

# Yong Pei

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

141  
papers

6,656  
citations

48  
h-index

78  
g-index

150  
ext. papers

7,757  
ext. citations

8.7  
avg, IF

6.18  
L-index

#	Paper	IF	Citations
141	Fabrication of magnetic nickel incorporated carbon nanofibers for superfast adsorption of sulfadiazine: Performance and mechanisms exploration. <i>Journal of Hazardous Materials</i> , <b>2022</b> , 423, 12721-12729	13.8	4
140	Evolution from superatomic AuAg monomers into molecular-like AuAg dimeric nanoclusters.. <i>Chemical Science</i> , <b>2022</b> , 13, 2778-2782	9.4	3
139	Ligand Modification of Au Nanoclusters for Near-Infrared Photocatalytic Oxidative Functionalization.. <i>Journal of the American Chemical Society</i> , <b>2022</b> ,	16.4	3
138	Mechanism of Nucleation of Gold(I) Thiolate Oligomers into Gold(III) Thiolate Nanoclusters. <i>Journal of Physical Chemistry C</i> , <b>2022</b> , 126, 5980-5990	3.8	1
137	Ligand Shell Isomerization Induces Different Fluorescence Origins of Two Au Nanoclusters.. <i>Journal of Physical Chemistry Letters</i> , <b>2022</b> , 3718-3725	6.4	0
136	Insight into the Mechanism of Single-Metal-Atom Tailoring on the Surface of Au-Cu Alloy Nanoclusters.. <i>Journal of Physical Chemistry Letters</i> , <b>2022</b> , 4139-4144	6.4	0
135	Single Metal Atom Catalyst Supported on g-C3N4 for Formic Acid Dehydrogenation: A Combining Density Functional Theory and Machine Learning Study. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 22513-22527	3.8	7
134	Origin of the structural stability of cage-like Au clusters. <i>Nanoscale</i> , <b>2021</b> , 13, 18134-18139	7.7	0
133	Exploration of Formation and Size-Evolution Pathways of Thiolate-Gold Nanoclusters in the CO-Directed [Au (SR) ] Synthesis. <i>Small</i> , <b>2021</b> , 17, e2000627	11	5
132	Structure and Catalytic Activity of Gold Clusters Supported on Nitrogen-Doped Graphene. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 5006-5019	3.8	3
131	NiMoO4 Nanosheets Anchored on N/S Doped Carbon Clothes with Hierarchical Structure as a Bidirectional Catalyst toward Accelerating Polysulfides Conversion for Li/S Battery. <i>Advanced Functional Materials</i> , <b>2021</b> , 31, 2101285	15.6	28
130	An AuS network model for exploring the structural origin, evolution, and two-electron (2e) reduction growth mechanism of Au(SR) clusters. <i>Journal of Chemical Physics</i> , <b>2021</b> , 154, 244308	3.9	1
129	Single Metal Atom Supported on N-Doped 2D Nitride Black Phosphorus: An Efficient Electrocatalyst for the Oxygen Evolution and Oxygen Reduction Reactions. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 12541-12550	3.8	8
128	[AuAgH(SPhCl)]: An Au-Ag Alloy Nanocluster with 12 Hydrides and Its Enlightenment on Nanocluster Structural Evolution. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 11640-11647	5.1	4
127	Anisotropic Evolution of Nanoclusters from Ag to Ag: Halogen- and Defect-Induced Epitaxial Growth in Nanoclusters. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 6654-6660	6.4	4
126	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. <i>ACS Omega</i> , <b>2021</b> , 6, 18024-18032	3.9	
125	Total structural determination of alloyed AuCu(S-Adm) nanoclusters with double superatomic chains. <i>Chemical Communications</i> , <b>2021</b> , 57, 2017-2020	5.8	3

