Hannu HÃ¤kkinen

List of Publications by Year
in descending order

230 papers	24,207 citations	10956 71 h-index	7496 151 g-index
240 all docs	240 docs citations	240 times ranked	13748 citing authors

#	Article	IF	Citations
1	A unified view of ligand-protected gold clusters as superatom complexes. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 9157-9162.	3.3	1,472
2	The goldâ€“sulfur interface at the nanoscale. Nature Chemistry, 2012, 4, 443-455.	6.6	1,418
3	Charging Effects on Bonding and Catalyzed Oxidation of CO on Au8 Clusters on MgO. Science, 2005, 307, 403-407.	6.0	1,358
4	On the Structure of Thiolate-Protected Au₂₅. Journal of the American Chemical Society, 2008, 130, 3756-3757.	6.6	682
5	All-thiol-stabilized Ag44 and Au12Ag32 nanoparticles with single-crystal structures. Nature Communications, 2013, 4, 2422.	5.8	675
6	Self-Passivating Edge Reconstructions of Graphene. Physical Review Letters, 2008, 101, 115502.	2.9	674
7	Atomic and electronic structure of gold clusters: understanding flakes, cages and superatoms from simple concepts. Chemical Society Reviews, 2008, 37, 1847.	18.7	639
8	Bonding in Cu, Ag, and Au Clusters: Relativistic Effects, Trends, and Surprises. Physical Review Letters, 2002, 89, 033401.	2.9	611
9	On the Electronic and Atomic Structures of Small AuN- (N = 4â^'14) Clusters:â€‰ A Photoelectron Spectroscopy and Density-Functional Study. Journal of Physical Chemistry A, 2003, 107, 6168-6175.	1.1	598
10	Structural, Electronic, and Impurity-Doping Effects in Nanoscale Chemistry: Supported Gold Nanoclusters. Angewandte Chemie - International Edition, 2003, 42, 1297-1300.	7.2	547
11	Gold clusters(AuN,2<~N<~10)and their anions. Physical Review B, 2000, 62, R2287-R2290.	1.1	454
12	Divide and Protect:Â Capping Gold Nanoclusters with Molecular Goldâ^'Thiolate Rings. Journal of Physical Chemistry B, 2006, 110, 9927-9931.	1.2	405
13	Chirality and Electronic Structure of the Thiolate-Protected Au₃₈ Nanocluster. Journal of the American Chemical Society, 2010, 132, 8210-8218.	6.6	401
14	Structure and Bonding in the Ubiquitous Icosahedral Metallic Gold Cluster Au₁₄₄(SR)₆₀. Journal of Physical Chemistry C, 2009, 113, 5035-5038.	1.5	393
15	Catalytic CO Oxidation by Free Au2-:Â Experiment and Theory. Journal of the American Chemical Society, 2003, 125, 10437-10445.	6.6	386
16	Interaction of O2 with Gold Clusters:â€‰ Molecular and Dissociative Adsorption. Journal of Physical Chemistry A, 2003, 107, 4066-4071.	1.1	349
17	N-heterocyclic carbene-functionalized magic-number gold nanoclusters. Nature Chemistry, 2019, 11, 419-425.	6.6	333
18	A Critical Size for Emergence of Nonbulk Electronic and Geometric Structures in Dodecanethiolate-Protected Au Clusters. Journal of the American Chemical Society, 2015, 137, 1206-1212.	6.6	322

#	Article	IF	Citations
19	Atomically Precise Alkynyl-Protected Metal Nanoclusters as a Model Catalyst: Observation of Promoting Effect of Surface Ligands on Catalysis by Metal Nanoparticles. Journal of the American Chemical Society, 2016, 138, 3278-3281.	6.6	297
