Yong Pei

List of Publications by Year in descending order

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150 papers	8,793 citations	34076 52 h-index	46771 89 g-index
150 all docs	150 docs citations	150 times ranked	7687 citing authors

#	Article	IF	Citations
1	MoS₂ Quantum Dot Growth Induced by S Vacancies in a ZnIn₂S₄ Monolayer: Atomic-Level Heterostructure for Photocatalytic Hydrogen Production. ACS Nano, 2018, 12, 751-758.	7.3	500
2	Structural Prediction of Thiolate-Protected Au₃₈: A Face-Fused Bi-icosahedral Au Core. Journal of the American Chemical Society, 2008, 130, 7830-7832.	6.6	272
3	Metal Exchange Method Using Au₂₅Nanoclusters as Templates for Alloy Nanoclusters with Atomic Precision. Journal of the American Chemical Society, 2015, 137, 4018-4021.	6.6	266
4	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.	10.8	246
5	Selfâ€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.	7.2	221
6	Investigating the structural evolution of thiolate protected gold clusters from first-principles. Nanoscale, 2012, 4, 4054.	2.8	219
7	A Theoretical Study of Single-Atom Catalysis of CO Oxidation Using Au Embedded 2D h-BN Monolayer: A CO-Promoted O2 Activation. Scientific Reports, 2014, 4, 5441.	1.6	211
8	The Structure and Optical Properties of the [Au₁₈(SR)₁₄] Nanocluster. Angewandte Chemie - International Edition, 2015, 54, 3145-3149.	7.2	205
9	Thiol Ligand-Induced Transformation of Au₃₈(SC₂H₄Ph)₂₄ to Au₃₆(SPh-t-Bu)₂₄. ACS Nano, 2013, 7, 6138-6145.	7.3	203
10	Catalytic Activities of Subnanometer Gold Clusters (Au₁₆â€“Au₁₈,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 387 7818-7829.	7.3	182
11	CO Self-Promoting Oxidation on Nanosized Gold Clusters: Triangular Au₃ Active Site and CO Induced Oâ€“O Scission. Journal of the American Chemical Society, 2013, 135, 2583-2595.	6.6	178
12	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, 15559-15565.	6.6	176
13	Photocatalytic wastewater purification with simultaneous hydrogen production using MoS 2 QD-decorated hierarchical assembly of ZnIn 2 S 4 on reduced graphene oxide photocatalyst. Water Research, 2017, 121, 11-19.	5.3	176
14	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, 10754-10757.	6.6	160
15	Thiolate-Protected Au₂₀(SR)₁₆ Cluster: Prolate Au₈ Core with New [Au₃(SR)₄] Staple Motif. Journal of the American Chemical Society, 2009, 131, 13619-13621.	6.6	156
16	B₂C Graphene, Nanotubes, and Nanoribbons. Nano Letters, 2009, 9, 1577-1582.	4.5	154
17	Planar Pentacoordinate Carbon in CAl₅⁺: A Global Minimum. Journal of the American Chemical Society, 2008, 130, 10394-10400.	6.6	153
18	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, 9438-9445.	6.6	149

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19	Monolayer MoS₂with S vacancies from interlayer spacing expanded counterparts for highly efficient electrochemical hydrogen production. Journal of Materials Chemistry A, 2016, 4, 16524-16530.	5.2	148
20	Ag₅₀(Dppm)₆(SR)₃₀ and Its Homologue Au_xAg_{50â€“x}(Dppm)₆(SR)₃₀ Alloy Nanocluster: Seeded Growth, Structure Determination, and Differences in Properties. Journal of the American Chemical Society, 2017, 139, 1618-1624.	6.6	138
21	CO Oxidation on TiO₂ (110) Supported Subnanometer Gold Clusters: Size and Shape Effects. Journal of the American Chemical Society, 2013, 135, 19336-19346.	6.6	127
22	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.	5.2	126