124	Structural determination of a metastable Ag <sub>27</sub> nanocluster and its transformations into Ag <sub>8</sub> and Ag <sub>29</sub> nanoclusters. <i>Inorganic Chemistry Frontiers</i> , <b>2021</b> , 8, 4407-4414	6.8	2
123	A homoleptic alkynyl-protected [AgCu(BuC <sub>3</sub> ) <sub>3</sub> ] superatom with free electrons: synthesis, structure analysis, and different properties compared with the AuAg cluster in the M series. <i>Chemical Science</i> , <b>2021</b> , 12, 12819-12826	9.4	3
122	Unraveling the Nucleation Process from a Au(I)-SR Complex to Transition-Size Nanoclusters. <i>Journal of the American Chemical Society</i> , <b>2021</b> , 143, 15224-15232	16.4	6
121	Evolution of Electronic Structure of Cuboid Thiolate-Monolayer-Protected Gold Nanocrystals. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 20670-20675	3.8	1
120	Activating a TiO <sub>2</sub> /BiVO <sub>4</sub> Film for Photoelectrochemical Water Splitting by Constructing a Heterojunction Interface with a Uniform Crystal Plane Orientation.. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2021</b> ,	9.5	4
119	From Monolayer-Protected Gold Cluster to Monolayer-Protected Gold-Sulfide Cluster: Geometrical and Electronic Structure Evolutions of AuS (SR) (n = 0-12). <i>ACS Omega</i> , <b>2020</b> , 5, 16901-16911	3.9	1
118	Effect of thiolate-ligand passivation on the electronic structure and optical absorption properties of ultrathin one and two-dimensional gold nanocrystals. <i>Nanoscale</i> , <b>2020</b> , 12, 5554-5566	7.7	5
117	The mechanism of metal exchange in non-metallic nanoclusters. <i>Nanoscale Advances</i> , <b>2020</b> , 2, 664-668	5.1	5
116	On the mechanism of inter-cluster alloying reactions: two-stage metal exchange of [Au <sub>25</sub> (PET) <sub>18</sub> ] <sup>+</sup> and [Ag <sub>25</sub> (DMBT) <sub>18</sub> ] <sup>+</sup> clusters. <i>Journal of Materials Chemistry A</i> , <b>2020</b> , 8, 10242-10251	13	7
115	Nanocluster growth "graft-onto": effects on geometric structures and optical properties. <i>Chemical Science</i> , <b>2020</b> , 11, 1691-1697	9.4	32
114	Structure Determination of Alkynyl-Protected Gold Nanocluster Au (BuC <sub>3</sub> ) <sub>3</sub> and Its Thermochromic Luminescence. <i>Angewandte Chemie - International Edition</i> , <b>2020</b> , 59, 2309-2312	16.4	55
113	Structure Determination of Alkynyl-Protected Gold Nanocluster Au <sub>22</sub> (tBuC <sub>3</sub> ) <sub>18</sub> and Its Thermochromic Luminescence. <i>Angewandte Chemie</i> , <b>2020</b> , 132, 2329-2332	3.6	14
112	Rational construction of a library of M nanoclusters from monometallic to tetrametallic. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2019</b> , 116, 18834-18840	11.5	50
111	Tellurium Surface Doping to Enhance the Structural Stability and Electrochemical Performance of Layered Ni-Rich Cathodes. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2019</b> , 11, 40022-40033	9.5	51
110	Insight into 6π Electrocyclic Reactions of 1,8-Dioxatetraene. <i>Angewandte Chemie - International Edition</i> , <b>2019</b> , 58, 2660-2664	16.4	4
109	Tuning Pb(II) Adsorption from Aqueous Solutions on Ultrathin Iron Oxychloride (FeOCl) Nanosheets. <i>Environmental Science &amp; Technology</i> , <b>2019</b> , 53, 2075-2085	10.3	71
108	Molecular isomeric engineering of naphthyl-quinoline-containing dinuclear platinum complexes to tune emission from deep red to near infrared. <i>Journal of Materials Chemistry C</i> , <b>2019</b> , 7, 630-638	7.1	23
107	Total structural determination of [AuAg(Dppm)(SR)] comprising an open icosahedral AuAg core with six free valence electrons. <i>Chemical Communications</i> , <b>2019</b> , 55, 6457-6460	5.8	11

