Yong Pei

List of Publications by Citations

141	6,656	48	78
papers	citations	h-index	g-index
150	7,757	8.7	6.18
ext. papers	ext. citations	avg, IF	L-index

#	Paper	IF	Citations
141	MoS Quantum Dot Growth Induced by S Vacancies in a ZnInS Monolayer: Atomic-Level Heterostructure for Photocatalytic Hydrogen Production. *ACS Nano*, **2018**, 12, 751-758	16.7	296
140	Structural prediction of thiolate-protected Au38: a face-fused bi-icosahedral Au core. *Journal of the American Chemical Society*, **2008**, 130, 7830-2	16.4	261
139	Metal exchange method using Au25 nanoclusters as templates for alloy nanoclusters with atomic precision. *Journal of the American Chemical Society*, **2015**, 137, 4018-21	16.4	218
138	Investigating the structural evolution of thiolate protected gold clusters from first-principles. *Nanoscale*, **2012**, 4, 4054-72	7.7	205
137	A theoretical study of single-atom catalysis of CO oxidation using Au embedded 2D h-BN monolayer: a CO-promoted O$_2$ activation. *Scientific Reports*, **2014**, 4, 5441	4.9	177
136	The structure and optical properties of the [Au18(SR)14] nanocluster. *Angewandte Chemie - International Edition*, **2015**, 54, 3145-9	16.4	177
135	Self-Optimization of the Active Site of Molybdenum Disulfide by an Irreversible Phase Transition during Photocatalytic Hydrogen Evolution. *Angewandte Chemie - International Edition*, **2017**, 56, 7610-7614	16.4	175
134	Photocatalytic degradation of organic pollutants coupled with simultaneous photocatalytic H2 evolution over graphene quantum dots/Mn-N-TiO2/g-C3N4 composite catalysts: Performance and mechanism. *Applied Catalysis B: Environmental*, **2018**, 227, 312-321	21.8	175
133	Thiol ligand-induced transformation of Au38(SC2H4Ph)24 to Au36(SPh-t-Bu)24. *ACS Nano*, **2013**, 7, 6138-45	16.7	168
132	Catalytic activities of subnanometer gold clusters (Au$_x$, Au$_y$, and Au$_z$) for CO oxidation. *ACS Nano*, **2011**, 5, 7818-29	16.7	163
131	CO self-promoting oxidation on nanosized gold clusters: triangular Au3 active site and CO induced O-O scission. *Journal of the American Chemical Society*, **2013**, 135, 2583-95	16.4	162
130	Thiolate-protected Au20(SR)16 cluster: prolate Au8 core with new [Au3(SR)4] staple motif. *Journal of the American Chemical Society*, **2009**, 131, 13619-21	16.4	154
129	Crystal structure and optical properties of the [Ag62S12(SBu(t))32](2+) nanocluster with a complete face-centered cubic kernel. *Journal of the American Chemical Society*, **2014**, 136, 15559-65	16.4	150
128	B2C graphene, nanotubes, and nanoribbons. *Nano Letters*, **2009**, 9, 1577-82	11.5	133
127	Photocatalytic wastewater purification with simultaneous hydrogen production using MoS QD-decorated hierarchical assembly of ZnInS on reduced graphene oxide photocatalyst. *Water Research*, **2017**, 121, 11-19	12.5	129
126	Unraveling the mechanisms of O2 activation by size-selected gold clusters: transition from superoxo to peroxo chemisorption. *Journal of the American Chemical Society*, **2012**, 134, 9438-45	16.4	129
125	Total Structure Determination of Au21(S-Adm)15 and Geometrical/Electronic Structure Evolution of Thiolated Gold Nanoclusters. *Journal of the American Chemical Society*, **2016**, 138, 10754-7	16.4	128

124	Planar pentacoordinate carbon in CAl5(+): a global minimum. *Journal of the American Chemical Society*, **2008**, 130, 10394-400	16.4	120
123	Interlocked catenane-like structure predicted in Au24(SR)20: implication to structural evolution of thiolated gold clusters from homoleptic gold(I) thiolates to core-stacked nanoparticles. *Journal of the American Chemical Society*, **2012**, 134, 3015-24	16.4	117
