-precise dopant-controlled single cluster catalysis for electrochemical nitrogen reduction. *Nature Communications*, **2020**, 11, 4389	17.4	52

380	Coordination engineering of iridium nanocluster bifunctional electrocatalyst for highly efficient and pH-universal overall water splitting. *Nature Communications*, **2020**, 11, 4246	17.4	92
379	Chromium Single-Atom Catalyst with Graphyne Support: A Theoretical Study of NO Oxidation and Reduction. *ACS Catalysis*, **2020**, 10, 11951-11961	13.1	21
378	Efficient GoldPalladium Nanoparticles Stabilized by Poly(amic acid) Salt: Synthesis and Application in Catalytic Oxidation of Amines to Imines. *Journal of Inorganic and Organometallic Polymers and Materials*, **2020**, 30, 1384-1392	3.2	2
377	Dual Metal Active Sites in an Ir1/FeOx Single-Atom Catalyst: A Redox Mechanism for the Water-Gas Shift Reaction. *Angewandte Chemie*, **2020**, 132, 12968-12975	3.6	13
376	Excited-State Chemistry: Photocatalytic Methanol Oxidation by Uranyl@Zeolite through Oxygen-Centered Radicals. *Inorganic Chemistry*, **2020**, 59, 6287-6300	5.1	4
375	Isolated Ni Atoms Dispersed on Ru Nanosheets: High-Performance Electrocatalysts toward Hydrogen Oxidation Reaction. *Nano Letters*, **2020**, 20, 3442-3448	11.5	80
374	Dual Metal Active Sites in an Ir /FeO Single-Atom Catalyst: A Redox Mechanism for the Water-Gas Shift Reaction. *Angewandte Chemie - International Edition*, **2020**, 59, 12868-12875	16.4	49
373	Rational design of an efficient descriptor for single-atom catalysts in the hydrogen evolution reaction. *Journal of Materials Chemistry A*, **2020**, 8, 9202-9208	13	20
372	Distinct electronic structures and bonding interactions in inverse-sandwich samarium and ytterbium biphenyl complexes. *Chemical Science*, **2020**, 12, 227-238	9.4	6
371	Understanding Periodic and Non-periodic Chemistry in Periodic Tables. *Frontiers in Chemistry*, **2020**, 8, 813	5	8
370	Giant Emission Enhancement of Solid-State Gold Nanoclusters by Surface Engineering. *Angewandte Chemie - International Edition*, **2020**, 59, 8270-8276	16.4	28
369	Remarkable active-site dependent HO promoting effect in CO oxidation. *Nature Communications*, **2019**, 10, 3824	17.4	53
368	Probing the electronic structure of the CoB16drum complex: Unusual oxidation state of Co *Chinese Journal of Chemical Physics*, **2019**, 32, 241-247	0.9	3
367	Regulating the coordination structure of single-atom Fe-NC catalytic sites for benzene oxidation. *Nature Communications*, **2019**, 10, 4290	17.4	173
366	Unravelling a general mechanism of converting ionic B/N complexes into neutral B/N analogues of alkanes: HH dihydrogen bonding assisted dehydrogenation. *Chemical Communications*, **2019**, 55, 12239-12242	5.8	16
365	Unraveling the coordination structure-performance relationship in Pt/FeO single-atom catalyst. *Nature Communications*, **2019**, 10, 4500	17.4	137
364	Norm-Conserving Pseudopotentials and Basis Sets To Explore Lanthanide Chemistry in Complex Environments. *Journal of Chemical Theory and Computation*, **2019**, 15, 5987-5997	6.4	22
363	Copper atom-pair catalyst anchored on alloy nanowires for selective and efficient electrochemical reduction of CO. *Nature Chemistry*, **2019**, 11, 222-228	17.6	337

362	Synergy of the catalytic activation on Ni and the CeO2TiO2/Ce2Ti2O7 stoichiometric redox cycle for dramatically enhanced solar fuel production. *Energy and Environmental Science*, **2019**, 12, 767-779	35.4	57
361	Breaking Long-Range Order in Iridium Oxide by Alkali Ion for Efficient Water Oxidation. *Journal of the American Chemical Society*, **2019**, 141, 3014-3023	16.4	172
360	[La(-B)La] (= 7-9): a new class of inverse sandwich complexes. *Chemical Science*, **2019**, 10, 2534-2542	9.4	42
359	Structure and Bonding in [Sb@In8Sb12]3and [Sb@In8Sb12]5*Angewandte Chemie*, **2019**, 131, 8455-8459	3.6	8
358	Highly active enzymetal nanohybrids synthesized in proteinolymer conjugates. *Nature Catalysis*, **2019**, 2, 718-725	36.5	60