106	Fe-Catalyzed decarbonylative cascade reaction of N-aryl cinnamamides with aliphatic aldehydes to construct 3,4-dihydroquinolin-2(1H)-ones. <i>Organic and Biomolecular Chemistry</i> , <b>2019</b> , 17, 5262-5268	3.9	9
105	Isomer Structural Transformation in AuCu Alloy Nanoclusters: Water Ripple-Like Transfer of Thiol Ligands. <i>Particle and Particle Systems Characterization</i> , <b>2019</b> , 36, 1800494	3.1	12
104	Insight into 6 $\pi$ Electrocyclic Reactions of 1,8-Dioxatetraene. <i>Angewandte Chemie</i> , <b>2019</b> , 131, 2686-2690	3.6	
103	Reversible nanocluster structure transformation between face-centered cubic and icosahedral isomers. <i>Chemical Science</i> , <b>2019</b> , 10, 8685-8693	9.4	45
102	Three-Component Cascade Synthesis of Carbazoles through [1s,6s] Sigmatropic Shift under Metal-Free Conditions. <i>Journal of Organic Chemistry</i> , <b>2019</b> , 84, 3121-3131	4.2	12
101	Hydroxyl group modification improves the electrocatalytic ORR and OER activity of graphene supported single and bi-metal atomic catalysts (Ni, Co, and Fe). <i>Journal of Materials Chemistry A</i> , <b>2019</b> , 7, 24583-24593	13	59
100	Molecular Dynamics Simulation of Surfactant Flooding Driven Oil-Detachment in Nano-Silica Channels. <i>Journal of Physical Chemistry B</i> , <b>2019</b> , 123, 277-288	3.4	23
99	Phenyl Ring Transfer Mechanism of Styrene Selective Oxidation to Phenyl Acetaldehyde on Gold Catalysts from Density Functional Theory (DFT) Studies. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 1710-1719	3.8	3
98	Growth-Rule-Guided Structural Exploration of Thiolate-Protected Gold Nanoclusters. <i>Accounts of Chemical Research</i> , <b>2019</b> , 52, 23-33	24.3	56
97	The Fourth Alloying Mode by Way of Anti-Galvanic Reaction. <i>Angewandte Chemie - International Edition</i> , <b>2018</b> , 57, 4500-4504	16.4	57
96	Photocatalytic degradation of organic pollutants coupled with simultaneous photocatalytic H <sub>2</sub> evolution over graphene quantum dots/Mn-N-TiO <sub>2</sub> /g-C <sub>3</sub> N <sub>4</sub> composite catalysts: Performance and mechanism. <i>Applied Catalysis B: Environmental</i> , <b>2018</b> , 227, 312-321	21.8	175
95	Effect on absorption and electron transfer by using Cd(ii) or Cu(ii) complexes with phenanthroline as auxiliary electron acceptors (A) in D-A- $\pi$ A motif sensitizers for dye-sensitized solar cells. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 6688-6697	3.6	3
94	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. <i>Journal of Physical Chemistry B</i> , <b>2018</b> , 122, 1905-1918	3.4	24
93	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. <i>Nanoscale</i> , <b>2018</b> , 10, 3918-3929	7.7	5
92	Combining the Single-Atom Engineering and Ligand-Exchange Strategies: Obtaining the Single-Heteroatom-Doped AuAg(S-Adm) Nanocluster with Atomically Precise Structure. <i>Inorganic Chemistry</i> , <b>2018</b> , 57, 335-342	5.1	35
91	MoS Quantum Dot Growth Induced by S Vacancies in a ZnInS Monolayer: Atomic-Level Heterostructure for Photocatalytic Hydrogen Production. <i>ACS Nano</i> , <b>2018</b> , 12, 751-758	16.7	296
90	Degradation of dyes by peroxymonosulfate activated by ternary CoFeNi-layered double hydroxide: Catalytic performance, mechanism and kinetic modeling. <i>Journal of Colloid and Interface Science</i> , <b>2018</b> , 515, 92-100	9.3	62
89	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.. <i>RSC Advances</i> , <b>2018</b> , 8, 11134-11144	3.7	6