23	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, 3015-3024.	6.6	123
24	Tuning Pb(II) Adsorption from Aqueous Solutions on Ultrathin Iron Oxychloride (FeOCl) Nanosheets. Environmental Science & Technology, 2019, 53, 2075-2085.	4.6	121
25	NiMoO₄ Nanosheets Anchored on Nï£¿S Doped Carbon Clothes with Hierarchical Structure as a Bidirectional Catalyst toward Accelerating Polysulfides Conversion for Lïï£¿S Battery. Advanced Functional Materials, 2021, 31, 2101285.	7.8	119
26	Icosahedral Crown Gold Nanocluster Au₄₃Cu₁₂ with High Catalytic Activity. Nano Letters, 2010, 10, 1055-1062.	4.5	115
27	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.	3.2	102
28	Crystal structure of Au₂₅(SePh)₁₈ nanoclusters and insights into their electronic, optical and catalytic properties. Nanoscale, 2014, 6, 13977-13985.	2.8	97
29	Probing the Planar Tetra-, Penta-, and Hexacoordinate Carbon in Carbonâ^'Boron Mixed Clusters. Journal of the American Chemical Society, 2008, 130, 2580-2592.	6.6	95
30	Auâ€“Carbon Electronic Interaction Mediated Selective Oxidation of Styrene. ACS Catalysis, 2017, 7, 3483-3488.	5.5	92
31	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.	5.0	92
32	Growth-Rule-Guided Structural Exploration of Thiolate-Protected Gold Nanoclusters. Accounts of Chemical Research, 2019, 52, 23-33.	7.6	91
33	Structure Prediction of Au44(SR)28: A Chiral Superatom Cluster. Journal of the American Chemical Society, 2013, 135, 19060-19063.	6.6	89
34	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.	1.7	88
35	Highly Bright Self-Assembled Copper Nanoclusters: A Novel Photoluminescent Probe for Sensitive Detection of Histamine. Analytical Chemistry, 2018, 90, 9060-9067.	3.2	87
36	Rational construction of a library of M ₂₉ nanoclusters from monometallic to tetrametallic. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 18834-18840.	3.3	86

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37	Tellurium Surface Doping to Enhance the Structural Stability and Electrochemical Performance of Layered Ni-Rich Cathodes. ACS Applied Materials & Interfaces, 2019, 11, 40022-40033.	4.0	85
38	Structure Determination of Alkynylâ€Protected Gold Nanocluster Au₂₂(^tBuCâ‰¡C)₁₈ and Its Thermochromic Luminescence. Angewandte Chemie - International Edition, 2020, 59, 2309-2312.	7.2	85
39	The Fourth Alloying Mode by Way of Antiâ€Galvanic Reaction. Angewandte Chemie - International Edition, 2018, 57, 4500-4504.	7.2	81
40	Total Structure Determination of Au₁₆(S-Adm)₁₂ and Cd₁Au₁₄(StBu)₁₂ and Implications for the Structure of Au₁₅(SR)₁₃. Journal of the American Chemical Society, 2018, 140, 10988-10994.	6.6	81
41	Investigating Active Site of Gold Nanoparticle Au₅₅(PPh₃)₁₂Cl₆ in Selective Oxidation. ACS Nano, 2010, 4, 2009-2020.	7.3	76
42	Planar Tetracoordinate Carbon Strips in Edge Decorated Graphene Nanoribbon. Journal of the American Chemical Society, 2010, 132, 5554-5555.	6.6	75
43	Ultrafast Relaxation Dynamics of Luminescent Rod-Shaped, Silver-Doped Ag_xAu_{25â€“x} Clusters. Journal of Physical Chemistry C, 2015, 119, 18790-18797.	1.5	75
44	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, 1390-1395.	2.1	71
45	Shapeâ€Controlled Synthesis of Trimetallic Nanoclusters: Structure Elucidation and Properties Investigation. Chemistry - A European Journal, 2016, 22, 17145-17150.	1.7	67
46	Quasiâ€Dualâ€Packedâ€Kerneled Au₄₉(2,4â€DMBT)₂₇ Nanoclusters and the Influence of Kernel Packing on the Electrochemical Gap. Angewandte Chemie - International Edition, 2017, 56, 12644-12648.	7.2	66