357	The df-d Dative Bonding in a Uranium-Cobalt Heterobimetallic Complex for Efficient Nitrogen Fixation. *Inorganic Chemistry*, **2019**, 58, 7433-7439	5.1	9
356	Re B and Re B: New Members of the Transition-Metal-Centered Borometallic Molecular Wheel Family. *Journal of Physical Chemistry A*, **2019**, 123, 5317-5324	2.8	23
355	LaB: an inverse triple-decker lanthanide boron cluster. *Chemical Communications*, **2019**, 55, 7864-7867	5.8	25
354	Probing the structures and bonding of size-selected boron and doped-boron clusters. *Chemical Society Reviews*, **2019**, 48, 3550-3591	58.5	90
353	Dynamic Frustrated Lewis Pairs on Ceria for Direct Nonoxidative Coupling of Methane. *ACS Catalysis*, **2019**, 9, 5523-5536	13.1	25
352	Structure and Bonding in [Sb@In Sb] and [Sb@In Sb]. *Angewandte Chemie - International Edition*, **2019**, 58, 8367-8371	16.4	23
351	Mechanistic Investigations on Thermal Hydrogenation of CO2 to Methanol by Nanostructured CeO2(100): The Crystal-Plane Effect on Catalytic Reactivity. *Journal of Physical Chemistry C*, **2019**, 123, 11763-11771	3.8	15
350	CeO(111) electronic reducibility tuned by ultra-small supported bimetallic Pt-Cu clusters. *Physical Chemistry Chemical Physics*, **2019**, 21, 15286-15296	3.6	13
349	Selective photoelectrochemical oxidation of glycerol to high value-added dihydroxyacetone. *Nature Communications*, **2019**, 10, 1779	17.4	83
348	Triple bonds between iron and heavier group-14 elements in the AFe(CO) complexes (A = Ge, Sn, and Pb). *Chemical Communications*, **2019**, 55, 5685-5688	5.8	13
347	Structure regulation of noble-metal-based nanomaterials at an atomic level. *Nano Today*, **2019**, 26, 164-175	17.9	24
346	Quantifying the Bonding Strength of Gold-Chalcogen Bonds in Block Copolymer Systems. *Chemistry - an Asian Journal*, **2019**, 14, 1481-1486	4.5	13
345	Heterogeneous Single-Cluster Catalysts for Selective Semihydrogenation of Acetylene with Graphdiyne-Supported Triatomic Clusters. *Journal of Physical Chemistry C*, **2019**, 123, 10494-10500	3.8	27

344	Structural exploration of Au M (M = Si, Ge, Sn; = 9-12) clusters with a revised genetic algorithm.. *RSC Advances*, **2019**, 9, 7432-7439	3.7	4
343	High Uptake of ReO and CO Conversion by a Radiation-Resistant Thorium-Nickle [Th Ni] Nanocage-Based Metal-Organic Framework. *Angewandte Chemie - International Edition*, **2019**, 58, 6022-6027	16.4	77
342	High Uptake of ReO4 and CO2 Conversion by a Radiation-Resistant Thorium Nickle [Th48Ni6] Nanocage-Based Metal Organic Framework. *Angewandte Chemie*, **2019**, 131, 6083-6088	3.6	13
341	Atomically Dispersed Ruthenium Species Inside Metal-Organic Frameworks: Combining the High Activity of Atomic Sites and the Molecular Sieving Effect of MOFs. *Angewandte Chemie - International Edition*, **2019**, 58, 4271-4275	16.4	92
340	Atomically Dispersed Ruthenium Species Inside Metal Organic Frameworks: Combining the High Activity of Atomic Sites and the Molecular Sieving Effect of MOFs. *Angewandte Chemie*, **2019**, 131, 4315-4319	3.6	12
339	A Ligand-Protected Golden Fullerene: The Dipyridylamido Au328+ Nanocluster. *Angewandte Chemie*, **2019**, 131, 5967-5970	3.6	25
338	An Ultrastable Matryoshka [Hf] Nanocluster as a Luminescent Sensor for Concentrated Alkali and Acid. *Angewandte Chemie - International Edition*, **2019**, 58, 16610-16616	16.4	26
337	An Ultrastable Matryoshka [Hf13] Nanocluster as a Luminescent Sensor for Concentrated Alkali and Acid. *Angewandte Chemie*, **2019**, 131, 16763-16769	3.6	4
336	The Key Role of Support Surface Hydrogenation in the CH4 to CH3OH Selective Oxidation by a ZrO2-Supported Single-Atom Catalyst. *ACS Catalysis*, **2019**, 9, 8903-8909	13.1	33
335	Fluorine substitution enabling pseudocapacitive intercalation of sodium ions in niobium oxyfluoride. *Journal of Materials Chemistry A*, **2019**, 7, 20813-20823	13	10
