Jun Li

List of Publications by Citations

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	Single-atom catalysis of CO oxidation using Pt1/FeOx. *Nature Chemistry*, **2011**, 3, 634-41	17.6	3489
468	Single-atom catalysts: a new frontier in heterogeneous catalysis. *Accounts of Chemical Research*, **2013**, 46, 1740-8	24.3	2437
467	Basis set exchange: a community database for computational sciences. *Journal of Chemical Information and Modeling*, **2007**, 47, 1045-52	6.1	2306
466	Heterogeneous single-atom catalysis. *Nature Reviews Chemistry*, **2018**, 2, 65-81	34.6	1624
465	Au20: a tetrahedral cluster. *Science*, **2003**, 299, 864-7	33.3	990
464	An efficient molybdenum disulfide/cobalt diselenide hybrid catalyst for electrochemical hydrogen generation. *Nature Communications*, **2015**, 6, 5982	17.4	771
463	Remarkable performance of Ir1/FeO(x) single-atom catalyst in water gas shift reaction. *Journal of the American Chemical Society*, **2013**, 135, 15314-7	16.4	646
462	Design of Single-Atom Co-N Catalytic Site: A Robust Electrocatalyst for CO Reduction with Nearly 100% CO Selectivity and Remarkable Stability. *Journal of the American Chemical Society*, **2018**, 140, 4218-4221	16.4	634
461	Observation of an all-boron fullerene. *Nature Chemistry*, **2014**, 6, 727-31	17.6	590
460	Hydrocarbon analogues of boron clusters--planarity, aromaticity and antiaromaticity. *Nature Materials*, **2003**, 2, 827-33	27	567
459	Planar hexagonal B(36) as a potential basis for extended single-atom layer boron sheets. *Nature Communications*, **2014**, 5, 3113	17.4	503
458	Direct observation of noble metal nanoparticles transforming to thermally stable single atoms. *Nature Nanotechnology*, **2018**, 13, 856-861	28.7	471
457	Ultrathin rhodium nanosheets. *Nature Communications*, **2014**, 5, 3093	17.4	350
456	Fe Isolated Single Atoms on S, N Codoped Carbon by Copolymer Pyrolysis Strategy for Highly Efficient Oxygen Reduction Reaction. *Advanced Materials*, **2018**, 30, e1800588	24	338
455	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
454	Ultrastable single-atom gold catalysts with strong covalent metal-support interaction (CMSI). *Nano Research*, **2015**, 8, 2913-2924	10	324
453	Experimental observation and confirmation of icosahedral W@Au12 and Mo@Au12 molecules. *Angewandte Chemie - International Edition*, **2002**, 41, 4786-9	16.4	299

452	Highly Efficient Catalysis of Preferential Oxidation of CO in H2-Rich Stream by Gold Single-Atom Catalysts. *ACS Catalysis*, **2015**, 5, 6249-6254	13.1	290
451	Dynamic formation of single-atom catalytic active sites on ceria-supported gold nanoparticles. *Nature Communications*, **2015**, 6, 6511	17.4	278
450	Insight into methanol synthesis from CO2 hydrogenation on Cu(1 1 1): Complex reaction network and the effects of H2O. *Journal of Catalysis*, **2011**, 281, 199-211	7.3	274
449	Non defect-stabilized thermally stable single-atom catalyst. *Nature Communications*, **2019**, 10, 234	17.4	274
448	High-Performance RhP Electrocatalyst for Efficient Water Splitting. *Journal of the American Chemical Society*, **2017**, 139, 5494-5502	16.4	267
447	Multi-site electrocatalysts for hydrogen evolution in neutral media by destabilization of water molecules. *Nature Energy*, **2019**, 4, 107-114	62.3	264
446	The role of reducible oxide-metal cluster charge transfer in catalytic processes: new insights on the catalytic mechanism of CO oxidation on Au/TiO2 from ab initio molecular dynamics. *Journal of the American Chemical Society*, **2013**, 135, 10673-83	16.4	251
445	The B35 cluster with a double-hexagonal vacancy: a new and more flexible structural motif for borophene. *Journal of the American Chemical Society*, **2014**, 136, 12257-60	16.4	250