122	Ag(Dppm)(SR) and Its Homologue AuAg(Dppm)(SR) Alloy Nanocluster: Seeded Growth, Structure Determination, and Differences in Properties. *Journal of the American Chemical Society*, **2017**, 139, 1618-1624	16.4	114
121	CO oxidation on TiO(2) (110) supported subnanometer gold clusters: size and shape effects. *Journal of the American Chemical Society*, **2013**, 135, 19336-46	16.4	113
120	Monolayer MoS2 with S vacancies from interlayer spacing expanded counterparts for highly efficient electrochemical hydrogen production. *Journal of Materials Chemistry A*, **2016**, 4, 16524-16530	13	107
119	Icosahedral crown gold nanocluster au(43)cu(12) with high catalytic activity. *Nano Letters*, **2010**, 10, 1055-62	11.5	107
118	Probing the planar tetra-, penta-, and hexacoordinate carbon in carbon-boron mixed clusters. *Journal of the American Chemical Society*, **2008**, 130, 2580-92	16.4	88
117	Crystal structure of Au□(SePh)□ nanoclusters and insights into their electronic, optical and catalytic properties. *Nanoscale*, **2014**, 6, 13977-85	7.7	86
116	Structure prediction of Au(44)(SR)(28): a chiral superatom cluster. *Journal of the American Chemical Society*, **2013**, 135, 19060-3	16.4	81
115	Planar tetracoordinate carbon strips in edge decorated graphene nanoribbon. *Journal of the American Chemical Society*, **2010**, 132, 5554-5	16.4	73
114	Tuning Pb(II) Adsorption from Aqueous Solutions on Ultrathin Iron Oxychloride (FeOCl) Nanosheets. *Environmental Science & Technology*, **2019**, 53, 2075-2085	10.3	71
113	Investigating active site of gold nanoparticle Au55(PPh3)12Cl6 in selective oxidation. *ACS Nano*, **2010**, 4, 2009-20	16.7	68
112	Au□carbon Electronic Interaction Mediated Selective Oxidation of Styrene. *ACS Catalysis*, **2017**, 7, 3483-3488	13.1	65
111	Ultrafast Relaxation Dynamics of Luminescent Rod-Shaped, Silver-Doped AgxAu25□ Clusters. *Journal of Physical Chemistry C*, **2015**, 119, 18790-18797	3.8	63
110	Degradation of dyes by peroxymonosulfate activated by ternary CoFeNi-layered double hydroxide: Catalytic performance, mechanism and kinetic modeling. *Journal of Colloid and Interface Science*, **2018**, 515, 92-100	9.3	62
109	Ab initio study of graphene-like monolayer molybdenum disulfide as a promising anode material for rechargeable sodium ion batteries. *RSC Advances*, **2014**, 4, 43183-43188	3.7	62
108	New Structure Model of Au22(SR)18: Bitetrahederon Golden Kernel Enclosed by [Au6(SR)6] Au(I) Complex. *Journal of Physical Chemistry Letters*, **2015**, 6, 1390-5	6.4	60
107	Photodegradation of Organic Pollutants Coupled with Simultaneous Photocatalytic Evolution of Hydrogen Using Quantum-Dot-Modified g-C3N4 Catalysts under Visible-Light Irradiation. *ACS Sustainable Chemistry and Engineering*, **2018**, 6, 12695-12705	8.3	60

106	Hydroxyl group modification improves the electrocatalytic ORR and OER activity of graphene supported single and bi-metal atomic catalysts (Ni, Co, and Fe). *Journal of Materials Chemistry A*, **2019**, 7, 24583-24593	13	59
105	Inorganic nanoribbons with unpassivated zigzag edges: Half metallicity and edge reconstruction. *Nano Research*, **2011**, 4, 233-239	10	58
104	Highly Bright Self-Assembled Copper Nanoclusters: A Novel Photoluminescent Probe for Sensitive Detection of Histamine. *Analytical Chemistry*, **2018**, 90, 9060-9067	7.8	58
103	The Fourth Alloying Mode by Way of Anti-Galvanic Reaction. *Angewandte Chemie - International Edition*, **2018**, 57, 4500-4504	16.4	57
102	Total Structure Determination of Au(S-Adm) and CdAu(S tBu) and Implications for the Structure of Au(SR). *Journal of the American Chemical Society*, **2018**, 140, 10988-10994	16.4	56
101	Quasi-Dual-Packed-Kerneled Au (2,4-DMBT) Nanoclusters and the Influence of Kernel Packing on the Electrochemical Gap. *Angewandte Chemie - International Edition*, **2017**, 56, 12644-12648	16.4	56