334	Understanding Heterolytic H2 Cleavage and Water-Assisted Hydrogen Spillover on Fe3O4(001)-Supported Single Palladium Atoms. *ACS Catalysis*, **2019**, 9, 7876-7887	13.1	39
333	Destruction of the Uranyl Moiety in a U(V) "Cation-Cation" Interaction. *Inorganic Chemistry*, **2019**, 58, 10148-10159	5.1	12
332	NMR studies of daidzein and puerarin: active anti-oxidants in traditional Chinese medicine. *Journal of Molecular Modeling*, **2019**, 25, 202	2	10
331	Self-Selective Catalyst Synthesis for CO2 Reduction. *Joule*, **2019**, 3, 1927-1936	27.8	35
330	Three-dimensional open nano-netcage electrocatalysts for efficient pH-universal overall water splitting. *Nature Communications*, **2019**, 10, 4875	17.4	119
329	PdAg bimetallic electrocatalyst for highly selective reduction of CO2 with low COOH* formation energy and facile CO desorption. *Nano Research*, **2019**, 12, 2866-2871	10	38
328	A Supramolecular Radical Dimer: High-Efficiency NIR-II Photothermal Conversion and Therapy. *Angewandte Chemie - International Edition*, **2019**, 58, 15526-15531	16.4	97
327	A Supramolecular Radical Dimer: High-Efficiency NIR-II Photothermal Conversion and Therapy. *Angewandte Chemie*, **2019**, 131, 15672-15677	3.6	29

326	Quadruple bonding between iron and boron in the BFe(CO) complex. *Nature Communications*, **2019**, 10, 4713	17.4	26
325	Ag2S decorated nanocubes with enhanced near-infrared photothermal and photodynamic properties for rapid sterilization. *Colloids and Interface Science Communications*, **2019**, 33, 100201	5.4	31
324	Insight into the elastic anisotropy and thermodynamics properties of Tantalum borides. *Vacuum*, **2019**, 169, 108883	3.7	15
323	A Ligand-Protected Golden Fullerene: The Dipyridylamido Au Nanocluster. *Angewandte Chemie - International Edition*, **2019**, 58, 5906-5909	16.4	60
322	Planar B and B clusters with double-hexagonal vacancies. *Nanoscale*, **2019**, 11, 23286-23295	7.7	29
321	Interfacial synergy of ultralong jagged Pt85Mo15 nanowires with abundant active sites on enhanced hydrogen evolution in an alkaline solution. *Journal of Materials Chemistry A*, **2019**, 7, 24328-24336	13	28
320	Physical origin of chemical periodicities in the system of elements. *Pure and Applied Chemistry*, **2019**, 91, 1969-1999	2.1	10
319	Rh single atoms on TiO dynamically respond to reaction conditions by adapting their site. *Nature Communications*, **2019**, 10, 4488	17.4	99
318	Molecular nitrogen promotes catalytic hydrodeoxygenation. *Nature Catalysis*, **2019**, 2, 1078-1087	36.5	33
317	Hydrogen evolution reaction catalyzed by nickel/nickel phosphide nanospheres synthesized through electrochemical methods. *Electrochimica Acta*, **2019**, 298, 229-236	6.7	12
316	Non defect-stabilized thermally stable single-atom catalyst. *Nature Communications*, **2019**, 10, 234	17.4	274
315	N2 Reduction on Fe-Based Complexes with Different Supporting Main-Group Elements: Critical Roles of Anchor and Peripheral Ligands. *Small Methods*, **2019**, 3, 1800340	12.8	13
314	Multi-site electrocatalysts for hydrogen evolution in neutral media by destabilization of water molecules. *Nature Energy*, **2019**, 4, 107-114	62.3	264
313	Impact of a Single Hydrogen Substitution by Fluorine on the Molecular Interaction and Miscibility between Sorafenib and Polymers. *Molecular Pharmaceutics*, **2019**, 16, 318-326	5.6	11
312	Lanthanides with Unusually Low Oxidation States in the PrB and PrB Boride Clusters. *Inorganic Chemistry*, **2019**, 58, 411-418	5.1	23
311	Implanting Mo Atoms into Surface Lattice of Pt3Mn Alloys Enclosed by High-Indexed Facets: Promoting Highly Active Sites for Ethylene Glycol Oxidation. *ACS Catalysis*, **2019**, 9, 442-455	13.1	44
310	TGMin: An efficient global minimum searching program for free and surface-supported clusters. *Journal of Computational Chemistry*, **2019**, 40, 1105-1112	3.5	27
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