444	Toward Rational Design of Oxide-Supported Single-Atom Catalysts: Atomic Dispersion of Gold on Ceria. *Journal of the American Chemical Society*, **2017**, 139, 6190-6199	16.4	240
443	Synthesis of Thermally Stable and Highly Active Bimetallic Au□Ag Nanoparticles on Inert Supports. *Chemistry of Materials*, **2009**, 21, 410-418	9.6	239
442	Isolated Single-Atom Pd Sites in Intermetallic Nanostructures: High Catalytic Selectivity for Semihydrogenation of Alkynes. *Journal of the American Chemical Society*, **2017**, 139, 7294-7301	16.4	238
441	PdZn Intermetallic Nanostructure with Pd□nPd Ensembles for Highly Active and Chemoselective Semi-Hydrogenation of Acetylene. *ACS Catalysis*, **2016**, 6, 1054-1061	13.1	234
440	Heterogeneous Fe single-cluster catalyst for ammonia synthesis via an associative mechanism. *Nature Communications*, **2018**, 9, 1610	17.4	233
439	Tuning defects in oxides at room□temperature by lithium reduction. *Nature Communications*, **2018**, 9, 1302	17.4	225
438	Synergetic Integration of Cu1.94S-ZnxCd1-xS Heteronanorods for Enhanced Visible-Light-Driven Photocatalytic Hydrogen Production. *Journal of the American Chemical Society*, **2016**, 138, 4286-9	16.4	212
437	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
436	Noble gas-actinide compounds: complexation of the CUO molecule by Ar, Kr, and Xe atoms in noble gas matrices. *Science*, **2002**, 295, 2242-5	33.3	205
435	Experimental and theoretical evidence of an axially chiral borospherene. *ACS Nano*, **2015**, 9, 754-60	16.7	195

434	Constructing NiCo/FeO Heteroparticles within MOF-74 for Efficient Oxygen Evolution Reactions. *Journal of the American Chemical Society*, **2018**, 140, 15336-15341	16.4	193
433	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
432	Catalysis on singly dispersed bimetallic sites. *Nature Communications*, **2015**, 6, 7938	17.4	182
431	Regulating the coordination structure of single-atom Fe-NC catalytic sites for benzene oxidation. *Nature Communications*, **2019**, 10, 4290	17.4	173
430	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
429	Cooperative CO2-to-ethanol conversion via enriched intermediates at molecule–metal catalyst interfaces. *Nature Catalysis*, **2020**, 3, 75-82	36.5	164
428	Efficient electrically powered CO2-to-ethanol via suppression of deoxygenation. *Nature Energy*, **2020**, 5, 478-486	62.3	163
427	A Durable Nickel Single-Atom Catalyst for Hydrogenation Reactions and Cellulose Valorization under Harsh Conditions. *Angewandte Chemie - International Edition*, **2018**, 57, 7071-7075	16.4	163
426	Surface Single-Cluster Catalyst for N-to-NH Thermal Conversion. *Journal of the American Chemical Society*, **2018**, 140, 46-49	16.4	163
425	Design of Efficient Catalysts with Double Transition Metal Atoms on C2N Layer. *Journal of Physical Chemistry Letters*, **2016**, 7, 1750-5	6.4	155
424	Shape control of CdSe nanocrystals with zinc blende structure. *Journal of the American Chemical Society*, **2009**, 131, 16423-9	16.4	144
423	Sn12(2-): stannaspherene. *Journal of the American Chemical Society*, **2006**, 128, 8390-1	16.4	140
422	Unraveling the coordination structure-performance relationship in Pt/FeO single-atom catalyst. *Nature Communications*, **2019**, 10, 4500	17.4	137
421	Identification of an iridium-containing compound with a formal oxidation state of IX. *Nature*, **2014**, 514, 475-7	50.4	137
420	Evidence of significant covalent bonding in Au(CN)(2)(-). *Journal of the American Chemical Society*, **2009**, 131, 16368-70	16.4	137
419	Icosahedral gold cage clusters: M@Au12- (M=V, Nb, and Ta). *Journal of Chemical Physics*, **2004**, 121, 8369-74	3.4	127