20	Quantum size effects in ambient CO oxidation catalysed by ligand-protected gold clusters. Nature Chemistry, 2010, 2, 329-334.	6.6	295
21	Photoelectron spectra of aluminum cluster anions: Temperature effects andab initiosimulations. Physical Review B, 1999, 60, R11297-R11300.	1.1	289
22	Evidence for graphene edges beyond zigzag and armchair. Physical Review B, 2009, 80, .	1.1	274
23	Single Crystal XRD Structure and Theoretical Analysis of the Chiral Au₃₀S(S-<i>t</i>-Bu)₁₈ Cluster. Journal of the American Chemical Society, 2014, 136, 5000-5005.	6.6	270
24	Electron microscopy of gold nanoparticles at atomic resolution. Science, 2014, 345, 909-912.	6.0	269
25	Symmetry and Electronic Structure of Noble-Metal Nanoparticles and the Role of Relativity. Physical Review Letters, 2004, 93, 093401.	2.9	241
26	Birth of the Localized Surface Plasmon Resonance in Monolayer-Protected Gold Nanoclusters. ACS Nano, 2013, 7, 10263-10270.	7.3	240
27	Plasmonic twinned silver nanoparticles with molecular precision. Nature Communications, 2016, 7, 12809.	5.8	235
28	Gas-Phase Catalytic Oxidation of CO by Au2-. Journal of the American Chemical Society, 2001, 123, 9704-9705.	6.6	230
29	Total Structure and Electronic Structure Analysis of Doped Thiolated Silver [MAg₂₄(SR)₁₈]^{2â€“} (M = Pd, Pt) Clusters. Journal of the American Chemical Society, 2015, 137, 11880-11883.	6.6	221
30	Structural and Theoretical Basis for Ligand Exchange on Thiolate Monolayer Protected Gold Nanoclusters. Journal of the American Chemical Society, 2012, 134, 13316-13322.	6.6	199
31	Size-Dependent Structural Evolution and Chemical Reactivity of Gold Clusters. ChemPhysChem, 2007, 8, 157-161.	1.0	197
32	Asymmetric Synthesis of Chiral Bimetallic [Ag₂₈Cu₁₂(SR)₂₄]^{4â€“} Nanoclusters via Ion Pairing. Journal of the American Chemical Society, 2016, 138, 12751-12754.	6.6	196
33	Time-dependent density-functional theory in the projector augmented-wave method. Journal of Chemical Physics, 2008, 128, 244101.	1.2	187
34	Robust, Highly Luminescent Au₁₃ Superatoms Protected by N-Heterocyclic Carbenes. Journal of the American Chemical Society, 2019, 141, 14997-15002.	6.6	185
35	Structural, chemical, and dynamical trends in graphene grain boundaries. Physical Review B, 2010, 81, .	1.1	184
36	An Intermetallic Au₂₄Ag₂₀ Superatom Nanocluster Stabilized by Labile Ligands. Journal of the American Chemical Society, 2015, 137, 4324-4327.	6.6	175

#	Article	IF	Citations
37	[Ag₆₇(SPhMe₂)₃₂(PPh₃)₈]³⁺: Synthesis, Total Structure, and Optical Properties of a Large Box-Shaped Silver Nanocluster. Journal of the American Chemical Society, 2016, 138, 14727-14732.	6.6	167
38	Ligand-Stabilized Au₁₃Cu_{<i>x</i>} (<i>x</i> = 2, 4, 8) Bimetallic Nanoclusters: Ligand Engineering to Control the Exposure of Metal Sites. Journal of the American Chemical Society, 2013, 135, 9568-9571.	6.6	162
39	Jahnâ€"Teller effects in Au₂₅(SR)₁₈. Chemical Science, 2016, 7, 1882-1890.	3.7	149
40	Structural Evolution of Atomically Precise Thiolated Bimetallic [Au_{12+<i>n</i>}Cu₃₂(SR)_{30+<i>n</i>}]^{4â€"} (<i>n</i> = 0,) Tj ETQq0 0 0 rgBT /Over	6.6	145