100	Growth-Rule-Guided Structural Exploration of Thiolate-Protected Gold Nanoclusters. *Accounts of Chemical Research*, **2019**, 52, 23-33	24.3	56
99	Shape-Controlled Synthesis of Trimetallic Nanoclusters: Structure Elucidation and Properties Investigation. *Chemistry - A European Journal*, **2016**, 22, 17145-17150	4.8	55
98	Semiring chemistry of Au25(SR)18: fragmentation pathway and catalytic active site. *Journal of the American Chemical Society*, **2013**, 135, 18067-79	16.4	55
97	Structure Determination of Alkynyl-Protected Gold Nanocluster Au (BuC?C) and Its Thermochromic Luminescence. *Angewandte Chemie - International Edition*, **2020**, 59, 2309-2312	16.4	55
96	X-Ray crystal structure, and optical and electrochemical properties of the Au15Ag3(SC6H11)14 nanocluster with a core-shell structure. *Nanoscale*, **2015**, 7, 18278-83	7.7	52
95	Tellurium Surface Doping to Enhance the Structural Stability and Electrochemical Performance of Layered Ni-Rich Cathodes. *ACS Applied Materials & Interfaces*, **2019**, 11, 40022-40033	9.5	51
94	Rational construction of a library of M nanoclusters from monometallic to tetrametallic. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 18834-18840	11.5	50
93	Self-Optimization of the Active Site of Molybdenum Disulfide by an Irreversible Phase Transition during Photocatalytic Hydrogen Evolution. *Angewandte Chemie*, **2017**, 129, 7718-7722	3.6	46
92	Reversible nanocluster structure transformation between face-centered cubic and icosahedral isomers. *Chemical Science*, **2019**, 10, 8685-8693	9.4	45
91	Ultrasmall Au nanocatalysts supported on nitrided carbon for electrocatalytic CO reduction: the role of the carbon support in high selectivity. *Nanoscale*, **2018**, 10, 14678-14686	7.7	42
90	Asymmetric Synthesis of 1,3-Butadienyl-2-carbinols by the Homoallenylboration of Aldehydes with a Chiral Phosphoric Acid Catalyst. *Angewandte Chemie - International Edition*, **2015**, 54, 7299-302	16.4	41
89	Structure and Electronic Structure Evolution of Thiolate-Protected Gold Nanoclusters Containing Quasi Face-Centered-Cubic Kernels. *Journal of Physical Chemistry C*, **2018**, 122, 14898-14907	3.8	39

88	The Structure and Optical Properties of the [Au18(SR)14] Nanocluster. *Angewandte Chemie*, **2015**, 127, 3188-3192	3.6	38
87	Onset of double helical structure in small-sized homoleptic gold thiolate clusters. *Journal of Physical Chemistry A*, **2009**, 113, 629-32	2.8	37
86	Electric field induced switching behaviors of monolayer-modified silicon surfaces: surface designs and molecular dynamics simulations. *Journal of the American Chemical Society*, **2005**, 127, 6802-13	16.4	36
85	Combining the Single-Atom Engineering and Ligand-Exchange Strategies: Obtaining the Single-Heteroatom-Doped AuAg(S-Adm) Nanocluster with Atomically Precise Structure. *Inorganic Chemistry*, **2018**, 57, 335-342	5.1	35
84	Density Functional Theory Studies on Structure, Ligand Exchange, and Optical Properties of Ligand-Protected Gold Nanoclusters: Thiolate versus Selenolate. *Journal of Physical Chemistry C*, **2015**, 119, 9205-9214	3.8	33
83	Bonding of Two 8-Electron Superatom Clusters. *Angewandte Chemie - International Edition*, **2018**, 57, 16768-16772	16.4	33
82	Hollow polyhedral structures in small gold-sulfide clusters. *ACS Nano*, **2011**, 5, 1441-9	16.7	32
81	Nanocluster growth "graft-onto": effects on geometric structures and optical properties. *Chemical Science*, **2020**, 11, 1691-1697	9.4	32
80	Two Electron Reduction: From Quantum Dots to Metal Nanoclusters. *Chemistry of Materials*, **2016**, 28, 7905-7911	9.6	31
79	Geometric structure, electronic structure and optical absorption properties of one-dimensional thiolate-protected gold clusters containing a quasi-face-centered-cubic (quasi-fcc) Au-core: a density-functional theoretical study. *Nanoscale*, **2016**, 8, 17044-17054	7.7	30