418	Theoretical and Experimental Investigations on Single-Atom Catalysis: Ir1/FeOx for CO Oxidation. *Journal of Physical Chemistry C*, **2014**, 118, 21945-21951	3.8	126
417	Theoretical Understandings of Graphene-based Metal Single-Atom Catalysts: Stability and Catalytic Performance. *Chemical Reviews*, **2020**, 120, 12315-12341	68.1	125

416	Experimental and theoretical investigation of the electronic and geometrical structures of the Au32 cluster. *Angewandte Chemie - International Edition*, **2005**, 44, 7119-23	16.4	124
415	CO Oxidation on Au/TiO2: Condition-Dependent Active Sites and Mechanistic Pathways. *Journal of the American Chemical Society*, **2016**, 138, 10467-76	16.4	123
414	Three-dimensional open nano-netcage electrocatalysts for efficient pH-universal overall water splitting. *Nature Communications*, **2019**, 10, 4875	17.4	119
413	Observation and characterization of the smallest borospherene, B28(-) and B28. *Journal of Chemical Physics*, **2016**, 144, 064307	3.9	119
412	From planar boron clusters to borophenes and metalloborophenes. *Nature Reviews Chemistry*, **2017**, 1,	34.6	118
411	Noble gas-actinide complexes of the CUO molecule with multiple Ar, Kr, and Xe atoms in noble-gas matrices. *Journal of the American Chemical Society*, **2003**, 125, 3126-39	16.4	117
410	[B]: a quasiplanar chiral boron cluster. *Angewandte Chemie - International Edition*, **2014**, 53, 5540-5	16.4	116
409	Bimetallic AuPd Alloy Catalysts for N2O Decomposition: Effects of Surface Structures on Catalytic Activity. *Journal of Physical Chemistry C*, **2012**, 116, 6222-6232	3.8	116
408	Theoretical understanding of the stability of single-atom catalysts. *National Science Review*, **2018**, 5, 638-641	10.8	111
407	Size-dependent dynamic structures of supported gold nanoparticles in CO oxidation reaction condition. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 7700-7705	11.5	109
406	Pd(2)@Sn(18)(4-): fusion of two endohedral stannaspherenes. *Journal of the American Chemical Society*, **2007**, 129, 9560-1	16.4	109
405	Pb12 2-: plumbaspherene. *Journal of Physical Chemistry A*, **2006**, 110, 10169-72	2.8	105
404	Reaction of Laser-Ablated Uranium Atoms with CO: Infrared Spectra of the CUO, CUO-, OUCCO, (2-C2)UO2, and U(CO)x (x = 1) Molecules in Solid Neon. *Journal of the American Chemical Society*, **1999**, 121, 9712-9721	16.4	103
403	Electronic structure differences in ZrO2 vs HfO2. *Journal of Physical Chemistry A*, **2005**, 109, 11521-5	2.8	102
402	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	10	101
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400	Endohedral stannaspherenes M@Sn12(-): a rich class of stable molecular cage clusters. *Angewandte Chemie - International Edition*, **2007**, 46, 742-5	16.4	100
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397	Au34-: A Fluxional Core□Shell Cluster. *Journal of Physical Chemistry C*, **2007**, 111, 8228-8232	3.8	98
396	A Supramolecular Radical Dimer: High-Efficiency NIR-II Photothermal Conversion and Therapy. *Angewandte Chemie - International Edition*, **2019**, 58, 15526-15531	16.4	97
395	Unique CO chemisorption properties of gold hexamer: Au6(CO)n- (n = 0-3). *Journal of the American Chemical Society*, **2005**, 127, 12098-106	16.4	96
394	Toward the Solution Synthesis of the Tetrahedral Au20 Cluster. *Journal of Physical Chemistry B*, **2004**, 108, 12259-12263	3.4	96
393	Maximizing the Number of Interfacial Sites in Single-Atom Catalysts for the Highly Selective, Solvent-Free Oxidation of Primary Alcohols. *Angewandte Chemie - International Edition*, **2018**, 57, 7795-7799	16.4	93
392	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