88	The Fourth Alloying Mode by Way of Anti-Galvanic Reaction. <i>Angewandte Chemie</i> , <b>2018</b> , 130, 4590-4594	3.6	17
87	Electrocatalytic dechlorination of halogenated antibiotics via synergistic effect of chlorine-cobalt bond and atomic H. <i>Journal of Hazardous Materials</i> , <b>2018</b> , 358, 294-301	12.8	22
86	Electronic Structure and Spin Transport Properties of a New Class of Semiconductor Surface-Confined One-Dimensional Half-Metallic [Eu-(C <sub>n</sub> H <sub>n</sub> O)] <sub>n</sub> (n = 7-9) Sandwich Compounds and Molecular Wires: First Principle Studies. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 16168-16177	3.8	6
85	Ultrasml Au nanocatalysts supported on nitrated carbon for electrocatalytic CO reduction: the role of the carbon support in high selectivity. <i>Nanoscale</i> , <b>2018</b> , 10, 14678-14686	7.7	42
84	A revisit to the structure of Au(SCHCHPh): a cubic nanocrystal-like gold kernel. <i>Nanoscale</i> , <b>2018</b> , 10, 10357-10364	7.7	64
83	Photodegradation of Organic Pollutants Coupled with Simultaneous Photocatalytic Evolution of Hydrogen Using Quantum-Dot-Modified g-C <sub>3</sub> N <sub>4</sub> Catalysts under Visible-Light Irradiation. <i>ACS Sustainable Chemistry and Engineering</i> , <b>2018</b> , 6, 12695-12705	8.3	60
82	Total Structure Determination of Au(S-Adm) and CdAu(S tBu) and Implications for the Structure of Au(SR). <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 10988-10994	16.4	56
81	Resolution and evaluation of 3-chlorophenyl-3-hydroxypropionylhydroxamic acid as antivirulence agent with excellent eradication efficacy in <i>Helicobacter pylori</i> infected mice. <i>European Journal of Pharmaceutical Sciences</i> , <b>2018</b> , 121, 293-300	5.1	3
80	Structure and Electronic Structure Evolution of Thiolate-Protected Gold Nanoclusters Containing Quasi Face-Centered-Cubic Kernels. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 14898-14907	3.8	39
79	Bonding of Two 8-Electron Superatom Clusters. <i>Angewandte Chemie</i> , <b>2018</b> , 130, 17010-17014	3.6	4
78	Bonding of Two 8-Electron Superatom Clusters. <i>Angewandte Chemie - International Edition</i> , <b>2018</b> , 57, 16768-16772	16.4	33
77	Theoretical prediction of a new stable structure of Au <sub>28</sub> (SR) <sub>20</sub> cluster. <i>Chemical Physics Letters</i> , <b>2018</b> , 704, 68-75	2.5	12
76	Highly Bright Self-Assembled Copper Nanoclusters: A Novel Photoluminescent Probe for Sensitive Detection of Histamine. <i>Analytical Chemistry</i> , <b>2018</b> , 90, 9060-9067	7.8	58
75	Ag(Dppm)(SR) and Its Homologue AuAg(Dppm)(SR) Alloy Nanocluster: Seeded Growth, Structure Determination, and Differences in Properties. <i>Journal of the American Chemical Society</i> , <b>2017</b> , 139, 1618-1624	16.4	114
74	A ten-electron (10e) thiolate-protected Au(SR) cluster: structure prediction and a gold-atom insertion, thiolate-group elimination mechanism. <i>Nanoscale</i> , <b>2017</b> , 9, 2895-2902	7.7	21
73	Theoretical Predictions of a New ~14 kDa Core-Mass Thiolate-Protected Gold Nanoparticle: Au(SR). <i>Journal of Physical Chemistry Letters</i> , <b>2017</b> , 8, 1248-1252	6.4	15
72	Au-Carbon Electronic Interaction Mediated Selective Oxidation of Styrene. <i>ACS Catalysis</i> , <b>2017</b> , 7, 3483-3488	3.8	65
71	Thiolate-protected gold nanoclusters: structural prediction and the understandings of electronic stability from first principles simulations. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , <b>2017</b> , 7, e1315	7.9	15