78	Comparative study on reactions and self-directed growth mechanisms of styrene molecules on H-terminated Si(111) and Si(100): combining quantum chemistry and molecular mechanics simulations. *Langmuir*, **2006**, 22, 3040-8	4	30
77	De-assembly of assembled PtAg units: tailoring the photoluminescence of atomically precise nanoclusters. *Chemical Communications*, **2017**, 53, 12564-12567	5.8	29
76	The Nucleation and Growth Mechanism of Thiolate-Protected Au Nanoclusters. *Journal of the American Chemical Society*, **2015**, 137, 15809-16	16.4	28
75	NiMoO4 Nanosheets Anchored on N?S Doped Carbon Clothes with Hierarchical Structure as a Bidirectional Catalyst toward Accelerating Polysulfides Conversion for Li?S Battery. *Advanced Functional Materials*, **2021**, 31, 2101285	15.6	28
74	Wide bandgap copolymers with vertical benzodithiophene dicarboxylate for high-performance polymer solar cells with an efficiency up to 7.49%. *Journal of Materials Chemistry A*, **2016**, 4, 18792-18803	13	28
73	Improved photovoltaic performance of star-shaped molecules with a triphenylamine core by tuning the substituted position of the carbazolyl unit at the terminal. *Journal of Materials Chemistry A*, **2015**, 3, 10883-10889	13	27
72	Density Functional Theory (DFT) Studies of CO Oxidation over Nanoporous Gold: Effects of Residual Ag and CO Self-Promoting Oxidation. *Journal of Physical Chemistry C*, **2015**, 119, 10345-10354	3.8	26
71	Correlating the Structure and Optical Absorption Properties of Au76(SR)44 Cluster. *Journal of Physical Chemistry C*, **2016**, 120, 13739-13748	3.8	25

70	Molecular Dynamics Simulations of the Oil-Detachment from the Hydroxylated Silica Surface: Effects of Surfactants, Electrostatic Interactions, and Water Flows on the Water Molecular Channel Formation. *Journal of Physical Chemistry B*, **2018**, 122, 1905-1918	3.4	24
69	Tri-Wing Graphene Nano-Paddle-Wheel with a Single-File Metal Joint: Formation of Multi-Planar Tetracoordinated-Carbon (ptC) Strips. *Journal of Physical Chemistry C*, **2012**, 116, 11378-11385	3.8	24
68	Molecular isomeric engineering of naphthyl-quinoline-containing dinuclear platinum complexes to tune emission from deep red to near infrared. *Journal of Materials Chemistry C*, **2019**, 7, 630-638	7.1	23
67	Molecular Dynamics Simulation of Surfactant Flooding Driven Oil-Detachment in Nano-Silica Channels. *Journal of Physical Chemistry B*, **2019**, 123, 277-288	3.4	23
66	Electrocatalytic dechlorination of halogenated antibiotics via synergistic effect of chlorine-cobalt bond and atomic H. *Journal of Hazardous Materials*, **2018**, 358, 294-301	12.8	22
65	A ten-electron (10e) thiolate-protected Au(SR) cluster: structure prediction and a □gold-atom insertion, thiolate-group elimination□mechanism. *Nanoscale*, **2017**, 9, 2895-2902	7.7	21
64	First-principles investigation on the structural, electronic properties and diffusion barriers of Mg/Al doped NaCoO2 as the cathode material of rechargeable sodium batteries. *RSC Advances*, **2015**, 5, 27229-27234	3.7	21
63	Density functional theory (DFT) studies of CO oxidation reaction on M13 and Au18M clusters (M = Au, Ag, Cu, Pt and Pd): the role of co-adsorbed CO molecule. *RSC Advances*, **2016**, 6, 55867-55877	3.7	21
62	Mechanistic Insight into the Styrene-Selective Oxidation on Subnanometer Gold Clusters (Au16□Au20, Au27, Au28, Au30, and Au32□Au35): A Density Functional Theory Study. *Journal of Physical Chemistry C*, **2014**, 118, 20346-20356	3.8	19
61	Synthesis and photovoltaic properties of conjugated side chains polymers with different electron-withdrawing and donating end groups. *Journal of Polymer Science Part A*, **2012**, 50, 3848-3858	2.5	19