47	Reversible nanocluster structure transformation between face-centered cubic and icosahedral isomers. Chemical Science, 2019, 10, 8685-8693.	3.7	65
48	Inorganic nanoribbons with unpassivated zigzag edges: Half metallicity and edge reconstruction. Nano Research, 2011, 4, 233-239.	5.8	62
49	X-Ray crystal structure, and optical and electrochemical properties of the Au₁₅Ag₃(SC₆H₁₁)₁₄nanocluster with a coreâ€“shell structure. Nanoscale, 2015, 7, 18278-18283.	2.8	62
50	Selfâ€Optimization of the Active Site of Molybdenum Disulfide by an Irreversible Phase Transition during Photocatalytic Hydrogen Evolution. Angewandte Chemie, 2017, 129, 7718-7722.	1.6	61
51	Semiring Chemistry of Au₂₅(SR)₁₈: Fragmentation Pathway and Catalytic Active site. Journal of the American Chemical Society, 2013, 135, 18067-18079.	6.6	60
52	Ultrasmall Au nanocatalysts supported on nitrided carbon for electrocatalytic CO₂ reduction: the role of the carbon support in high selectivity. Nanoscale, 2018, 10, 14678-14686.	2.8	57
53	Asymmetric Synthesis of 1,3â€Butadienylâ€2â€carbinols by the Homoallenylboration of Aldehydes with a Chiral Phosphoric Acid Catalyst. Angewandte Chemie - International Edition, 2015, 54, 7299-7302.	7.2	49
54	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.	1.5	47

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55	Molecular Dynamics Simulation of Surfactant Flooding Driven Oil-Detachment in Nano-Silica Channels. Journal of Physical Chemistry B, 2019, 123, 277-288.	1.2	46
56	Controlling Nanoparticles with Atomic Precision. Accounts of Chemical Research, 2019, 52, 1-1.	7.6	46
57	Ligand Modification of Au₂₅ Nanoclusters for Near-Infrared Photocatalytic Oxidative Functionalization. Journal of the American Chemical Society, 2022, 144, 3787-3792.	6.6	45
58	Electrocatalytic dechlorination of halogenated antibiotics via synergistic effect of chlorine-cobalt bond and atomic H*. Journal of Hazardous Materials, 2018, 358, 294-301.	6.5	44
59	The Structure and Optical Properties of the [Au₁₈(SR)₁₄] Nanocluster. Angewandte Chemie, 2015, 127, 3188-3192.	1.6	43
60	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.	1.2	43
61	Combining the Single-Atom Engineering and Ligand-Exchange Strategies: Obtaining the Single-Heteroatom-Doped Au₁₆Ag₁(S-Adm)₁₃ Nanocluster with Atomically Precise Structure. Inorganic Chemistry, 2018, 57, 335-342.	1.9	43
62	Bonding of Two 8â€Electron Superatom Clusters. Angewandte Chemie - International Edition, 2018, 57, 16768-16772.	7.2	43
63	Nanocluster growth via â€œgraft-ontoâ€• effects on geometric structures and optical properties. Chemical Science, 2020, 11, 1691-1697.	3.7	41
64	Onset of Double Helical Structure in Small-Sized Homoleptic Gold Thiolate Clusters. Journal of Physical Chemistry A, 2009, 113, 629-632.	1.1	39
65	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.	2.8	39
66	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.	2.7	39
67	De-assembly of assembled Pt₁Ag₁₂ units: tailoring the photoluminescence of atomically precise nanoclusters. Chemical Communications, 2017, 53, 12564-12567.	2.2	37
68	Electric Field Induced Switching Behaviors of Monolayer-Modified Silicon Surfaces:Â Surface Designs and Molecular Dynamics Simulations. Journal of the American Chemical Society, 2005, 127, 6802-6813.	6.6	36