41	Atomically Precise, Thiolated Copperâ€"Hydride Nanoclusters as Single-Site Hydrogenation Catalysts for Ketones in Mild Conditions. ACS Nano, 2019, 13, 5975-5986.	7.3	138
42	Gold Nanowires and Their Chemical Modifications. Journal of Physical Chemistry B, 1999, 103, 8814-8816.	1.2	135
43	Goldâ^'Thiolate Complexes Form a Unique <i>c</i>(4 Ã— 2) Structure on Au(111). Journal of Physical Chemistry C, 2008, 112, 15940-15942.	1.5	125
44	Chiral Phase Transfer and Enantioenrichment of Thiolate-Protected Au₁₀₂ Clusters. Journal of the American Chemical Society, 2014, 136, 4129-4132.	6.6	125
45	Highly Robust but Surfaceâ€Active: An Nâ€Heterocyclic Carbeneâ€Stabilized Au₂₅ Nanocluster. Angewandte Chemie - International Edition, 2019, 58, 17731-17735.	7.2	125
46	Bulky Surface Ligands Promote Surface Reactivities of [Ag₁₄₁X₁₂(S-Adm)₄₀]³⁺ (X = Cl, Br, I) Nanoclusters: Models for Multiple-Twinned Nanoparticles. Journal of the American Chemical Society, 2017, 139, 13288-13291.	6.6	124
47	Theoretical Characterization of Cyclic Thiolated Gold Clusters. Journal of the American Chemical Society, 2006, 128, 10268-10275.	6.6	118
48	Embryonic Growth of Face-Center-Cubic Silver Nanoclusters Shaped in Nearly Perfect Half-Cubes and Cubes. Journal of the American Chemical Society, 2017, 139, 31-34.	6.6	113
49	Au₄₀(SR)₂₄ Cluster as a Chiral Dimer of 8-Electron Superatoms: Structure and Optical Properties. Journal of the American Chemical Society, 2012, 134, 19560-19563.	6.6	112
50	Aluminum cluster anions: Photoelectron spectroscopy andab initiosimulations. Physical Review B, 2000, 62, 13216-13228.	1.1	111
51	Thiolate-Protected Au₂₅ Superatoms as Building Blocks: Dimers and Crystals. Journal of Physical Chemistry C, 2010, 114, 15986-15994.	1.5	109
52	Effects of Silver Doping on the Geometric and Electronic Structure and Optical Absorption Spectra of the Au_{25â€"<i>n</i>}Ag_{<i>n</i>}(SH)₁₈^{â€"} (<i>n</i> = 1,) Tj ETQq0 0 0 rgBT /Ov	1.5	108
53	Nanowire Gold Chains:Â Formation Mechanisms and Conductance. Journal of Physical Chemistry B, 2000, 104, 9063-9066.	1.2	106
54	A density functional investigation of thiolate-protected bimetal PdAu24(SR)18z clusters: doping the superatom complex. Physical Chemistry Chemical Physics, 2009, 11, 7123.	1.3	100

#	Article	IF	Citations
55	A hollow tetrahedral cage of hexadecagold dianion provides a robust backbone for a tuneable sub-nanometer oxidation and reduction agent via endohedral doping. Physical Chemistry Chemical Physics, 2006, 8, 5407-5411.	1.3	98
56	Site-specific targeting of enterovirus capsid by functionalized monodisperse gold nanoclusters. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 1277-1281.	3.3	95
57	Co-crystallization of atomically precise metal nanoparticles driven by magic atomic and electronic shells. Nature Communications, 2018, 9, 3357.	5.8	95
58	Atomistic Simulations of Functional Au₁₄₄(SR)₆₀ Gold Nanoparticles in Aqueous Environment. Journal of Physical Chemistry C, 2012, 116, 9805-9815.	1.5	94