60	Two-dimensional to three-dimensional structural transition of gold cluster Au10 during soft landing on TiO2 surface and its effect on CO oxidation. *Journal of Chemical Physics*, **2010**, 133, 134707	3.9	19
59	Quasi-Dual-Packed-Kerneled Au49(2,4-DMBT)27 Nanoclusters and the Influence of Kernel Packing on the Electrochemical Gap. *Angewandte Chemie*, **2017**, 129, 12818-12822	3.6	18
58	Dual phosphorescence emission of dinuclear platinum(ii) complex incorporating cyclometallating pyrenyl-dipyridine-based ligand and its application in near-infrared solution-processed polymer light-emitting diodes. *Dalton Transactions*, **2017**, 46, 16257-16268	4.3	17
57	The Fourth Alloying Mode by Way of Anti-Galvanic Reaction. *Angewandte Chemie*, **2018**, 130, 4590-4594	3.6	17
56	Theoretical Predictions of a New ~14 kDa Core-Mass Thiolate-Protected Gold Nanoparticle: Au(SR). *Journal of Physical Chemistry Letters*, **2017**, 8, 1248-1252	6.4	15
55	Thiolate-protected gold nanoclusters: structural prediction and the understandings of electronic stability from first principles simulations. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2017**, 7, e1315	7.9	15
54	Spatially Confined Li□Oxygen Interaction in the Tunnel of □MnO2 Catalyst for Li□Air Battery: A First-Principles Study. *Journal of Physical Chemistry C*, **2017**, 121, 16193-16200	3.8	14
53	Structure Determination of Alkynyl-Protected Gold Nanocluster Au22(tBuC?C)18 and Its Thermochromic Luminescence. *Angewandte Chemie*, **2020**, 132, 2329-2332	3.6	14

52	Tuning the Isomeric Fused Heteroaromatic Core of Small Donor–Acceptor Molecules to Alter Their Crystalline Nature and Enhance Photovoltaic Performance. *European Journal of Organic Chemistry*, **2015**, 2015, 820-827	3.2	13
51	Isomer Structural Transformation in Au□Cu Alloy Nanoclusters: Water Ripple-Like Transfer of Thiol Ligands. *Particle and Particle Systems Characterization*, **2019**, 36, 1800494	3.1	12
50	Three-Component Cascade Synthesis of Carbazoles through [1s,6s] Sigmatropic Shift under Metal-Free Conditions. *Journal of Organic Chemistry*, **2019**, 84, 3121-3131	4.2	12
49	Theoretical prediction of a new stable structure of Au28(SR)20 cluster. *Chemical Physics Letters*, **2018**, 704, 68-75	2.5	12
48	Total structural determination of [AuAg(Dppm)(SR)] comprising an open icosahedral AuAg core with six free valence electrons. *Chemical Communications*, **2019**, 55, 6457-6460	5.8	11
47	Edge decorated SiC nanoribbons with metal: Coexistence of planar tetracoordinate carbon and silicon. *Chemical Physics Letters*, **2013**, 580, 78-81	2.5	10
46	Novel solution-processible small molecules based on benzo[1,2-b:3,4-b?:5,6-b??]trithiophene for effective organic photovoltaics with high open-circuit voltage. *RSC Advances*, **2015**, 5, 14540-14546	3.7	10
45	Exohedral silicon fullerenes: SiNPtN/2 (20. *Journal of Chemical Physics*, **2007**, 127, 044704	3.9	10
44	Fe-Catalyzed decarbonylative cascade reaction of N-aryl cinnamamides with aliphatic aldehydes to construct 3,4-dihydroquinolin-2(1H)-ones. *Organic and Biomolecular Chemistry*, **2019**, 17, 5262-5268	3.9	9
43	Single Metal Atom Supported on N-Doped 2D Nitride Black Phosphorus: An Efficient Electrocatalyst for the Oxygen Evolution and Oxygen Reduction Reactions. *Journal of Physical Chemistry C*, **2021**, 125, 12541-12550	3.8	8
42	On the mechanism of inter-cluster alloying reactions: two-stage metal exchange of [Au25(PET)18]□ and [Ag25(DMBT)18]□clusters. *Journal of Materials Chemistry A*, **2020**, 8, 10242-10251	13	7
41	A revisit to the structure of Au(SCHCHPh): a cubic nanocrystal-like gold kernel. *Nanoscale*, **2018**, 10, 10357-10364	7.7	7