70	Photocatalytic wastewater purification with simultaneous hydrogen production using MoS <sub>2</sub> QD-decorated hierarchical assembly of ZnInS on reduced graphene oxide photocatalyst. <i>Water Research</i> , <b>2017</b> , 121, 11-19	12.5	129
69	Self-Optimization of the Active Site of Molybdenum Disulfide by an Irreversible Phase Transition during Photocatalytic Hydrogen Evolution. <i>Angewandte Chemie - International Edition</i> , <b>2017</b> , 56, 7610-7614	16.4	175
68	Self-Optimization of the Active Site of Molybdenum Disulfide by an Irreversible Phase Transition during Photocatalytic Hydrogen Evolution. <i>Angewandte Chemie</i> , <b>2017</b> , 129, 7718-7722	3.6	46
67	De-assembly of assembled PtAg units: tailoring the photoluminescence of atomically precise nanoclusters. <i>Chemical Communications</i> , <b>2017</b> , 53, 12564-12567	5.8	29
66	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. <i>Dalton Transactions</i> , <b>2017</b> , 46, 16257-16268	4.3	17
65	Quasi-Dual-Packed-Kernelled Au (2,4-DMBT) Nanoclusters and the Influence of Kernel Packing on the Electrochemical Gap. <i>Angewandte Chemie - International Edition</i> , <b>2017</b> , 56, 12644-12648	16.4	56
64	Quasi-Dual-Packed-Kernelled Au <sub>49</sub> (2,4-DMBT) <sub>27</sub> Nanoclusters and the Influence of Kernel Packing on the Electrochemical Gap. <i>Angewandte Chemie</i> , <b>2017</b> , 129, 12818-12822	3.6	18
63	Spatially Confined Li-Oxygen Interaction in the Tunnel of MnO <sub>2</sub> Catalyst for Li-Air Battery: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 16193-16200	3.8	14
62	Interfacial adhesion properties of graphene sheet on nanoscale corrugated surface: a molecular dynamics simulation study. <i>Molecular Simulation</i> , <b>2016</b> , 42, 405-412	2	4
61	Total Structure Determination of Au <sub>21</sub> (S-Adm) <sub>15</sub> and Geometrical/Electronic Structure Evolution of Thiolated Gold Nanoclusters. <i>Journal of the American Chemical Society</i> , <b>2016</b> , 138, 10754-7	16.4	128
60	Monolayer MoS <sub>2</sub> with S vacancies from interlayer spacing expanded counterparts for highly efficient electrochemical hydrogen production. <i>Journal of Materials Chemistry A</i> , <b>2016</b> , 4, 16524-16530	13	107
59	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. <i>Nanoscale</i> , <b>2016</b> , 8, 17044-17054	7.7	30
58	Shape-Controlled Synthesis of Trimetallic Nanoclusters: Structure Elucidation and Properties Investigation. <i>Chemistry - A European Journal</i> , <b>2016</b> , 22, 17145-17150	4.8	55
57	Two Electron Reduction: From Quantum Dots to Metal Nanoclusters. <i>Chemistry of Materials</i> , <b>2016</b> , 28, 7905-7911	9.6	31
56	Correlating the Structure and Optical Absorption Properties of Au <sub>76</sub> (SR) <sub>44</sub> Cluster. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 13739-13748	3.8	25
55	Density functional theory (DFT) studies of CO oxidation reaction on M <sub>13</sub> and Au <sub>18</sub> M clusters (M = Au, Ag, Cu, Pt and Pd): the role of co-adsorbed CO molecule. <i>RSC Advances</i> , <b>2016</b> , 6, 55867-55877	3.7	21
54	First-Principles Study of Structural, Electronic, and Magnetic Properties of One-Dimensional Transition Metals Incorporated Vinylanthalene Molecular Wires on Hydrogen-Terminated Silicon Surface. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 27980-27988	3.8	5
53	Wide bandgap copolymers with vertical benzodithiophene dicarboxylate for high-performance polymer solar cells with an efficiency up to 7.49%. <i>Journal of Materials Chemistry A</i> , <b>2016</b> , 4, 18792-18803	13	28