59	Supramolecular Functionalization and Concomitant Enhancement in Properties of Au₂₅ Clusters. ACS Nano, 2014, 8, 139-152.	7.3	94
60	Gold in graphene: In-plane adsorption and diffusion. Applied Physics Letters, 2009, 94, .	1.5	93
61	Conformation and dynamics of the ligand shell of a water-soluble Au102 nanoparticle. Nature Communications, 2016, 7, 10401.	5.8	91
62	Solvent-mediated assembly of atom-precise goldâ€“silver nanoclusters to semiconducting one-dimensional materials. Nature Communications, 2020, 11, 2229.	5.8	91
63	From Symmetry Breaking to Unraveling the Origin of the Chirality of Ligated Au₁₃Cu₂ Nanoclusters. Angewandte Chemie - International Edition, 2018, 57, 3421-3425.	7.2	88
64	Templateâ€Free Supracolloidal Selfâ€Assembly of Atomically Precise Gold Nanoclusters: From 2D Colloidal Crystals to Spherical Capsids. Angewandte Chemie - International Edition, 2016, 55, 16035-16038.	7.2	86
65	Electronic and Vibrational Signatures of the Au₁₀₂(<i>p</i>-MBA)₄₄ Cluster. Journal of the American Chemical Society, 2011, 133, 3752-3755.	6.6	80
66	Carbon Dioxide Activation and Reaction Induced by Electron Transfer at an Oxideâ€“Metal Interface. Angewandte Chemie - International Edition, 2015, 54, 12484-12487.	7.2	80
67	Connections Between Theory and Experiment for Gold and Silver Nanoclusters. Annual Review of Physical Chemistry, 2018, 69, 205-229.	4.8	80
68	Ag₄₄(SeR)₃₀: A Hollow Cage Silver Cluster with Selenolate Protection. Journal of Physical Chemistry Letters, 2013, 4, 3351-3355.	2.1	78
69	A Unified AMBER-Compatible Molecular Mechanics Force Field for Thiolate-Protected Gold Nanoclusters. Journal of Chemical Theory and Computation, 2016, 12, 1342-1350.	2.3	76
70	Au Adsorption on Regular and Defected Thin MgO(100) Films Supported by Mo. Journal of Physical Chemistry C, 2007, 111, 4319-4327.	1.5	74
71	Charging of atoms, clusters, and molecules on metal-supported oxides: A general and long-ranged phenomenon. Physical Review B, 2008, 78, .	1.1	74
72	N-Heterocyclic Carbene-Stabilized Hydrido Au₂₄ Nanoclusters: Synthesis, Structure, and Electrocatalytic Reduction of CO₂. Journal of the American Chemical Society, 2022, 144, 9000-9006.	6.6	74

#	Article	IF	Citations
73	Polymerization at the Alkylthiolateâˆ'Au(111) Interface. Journal of Physical Chemistry B, 2007, 111, 3325-3327.	1.2	73
74	[Cu₃₂(PET)₂₄H₈Cl₂](PPh₄)₂: A Copper Hydride Nanocluster with a Bisquare Antiprismatic Core. Journal of the American Chemical Society, 2020, 142, 13974-13981.	6.6	73
75	Combinatorial Identification of Hydrides in a Ligated Ag₄₀ Nanocluster with Noncompact Metal Core. Journal of the American Chemical Society, 2019, 141, 11905-11911.	6.6	72
76	Electronic Structure and Bonding of Icosahedral Coreâ€“Shell Goldâ€“Silver Nanoalloy Clusters Au_{144â€“<i>x</i>}Ag_{<i>x</i>}(SR)₆₀. Journal of Physical Chemistry Letters, 2011, 2, 2316-2321.	2.1	71
77	Cd₁₂Ag₃₂(SePh)₃₆: Non-Noble Metal Doped Silver Nanoclusters. Journal of the American Chemical Society, 2019, 141, 8422-8425.	6.6	71