69	Hollow Polyhedral Structures in Small Goldâ^'Sulfide Clusters. ACS Nano, 2011, 5, 1441-1449.	7.3	35
70	The Nucleation and Growth Mechanism of Thiolate-Protected Au Nanoclusters. Journal of the American Chemical Society, 2015, 137, 15809-15816.	6.6	35
71	Two Electron Reduction: From Quantum Dots to Metal Nanoclusters. Chemistry of Materials, 2016, 28, 7905-7911.	3.2	35
72	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.	1.5	34

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73	First-principles investigation on the structural, electronic properties and diffusion barriers of Mg/Al doped NaCoO₂as the cathode material of rechargeable sodium batteries. RSC Advances, 2015, 5, 27229-27234.	1.7	33
74	Fluorescence or Phosphorescence? The Metallic Composition of the Nanocluster Kernel Does Matter. Angewandte Chemie - International Edition, 2022, 61, .	7.2	32
75	Comparative Study on Reactions and Self-Directed Growth Mechanisms of Styrene Molecules on Hâ˚Terminated Si(111) and Si(100):Â Combining Quantum Chemistry and Molecular Mechanics Simulations. Langmuir, 2006, 22, 3040-3048.	1.6	30
76	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.	5.2	30
77	Correlating the Structure and Optical Absorption Properties of Au₇₆(SR)₄₄ Cluster. Journal of Physical Chemistry C, 2016, 120, 13739-13748.	1.5	30
78	Activating a TiO₂/BiVO₄ Film for Photoelectrochemical Water Splitting by Constructing a Heterojunction Interface with a Uniform Crystal Plane Orientation. ACS Applied Materials & Interfaces, 2022, 14, 2316-2325.	4.0	30
79	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.	1.5	28
80	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.	1.5	28
81	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.	5.2	27
82	A homoleptic alkynyl-protected [Ag₉Cu₆(^tBuCî€,C)₁₂]⁺ superatom with free electrons: synthesis, structure analysis, and different properties compared with the Au₇Ag₈ cluster in the M₁₅⁺ series. Chemical Science, 2021, 12, 12819-12826.	3.7	27
83	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.	1.7	26
84	A ten-electron (10e) thiolate-protected Au₂₉(SR)₁₉cluster: structure prediction and a â€˜gold-atom insertion, thiolate-group eliminationâ€™ mechanism. Nanoscale, 2017, 9, 2895-2902.	2.8	26
85	Unraveling the Nucleation Process from a Au(I)-SR Complex to Transition-Size Nanoclusters. Journal of the American Chemical Society, 2021, 143, 15224-15232.	6.6	26
86	Evolution from superatomic Au₂₄Ag₂₀ monomers into molecular-like Au₄₃Ag₃₈ dimeric nanoclusters. Chemical Science, 2022, 13, 2778-2782.	3.7	25
87	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.	1.5	24
88	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.	1.5	24
89	Quantum-sized metal nanoclusters. Nanoscale, 2012, 4, 4026.	2.8	23
90	Structure Determination of Alkynylâ€Protected Gold Nanocluster Au₂₂(^tBuCâ‰¡C)₁₈ and Its Thermochromic Luminescence. Angewandte Chemie, 2020, 132, 2329-2332.	1.6	22

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91	Synthesis and photovoltaic properties of conjugated side chains polymers with different electronâ€withdrawing and donating end groups. Journal of Polymer Science Part A, 2012, 50, 3848-3858.	2.5	21
92	Thiolateâ€protected gold nanoclusters: structural prediction and the understandings of electronic stability from first principles simulations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1315.	6.2	21
93	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.	1.5	21