52	Tuning the Isomeric Fused Heteroaromatic Core of Small Donor-Acceptor Molecules to Alter Their Crystalline Nature and Enhance Photovoltaic Performance. <i>European Journal of Organic Chemistry</i> , <b>2015</b> , 2015, 820-827	3.2	13
51	First-principles investigation on the structural, electronic properties and diffusion barriers of Mg/Al doped NaCoO <sub>2</sub> as the cathode material of rechargeable sodium batteries. <i>RSC Advances</i> , <b>2015</b> , 5, 27229-27234 <sup>21</sup>	3.7	21
50	First-principles investigation on structural and electrochemical properties of NaCoO <sub>2</sub> for rechargeable Na-ion batteries. <i>Journal of Central South University</i> , <b>2015</b> , 22, 2036-2042	2.1	3
49	Electronic and magnetic properties of silicon supported organometallic molecular wires: a density functional theory (DFT) study. <i>Nanoscale</i> , <b>2015</b> , 7, 13734-46	7.7	6
48	Ultrafast Relaxation Dynamics of Luminescent Rod-Shaped, Silver-Doped Ag <sub>25</sub> Au <sub>25</sub> Clusters. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 18790-18797	3.8	63
47	Density Functional Theory Studies on Structure, Ligand Exchange, and Optical Properties of Ligand-Protected Gold Nanoclusters: Thiolate versus Selenolate. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 9205-9214	3.8	33
46	Metal exchange method using Au <sub>25</sub> nanoclusters as templates for alloy nanoclusters with atomic precision. <i>Journal of the American Chemical Society</i> , <b>2015</b> , 137, 4018-21	16.4	218
45	Improved photovoltaic performance of star-shaped molecules with a triphenylamine core by tuning the substituted position of the carbazolyl unit at the terminal. <i>Journal of Materials Chemistry A</i> , <b>2015</b> , 3, 10883-10889	13	27
44	New Structure Model of Au <sub>22</sub> (SR) <sub>18</sub> : Bitetrahedron Golden Kernel Enclosed by [Au <sub>6</sub> (SR) <sub>6</sub> ] Au(I) Complex. <i>Journal of Physical Chemistry Letters</i> , <b>2015</b> , 6, 1390-5	6.4	60
43	Density Functional Theory (DFT) Studies of CO Oxidation over Nanoporous Gold: Effects of Residual Ag and CO Self-Promoting Oxidation. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 10345-10354	3.8	26
42	Asymmetric Synthesis of 1,3-Butadienyl-2-carbinols by the Homoallylboronation of Aldehydes with a Chiral Phosphoric Acid Catalyst. <i>Angewandte Chemie - International Edition</i> , <b>2015</b> , 54, 7299-302	16.4	41
41	X-Ray crystal structure, and optical and electrochemical properties of the Au <sub>15</sub> Ag <sub>3</sub> (SC <sub>6</sub> H <sub>11</sub> ) <sub>14</sub> nanocluster with a core-shell structure. <i>Nanoscale</i> , <b>2015</b> , 7, 18278-83	7.7	52
40	The Nucleation and Growth Mechanism of Thiolate-Protected Au Nanoclusters. <i>Journal of the American Chemical Society</i> , <b>2015</b> , 137, 15809-16	16.4	28
39	The Structure and Optical Properties of the [Au <sub>18</sub> (SR) <sub>14</sub> ] Nanocluster. <i>Angewandte Chemie</i> , <b>2015</b> , 127, 3188-3192	3.6	38
38	The structure and optical properties of the [Au <sub>18</sub> (SR) <sub>14</sub> ] nanocluster. <i>Angewandte Chemie - International Edition</i> , <b>2015</b> , 54, 3145-9	16.4	177
37	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. <i>RSC Advances</i> , <b>2015</b> , 5, 14540-14546	3.7	10
36	A theoretical study of single-atom catalysis of CO oxidation using Au embedded 2D h-BN monolayer: a CO-promoted O <sub>2</sub> activation. <i>Scientific Reports</i> , <b>2014</b> , 4, 5441	4.9	177
35	Crystal structure and optical properties of the [Ag <sub>62</sub> S <sub>12</sub> (SBU(t)) <sub>32</sub> ](2+) nanocluster with a complete face-centered cubic kernel. <i>Journal of the American Chemical Society</i> , <b>2014</b> , 136, 15559-65	16.4	150