78	Surface Coordination of Multiple Ligands Endows Nâ€Heterocyclic Carbeneâ€Stabilized Gold Nanoclusters with High Robustness and Surface Reactivity. Angewandte Chemie - International Edition, 2021, 60, 3752-3758.	7.2	71
79	Cationic Au Nanoparticle Binding with Plasma Membrane-like Lipid Bilayers: Potential Mechanism for Spontaneous Permeation to Cells Revealed by Atomistic Simulations. Journal of Physical Chemistry C, 2014, 118, 11131-11141.	1.5	69
80	Trapping of 27 bpâ€“8 kbp DNA and immobilization of thiol-modified DNA using dielectrophoresis. Nanotechnology, 2007, 18, 295204.	1.3	68
81	Characterizing low-coordinated atoms at the periphery of MgO-supported Au islands using scanning tunneling microscopy and electronic structure calculations. Physical Review B, 2010, 81, .	1.1	67
82	Hydrogen Welding and Hydrogen Switches in a Monatomic Gold Nanowire. Nano Letters, 2004, 4, 1845-1852.	4.5	66
83	Molecule-like Photodynamics of Au₁₀₂(<i>p</i>MBA)₄₄ Nanocluster. ACS Nano, 2015, 9, 2328-2335.	7.3	66
84	Chiral Inversion of Thiolate-Protected Gold Nanoclusters via Core Reconstruction without Breaking a Auâ€“S Bond. Journal of the American Chemical Society, 2019, 141, 6006-6012.	6.6	66
85	Thiol-stabilized atomically precise, superatomic silver nanoparticles for catalysing cycloisomerization of alkynyl amines. National Science Review, 2018, 5, 694-702.	4.6	63
86	Liquid-Liquid Phase Coexistence in Gold Clusters: 2D or Not 2D?. Physical Review Letters, 2007, 98, 015701.	2.9	62
87	Experimental and Density Functional Theory Analysis of Serial Introductions of Electron-Withdrawing Ligands into the Ligand Shell of a Thiolate-Protected Au₂₅ Nanoparticle. Journal of Physical Chemistry C, 2010, 114, 8276-8281.	1.5	61
88	Site Preference in Multimetallic Nanoclusters: Incorporation of Alkali Metal Ions or Copper Atoms into the Alkynylâ€Protected Bodyâ€Centered Cubic Cluster [Au₇Ag₈(Câ‰¡C^{<i>t</i>}Bu)₁₂]⁺. Angewandte Chemie - International Edition, 2016, 55, 15152-15156.	7.2	60
89	Covalently linked multimers of gold nanoclusters Au₁₀₂(p-MBA)₄₄and Au_{âˆ¼250}(p-MBA)_n. Nanoscale, 2016, 8, 18665-18674.	2.8	59
90	Nondestructive Size Determination of Thiol-Stabilized Gold Nanoclusters in Solution by Diffusion Ordered NMR Spectroscopy. Analytical Chemistry, 2013, 85, 3489-3492.	3.2	57

#	Article	IF	Citations
91	Atomically Precise Nanocluster Assemblies Encapsulating Plasmonic Gold Nanorods. Angewandte Chemie - International Edition, 2018, 57, 6522-6526.	7.2	57
92	Electronic Structure and Optical Properties of the Thiolate-Protected Au₂₈(SMe)₂₀ Cluster. Journal of Physical Chemistry A, 2013, 117, 10526-10533.	1.1	56
93	Oxidation of magnesia-supported Pd-clusters leads to the ultimate limit of epitaxy with a catalytic function. Nature Materials, 2006, 5, 44-47.	13.3	55
94	Adsorption of gold clusters on metal-supported MgO: Correlation to electron affinity of gold. Physical Review B, 2007, 76, .	1.1	53
95	Einfluss der geometrischen und elektronischen Struktur sowie der elementaren Zusammensetzung von Clustern auf chemische Prozesse in der Nanometerskala. Angewandte Chemie, 2003, 115, 1335-1338.	1.6	52