40	Single Metal Atom Catalyst Supported on g-C3N4 for Formic Acid Dehydrogenation: A Combining Density Functional Theory and Machine Learning Study. *Journal of Physical Chemistry C*, **2021**, 125, 22513-22521	3.8	7
39	Electronic and magnetic properties of silicon supported organometallic molecular wires: a density functional theory (DFT) study. *Nanoscale*, **2015**, 7, 13734-46	7.7	6
38	Molecular dynamics simulations of the self-organization of side-chain decorated polyaromatic conjugation molecules: phase separated lamellar and columnar structures and dispersion behaviors in toluene solvent.. *RSC Advances*, **2018**, 8, 11134-11144	3.7	6
37	Electronic Structure and Spin Transport Properties of a New Class of Semiconductor Surface-Confined One-Dimensional Half-Metallic [Eu-(CnHn□)]N (n = 7−9) Sandwich Compounds and Molecular Wires: First Principle Studies. *Journal of Physical Chemistry C*, **2018**, 122, 16168-16177	3.8	6
36	Unraveling the Nucleation Process from a Au(I)-SR Complex to Transition-Size Nanoclusters. *Journal of the American Chemical Society*, **2021**, 143, 15224-15232	16.4	6
35	Effect of thiolate-ligand passivation on the electronic structure and optical absorption properties of ultrathin one and two-dimensional gold nanocrystals. *Nanoscale*, **2020**, 12, 5554-5566	7.7	5

34	The mechanism of metal exchange in non-metallic nanoclusters. *Nanoscale Advances*, **2020**, 2, 664-668	5.1	5
33	Exploring the structure evolution and core/ligand structure patterns of a series of large sized thiolate-protected gold clusters Au(SR) (N = 1-8): a first principles study. *Nanoscale*, **2018**, 10, 3918-3929	7.7	5
32	Radical Chain-Reaction of Terminal-Unsaturated Organic Molecules on Water-Saturated Si(100)-(2 □ 1): The Role of Surface Hydroxyl Groups. *Journal of Physical Chemistry C*, **2013**, 117, 14032-14042	3.8	5
31	Exploration of Formation and Size-Evolution Pathways of Thiolate-Gold Nanoclusters in the CO-Directed [Au (SR)] Synthesis. *Small*, **2021**, 17, e2000627	11	5
30	First-Principles Study of Structural, Electronic, and Magnetic Properties of One-Dimensional Transition Metals Incorporated Vinylnaphthalene Molecular Wires on Hydrogen-Terminated Silicon Surface. *Journal of Physical Chemistry C*, **2016**, 120, 27980-27988	3.8	5
29	Interfacial adhesion properties of graphene sheet on nanoscale corrugated surface: a molecular dynamics simulation study. *Molecular Simulation*, **2016**, 42, 405-412	2	4
28	Insight into 6□Electrocyclic Reactions of 1,8-Dioxatetraene. *Angewandte Chemie - International Edition*, **2019**, 58, 2660-2664	16.4	4
27	[AuAgH(SPhCl)]: An Au-Ag Alloy Nanocluster with 12 Hydrides and Its Enlightenment on Nanocluster Structural Evolution. *Inorganic Chemistry*, **2021**, 60, 11640-11647	5.1	4
26	Anisotropic Evolution of Nanoclusters from Ag to Ag: Halogen- and Defect-Induced Epitaxial Growth in Nanoclusters. *Journal of Physical Chemistry Letters*, **2021**, 12, 6654-6660	6.4	4
25	Bonding of Two 8-Electron Superatom Clusters. *Angewandte Chemie*, **2018**, 130, 17010-17014	3.6	4
24	Fabrication of magnetic nickel incorporated carbon nanofibers for superfast adsorption of sulfadiazine: Performance and mechanisms exploration. *Journal of Hazardous Materials*, **2022**, 423, 127219	12.8	4
23	Activating a TiO/BiVO Film for Photoelectrochemical Water Splitting by Constructing a Heterojunction Interface with a Uniform Crystal Plane Orientation.. *ACS Applied Materials & Interfaces*, **2021**,	9.5	4
22	First-principles investigation on structural and electrochemical properties of NaCoO2 for rechargeable Na-ion batteries. *Journal of Central South University*, **2015**, 22, 2036-2042	2.1	3