34	Crystal structure of Au(SePh) <sub>n</sub> nanoclusters and insights into their electronic, optical and catalytic properties. <i>Nanoscale</i> , <b>2014</b> , 6, 13977-85	7.7	86
33	Ab initio study of graphene-like monolayer molybdenum disulfide as a promising anode material for rechargeable sodium ion batteries. <i>RSC Advances</i> , <b>2014</b> , 4, 43183-43188	3.7	62
32	Mechanistic Insight into the Styrene-Selective Oxidation on Subnanometer Gold Clusters (Au <sub>16</sub> , Au <sub>20</sub> , Au <sub>27</sub> , Au <sub>28</sub> , Au <sub>30</sub> , and Au <sub>32</sub> -Au <sub>35</sub> ): A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 20346-20356	3.8	19
31	Edge decorated SiC nanoribbons with metal: Coexistence of planar tetracoordinate carbon and silicon. <i>Chemical Physics Letters</i> , <b>2013</b> , 580, 78-81	2.5	10
30	CO self-promoting oxidation on nanosized gold clusters: triangular Au <sub>3</sub> active site and CO induced O-O scission. <i>Journal of the American Chemical Society</i> , <b>2013</b> , 135, 2583-95	16.4	162
29	Thiol ligand-induced transformation of Au <sub>38</sub> (SC <sub>2</sub> H <sub>4</sub> Ph) <sub>24</sub> to Au <sub>36</sub> (SPh-t-Bu) <sub>24</sub> . <i>ACS Nano</i> , <b>2013</b> , 7, 6138-6147	16.7	168
28	Radical Chain-Reaction of Terminal-Unsaturated Organic Molecules on Water-Saturated Si(100)-(2 × 1): The Role of Surface Hydroxyl Groups. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 14032-14042	3.8	5
27	Structure prediction of Au(44)(SR)(28): a chiral superatom cluster. <i>Journal of the American Chemical Society</i> , <b>2013</b> , 135, 19060-3	16.4	81
26	CO oxidation on TiO <sub>2</sub> (110) supported subnanometer gold clusters: size and shape effects. <i>Journal of the American Chemical Society</i> , <b>2013</b> , 135, 19336-46	16.4	113
25	Semiring chemistry of Au <sub>25</sub> (SR) <sub>18</sub> : fragmentation pathway and catalytic active site. <i>Journal of the American Chemical Society</i> , <b>2013</b> , 135, 18067-79	16.4	55
24	Tri-Wing Graphene Nano-Paddle-Wheel with a Single-File Metal Joint: Formation of Multi-Planar Tetracoordinated-Carbon (ptC) Strips. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 11378-11385	3.8	24
23	Interlocked catenane-like structure predicted in Au <sub>24</sub> (SR) <sub>20</sub> : implication to structural evolution of thiolated gold clusters from homoleptic gold(I) thiolates to core-stacked nanoparticles. <i>Journal of the American Chemical Society</i> , <b>2012</b> , 134, 3015-24	16.4	117
22	Unraveling the mechanisms of O <sub>2</sub> activation by size-selected gold clusters: transition from superoxo to peroxo chemisorption. <i>Journal of the American Chemical Society</i> , <b>2012</b> , 134, 9438-45	16.4	129
21	Investigating the structural evolution of thiolate protected gold clusters from first-principles. <i>Nanoscale</i> , <b>2012</b> , 4, 4054-72	7.7	205
20	Synthesis and photovoltaic properties of conjugated side chains polymers with different electron-withdrawing and donating end groups. <i>Journal of Polymer Science Part A</i> , <b>2012</b> , 50, 3848-3858	2.5	19
19	Hollow polyhedral structures in small gold-sulfide clusters. <i>ACS Nano</i> , <b>2011</b> , 5, 1441-9	16.7	32
18	Catalytic activities of subnanometer gold clusters (Au <sub>n</sub> Au <sub>m</sub> Au <sub>p</sub> and Au <sub>n</sub> Au <sub>m</sub> ) for CO oxidation. <i>ACS Nano</i> , <b>2011</b> , 5, 7818-29	16.7	163
17	Exohedral Silicon Fullerenes: Si <sub>60</sub> Pn <sub>60</sub> and Si <sub>80</sub> Pn <sub>60</sub> (Pn = P, As, Sb and Bi). <i>Journal of Cluster Science</i> , <b>2011</b> , 22, 343-354	3	1