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390	Coordination engineering of iridium nanocluster bifunctional electrocatalyst for highly efficient and pH-universal overall water splitting. *Nature Communications*, **2020**, 11, 4246	17.4	92
389	Observation of a metal-centered B-Ta@B tubular molecular rotor and a perfect Ta@B boron drum with the record coordination number of twenty. *Chemical Communications*, **2017**, 53, 1587-1590	5.8	90
388	Probing the structures and bonding of size-selected boron and doped-boron clusters. *Chemical Society Reviews*, **2019**, 48, 3550-3591	58.5	90
387	On the Nature of Support Effects of Metal Dioxides MO2 (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	3.8	88
386	A Water-Promoted Mechanism of Alcohol Oxidation on a Au(111) Surface: Understanding the Catalytic Behavior of Bulk Gold. *ACS Catalysis*, **2013**, 3, 1693-1699	13.1	87
385	Formation and characterization of the boron dicarbonyl complex [B(CO)2](-). *Angewandte Chemie - International Edition*, **2015**, 54, 11078-83	16.4	86
384	Electronic Structure of Cycloheptatrienyl Sandwich Compounds of Actinides: An(□7-C7H7)2 (An = Th, Pa, U, Np, Pu, Am). *Journal of the American Chemical Society*, **1997**, 119, 9021-9032	16.4	84
383	Manganese-centered tubular boron cluster - MnB16 (-): A new class of transition-metal molecules. *Journal of Chemical Physics*, **2016**, 144, 154310	3.9	84
382	Selective photoelectrochemical oxidation of glycerol to high value-added dihydroxyacetone. *Nature Communications*, **2019**, 10, 1779	17.4	83
381	Thermodynamic studies and hydride transfer reactions from a rhodium complex to BX3 compounds. *Journal of the American Chemical Society*, **2009**, 131, 14454-65	16.4	82

380	Trivalent actinide and lanthanide separations by tetradentate nitrogen ligands: a quantum chemistry study. *Inorganic Chemistry*, **2011**, 50, 9230-7	5.1	81
379	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, 2554-7	16.4	80
378	Isolated Ni Atoms Dispersed on Ru Nanosheets: High-Performance Electrocatalysts toward Hydrogen Oxidation Reaction. *Nano Letters*, **2020**, 20, 3442-3448	11.5	80
377	Identification of the Electronic and Structural Dynamics of Catalytic Centers in Single-Fe-Atom Material. *CheM*, **2020**, 6, 3440-3454	16.2	79
376	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
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374	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
373	MOF-Confined Sub-2 nm Atomically Ordered Intermetallic PdZn Nanoparticles as High-Performance Catalysts for Selective Hydrogenation of Acetylene. *Advanced Materials*, **2018**, 30, e1801878	24	77
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369	A multicentre-bonded [Zn(I)]8 cluster with cubic aromaticity. *Nature Communications*, **2015**, 6, 6331	17.4	73
368	3-Fold-interpenetrated uranium-organic frameworks: new strategy for rationally constructing three-dimensional uranyl organic materials. *Inorganic Chemistry*, **2012**, 51, 3103-7	5.1	73
367	On the electronic structure of molecular UO2 in the presence of Ar atoms: evidence for direct U-Ar bonding. *Journal of the American Chemical Society*, **2004**, 126, 3424-5	16.4	73
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351	Observation of highly stable and symmetric lanthanide octa-boron inverse sandwich complexes. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, E6972-E6977	11.5	59
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334	Formation and Characterization of the Boron Dicarbonyl Complex [B(CO)2]− *Angewandte Chemie*, **2015**, 127, 11230-11235	3.6	50
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325	A diuranium carbide cluster stabilized inside a C fullerene cage. *Nature Communications*, **2018**, 9, 2753	17.4	47
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