94	Three-Component Cascade Synthesis of Carbazoles through [1s,6s] Sigmatropic Shift under Metal-Free Conditions. Journal of Organic Chemistry, 2019, 84, 3121-3131.	1.7	21
95	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.	1.2	20
96	Quasiâ€Dualâ€Packedâ€Kerneled Au 49 (2,4â€DMBT) 27 Nanoclusters and the Influence of Kernel Packing on the Electrochemical Gap. Angewandte Chemie, 2017, 129, 12818-12822.	1.6	20
97	The Fourth Alloying Mode by Way of Anti-Galvanic Reaction. Angewandte Chemie, 2018, 130, 4590-4594.	1.6	20
98	Mechanistic Insight into the Styrene-Selective Oxidation on Subnanometer Gold Clusters (Au₁₆â€“Au₂₀, Au₂₇, Au₂₈, Au₃₀, and) Tj ETQq0 0 0 rgBT /Overlock 1 C, 2014, 118, 20346-20356.	1.5	19
99	Theoretical Predictions of a New â¼14 kDa Core-Mass Thiolate-Protected Gold Nanoparticle: Au₆₈(SR)₃₆. Journal of Physical Chemistry Letters, 2017, 8, 1248-1252.	2.1	19
100	BiOI Nanopaper As a High-Capacity, Long-Life and Insertion-Type Anode for a Flexible Quasi-Solid-State Zn-Ion Battery. ACS Applied Materials & Interfaces, 2022, 14, 25516-25523.	4.0	19
101	Dual phosphorescence emission of dinuclear platinum(<scp>ii</scp>) 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.	1.6	18
102	Theoretical prediction of a new stable structure of Au28(SR)20 cluster. Chemical Physics Letters, 2018, 704, 68-75.	1.2	17
103	Total structural determination of [Au₁Ag₂₄(Dppm)₃(SR)₁₇]²⁺ comprising an open icosahedral Au₁Ag₁₂ core with six free valence electrons. Chemical Communications, 2019, 55, 6457-6460.	2.2	17
104	Isomer Structural Transformation in Auâ€“Cu Alloy Nanoclusters: Water Rippleâ€Like Transfer of Thiol Ligands. Particle and Particle Systems Characterization, 2019, 36, 1800494.	1.2	17
105	Spatially Confined Liâ€“Oxygen Interaction in the Tunnel of Î±-MnO₂ Catalyst for Liâ€“Air Battery: A First-Principles Study. Journal of Physical Chemistry C, 2017, 121, 16193-16200.	1.5	15
106	On the mechanism of inter-cluster alloying reactions: two-stage metal exchange of [Au₂₅(PET)₁₈]^{â^'}and [Ag₂₅(DMBT)₁₈]^{â^'}clusters. Journal of Materials Chemistry A, 2020, 8, 10242-10251.	5.2	14
107	Fabrication of magnetic nickel incorporated carbon nanofibers for superfast adsorption of sulfadiazine: Performance and mechanisms exploration. Journal of Hazardous Materials, 2022, 423, 127219.	6.5	14
108	Exohedral silicon fullerenes: SiNPtNâ•2â€(20â©½Nâ©½60). Journal of Chemical Physics, 2007, 127, 044704.	1.2	13

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109	Tuning the Isomeric Fused Heteroaromatic Core of Small Donorâ€“Acceptor Molecules to Alter Their Crystalline Nature and Enhance Photovoltaic Performance. European Journal of Organic Chemistry, 2015, 2015, 820-827.	1.2	13
110	Structural determination of a metastable Ag₂₇ nanocluster and its transformations into Ag₈ and Ag₂₉ nanoclusters. Inorganic Chemistry Frontiers, 2021, 8, 4407-4414.	3.0	13
111	Structure and Catalytic Activity of Gold Clusters Supported on Nitrogen-Doped Graphene. Journal of Physical Chemistry C, 2021, 125, 5006-5019.	1.5	13
112	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.	1.7	12
113	Novel solution-processible small molecules based on benzo[1,2-b:3,4-bâ€²:5,6-bâ€²â€²]trithiophene for effective organic photovoltaics with high open-circuit voltage. RSC Advances, 2015, 5, 14540-14546.	1.7	11