16	Inorganic nanoribbons with unpassivated zigzag edges: Half metallicity and edge reconstruction. <i>Nano Research</i> , <b>2011</b> , 4, 233-239	10	58
15	Two-dimensional to three-dimensional structural transition of gold cluster Au <sub>10</sub> during soft landing on TiO <sub>2</sub> surface and its effect on CO oxidation. <i>Journal of Chemical Physics</i> , <b>2010</b> , 133, 134707	3.9	19
14	Investigating active site of gold nanoparticle Au <sub>55</sub> (PPh <sub>3</sub> ) <sub>12</sub> Cl <sub>6</sub> in selective oxidation. <i>ACS Nano</i> , <b>2010</b> , 4, 2009-20	16.7	68
13	Planar tetracoordinate carbon strips in edge decorated graphene nanoribbon. <i>Journal of the American Chemical Society</i> , <b>2010</b> , 132, 5554-5	16.4	73
12	Icosahedral crown gold nanocluster Au <sub>43</sub> Cu <sub>12</sub> with high catalytic activity. <i>Nano Letters</i> , <b>2010</b> , 10, 1055-63	16.3	107
11	Onset of double helical structure in small-sized homoleptic gold thiolate clusters. <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 629-32	2.8	37
10	Thiolate-protected Au <sub>20</sub> (SR) <sub>16</sub> cluster: prolate Au <sub>8</sub> core with new [Au <sub>3</sub> (SR) <sub>4</sub> ] staple motif. <i>Journal of the American Chemical Society</i> , <b>2009</b> , 131, 13619-21	16.4	154
9	B <sub>2</sub> C graphene, nanotubes, and nanoribbons. <i>Nano Letters</i> , <b>2009</b> , 9, 1577-82	11.5	133
8	Probing the planar tetra-, penta-, and hexacoordinate carbon in carbon-boron mixed clusters. <i>Journal of the American Chemical Society</i> , <b>2008</b> , 130, 2580-92	16.4	88
7	Planar pentacoordinate carbon in CA <sub>5</sub> (+): a global minimum. <i>Journal of the American Chemical Society</i> , <b>2008</b> , 130, 10394-400	16.4	120
6	Structural prediction of thiolate-protected Au <sub>38</sub> : a face-fused bi-icosahedral Au core. <i>Journal of the American Chemical Society</i> , <b>2008</b> , 130, 7830-2	16.4	261
5	Exohedral silicon fullerenes: Si <sub>n</sub> P <sub>n</sub> T <sub>n</sub> /2 (20). <i>Journal of Chemical Physics</i> , <b>2007</b> , 127, 044704	3.9	10
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3	Electric field induced switching behaviors of monolayer-modified silicon surfaces: surface designs and molecular dynamics simulations. <i>Journal of the American Chemical Society</i> , <b>2005</b> , 127, 6802-13	16.4	36
2	(002) facets exposed and controllable thickness of CdS nanobelts drive desirable hydrogen-adsorption free energy (ΔG <sub>H</sub> ) for boosting visible-light photocatalytic performance. <i>Catalysis Science and Technology</i> ,	5.5	2
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