21	Effect on absorption and electron transfer by using Cd(ii) or Cu(ii) complexes with phenanthroline as auxiliary electron acceptors (A) in D-A-□A motif sensitizers for dye-sensitized solar cells. *Physical Chemistry Chemical Physics*, **2018**, 20, 6688-6697	3.6	3
20	Resolution and evaluation of 3-chlorophenyl-3-hydroxypropionylhydroxamic acid as antivirulence agent with excellent eradication efficacy in Helicobacter pylori infected mice. *European Journal of Pharmaceutical Sciences*, **2018**, 121, 293-300	5.1	3
19	Structure and Catalytic Activity of Gold Clusters Supported on Nitrogen-Doped Graphene. *Journal of Physical Chemistry C*, **2021**, 125, 5006-5019	3.8	3
18	Phenyl Ring Transfer Mechanism of Styrene Selective Oxidation to Phenyl Acetaldehyde on Gold Catalysts from Density Functional Theory (DFT) Studies. *Journal of Physical Chemistry C*, **2019**, 123, 1710-1719	3.8	3
17	Total structural determination of alloyed AuCu(S-Adm) nanoclusters with double superatomic chains. *Chemical Communications*, **2021**, 57, 2017-2020	5.8	3

List of Publications

16	A homoleptic alkynyl-protected [AgCu(BuC[triple bond, length as m-dash]C)] superatom with free electrons: synthesis, structure analysis, and different properties compared with the AuAg cluster in the M series. *Chemical Science*, **2021**, 12, 12819-12826	9.4	3
15	Evolution from superatomic AuAg monomers into molecular-like AuAg dimeric nanoclusters.. *Chemical Science*, **2022**, 13, 2778-2782	9.4	3
14	Ligand Modification of Au Nanoclusters for Near-Infrared Photocatalytic Oxidative Functionalization.. *Journal of the American Chemical Society*, **2022**,	16.4	3
13	Structural determination of a metastable Ag27 nanocluster and its transformations into Ag8 and Ag29 nanoclusters. *Inorganic Chemistry Frontiers*, **2021**, 8, 4407-4414	6.8	2
12	(002) facets exposed and controllable thickness of CdS nanobelts drive desirable hydrogen-adsorption free energy (?GH) for boosting visible-light photocatalytic performance. *Catalysis Science and Technology*,	5.5	2
11	From Monolayer-Protected Gold Cluster to Monolayer-Protected Gold-Sulfide Cluster: Geometrical and Electronic Structure Evolutions of AuS (SR) (= 0-12). *ACS Omega*, **2020**, 5, 16901-16911	3.9	1
10	Exohedral Silicon Fullerenes: Si60Pn60 and Si80Pn60 (Pn = P, As, Sb and Bi). *Journal of Cluster Science*, **2011**, 22, 343-354	3	1
9	An AuS network model for exploring the structural origin, evolution, and two-electron (2e) reduction growth mechanism of Au(SR) clusters. *Journal of Chemical Physics*, **2021**, 154, 244308	3.9	1
8	Evolution of Electronic Structure of Cuboid Thiolate-Monolayer-Protected Gold Nanocrystals. *Journal of Physical Chemistry C*, **2021**, 125, 20670-20675	3.8	1
7	Mechanism of Nucleation of Gold(I) Thiolate Oligomers into Gold□thiolate Nanoclusters. *Journal of Physical Chemistry C*, **2022**, 126, 5980-5990	3.8	1
6	Origin of the structural stability of cage-like Au clusters. *Nanoscale*, **2021**, 13, 18134-18139	7.7	0
5	Ligand Shell Isomerization Induces Different Fluorescence Origins of Two Au Nanoclusters.. *Journal of Physical Chemistry Letters*, **2022**, 3718-3725	6.4	0
4	Insight into the Mechanism of Single-Metal-Atom Tailoring on the Surface of Au-Cu Alloy Nanoclusters.. *Journal of Physical Chemistry Letters*, **2022**, 4139-4144	6.4	0
3	On the synergistic effect of asphaltene and surfactant to reduce n-dodecane□water interfacial tension: insights from molecular dynamics simulations. *Molecular Simulation*,1-10	2	0
2	Insight into 6□Electrocyclic Reactions of 1,8-Dioxatetraene. *Angewandte Chemie*, **2019**, 131, 2686-2690	3.6	
1	Symmetric Growth of Dual-Packed Kernel: Exploration of the Evolution of Au(SR) to Au(SR) and Au(SR) Clusters via the 2 -Reduction Cluster Growth Mechanism. *ACS Omega*, **2021**, 6, 18024-18032	3.9	