114	[Au₁₆Ag₄₃H₁₂(SPhCl₂)₃₄]^{5â€“}: An Auâ€“Ag Alloy Nanocluster with 12 Hydrides and Its Enlightenment on Nanocluster Structural Evolution. Inorganic Chemistry, 2021, 60, 11640-11647.	1.9	11
115	Anisotropic Evolution of Nanoclusters from Ag₄₀ to Ag₄₅: Halogen- and Defect-Induced Epitaxial Growth in Nanoclusters. Journal of Physical Chemistry Letters, 2021, 12, 6654-6660.	2.1	11
116	Edge decorated SiC nanoribbons with metal: Coexistence of planar tetracoordinate carbon and silicon. Chemical Physics Letters, 2013, 580, 78-81.	1.2	10
117	A revisit to the structure of Au20(SCH2CH2Ph)16: a cubic nanocrystal-like gold kernel. Nanoscale, 2018, 10, 10357-10364.	2.8	10
118	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.	1.9	10
119	Electronic Structure and Spin Transport Properties of a New Class of Semiconductor Surface-Confined One-Dimensional Half-Metallic [Eu-(C_nH_{nâ€“2})]_N (n = 7â€“9) Sandwich Compounds and Molecular Wires: First Principle Studies. Journal of Physical Chemistry C, 2018, 122, 16168-16177.	1.5	9
120	Insight into 6Ï€ Electrocyclic Reactions of 1,8â€Dioxatetraene. Angewandte Chemie - International Edition, 2019, 58, 2660-2664.	7.2	9
121	Exploration of Formation and Sizeâ€Evolution Pathways of Thiolateâ€Gold Nanoclusters in the COâ€Directed [Au 25 (SR) 18] â^' Synthesis. Small, 2020, 17, 2000627.	5.2	9
122	Electronic and magnetic properties of silicon supported organometallic molecular wires: a density functional theory (DFT) study. Nanoscale, 2015, 7, 13734-13746.	2.8	8
123	Exploring the structure evolution and core/ligand structure patterns of a series of large sized thiolate-protected gold clusters Au_{145-3N}(SR)_{60-2N} (N = 1â€“8): a first principles study. Nanoscale, 2018, 10, 3918-3929.	2.8	8
124	The mechanism of metal exchange in non-metallic nanoclusters. Nanoscale Advances, 2020, 2, 664-668.	2.2	8
125	Exposed (002) facets and controllable thickness of CdS nanobelts drive desirable hydrogen-adsorption free energy (Î”G_H) for boosting visible-light photocatalytic performance. Catalysis Science and Technology, 2021, 11, 7486-7492.	2.1	8
126	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.	1.5	7

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127	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.	1.5	7
128	Radical Chain-Reaction of Terminal-Unsaturated Organic Molecules on Water-Saturated Si(100)-(2 Ã— 1): The Role of Surface Hydroxyl Groups. Journal of Physical Chemistry C, 2013, 117, 14032-14042.	1.5	6
129	First-principles investigation on structural and electrochemical properties of NaCoO2 for rechargeable Na-ion batteries. Journal of Central South University, 2015, 22, 2036-2042.	1.2	6
130	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.	2.8	6
131	Interfacial adhesion properties of graphene sheet on nanoscale corrugated surface: a molecular dynamics simulation study. Molecular Simulation, 2016, 42, 405-412.	0.9	5
132	Bonding of Two 8â€Electron Superatom Clusters. Angewandte Chemie, 2018, 130, 17010-17014.	1.6	5
133	Total structural determination of alloyed Au_{15.37}Cu_{16.63}(S-Adm)₂₀ nanoclusters with double superatomic chains. Chemical Communications, 2021, 57, 2017-2020.	2.2	5
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135	Ligand Shell Isomerization Induces Different Fluorescence Origins of Two Au₂₈ Nanoclusters. Journal of Physical Chemistry Letters, 2022, 13, 3718-3725.	2.1	5
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