96	Theoretical Characterization of Cyclic Thiolated Copper, Silver, and Gold Clusters. Journal of Physical Chemistry C, 2010, 114, 13571-13576.	1.5	51
97	N-Heterocyclic Carbene-Stabilized Gold Nanoclusters with Organometallic Motifs for Promoting Catalysis. Journal of the American Chemical Society, 2022, 144, 10844-10853.	6.6	51
98	Electronic Structure of MgO-Supported Au Clusters: Quantum Dots Probed by Scanning Tunneling Microscopy. Physical Review Letters, 2007, 99, 096102.	2.9	49
99	Ultrafast Electronic Relaxation and Vibrational Cooling Dynamics of Au₁₄₄(SC₂H₄Ph)₆₀ Nanocluster Probed by Transient Mid-IR Spectroscopy. Journal of Physical Chemistry C, 2014, 118, 18233-18239.	1.5	49
100	Experimental and Theoretical Determination of the Optical Gap of the Au₁₄₄(SC₂H₄Ph)₆₀ Cluster and the (Au/Ag)₁₄₄(SC₂H₄Ph)₆₀ Nanoalloys. Journal of Physical Chemistry Letters, 2012, 3, 3076-3080.	2.1	48
101	Acidâ€“Base Properties and Surface Charge Distribution of the Water-Soluble Au₁₀₂(<i>p</i>MBA)₄₄ Nanocluster. Journal of Physical Chemistry C, 2016, 120, 10041-10050.	1.5	47
102	[Pt₂Cu₃₄(PET)₂₂Cl₄]^{2â€“}: An Atomically Precise, 10-Electron PtCu Bimetal Nanocluster with a Direct Ptâ€“Pt Bond. Journal of the American Chemical Society, 2021, 143, 12100-12107.	6.6	47
103	Pd₂Au₃₆(SR)₂₄cluster: structure studies. Nanoscale, 2015, 7, 17012-17019.	2.8	46
104	A 58-electron superatom-complex model for the magic phosphine-protected gold clusters (Schmid-gold, NanogoldÂ®) of 1.4-nm dimension. Chemical Science, 2011, 2, 1583.	3.7	44
105	Synthesis and Characterization of Enantiopure Chiral Bis NHC-Stabilized Edge-Shared Au₁₀ Nanocluster with Unique Prolate Shape. Journal of the American Chemical Society, 2022, 144, 2056-2061.	6.6	44
106	Oligomeric Goldâˆ'Thiolate Units Define the Properties of the Molecular Junction between Gold and Benzene Dithiols. Journal of Physical Chemistry Letters, 2010, 1, 1528-1532.	2.1	43
107	A Homoleptic Alkynylâ€Ligated [Au₁₃Ag₁₆L₂₄]^{3âˆ'} Cluster as a Catalytically Active Eightâ€Electron Superatom. Angewandte Chemie - International Edition, 2021, 60, 970-975.	7.2	43
108	Evidence of superatom electronic shells in ligand-stabilized aluminum clusters. Journal of Chemical Physics, 2011, 135, 094701.	1.2	42

#	Article	IF	Citations
109	Au₇₀S₂₀(PPh₃)₁₂: an intermediate sized metalloid gold cluster stabilized by the Au₄S₄ ring motif and Au-PPh₃ groups. Chemical Communications, 2018, 54, 248-251.	2.2	42
110	Enhanced Surface Ligands Reactivity of Metal Clusters by Bulky Ligands for Controlling Optical and Chiral Properties. Angewandte Chemie - International Edition, 2021, 60, 12897-12903.	7.2	42
111	Density functional study of gold atoms and clusters on a graphite (0001) surface with defects. Physical Review B, 2006, 74, .	1.1	41
112	The Al50Cp*12 Cluster - A 138-Electron Closed Shell (L = 6) Superatom. European Journal of Inorganic Chemistry, 2011, 2011, 2649-2652.	1.0	41
113	Formation of Gold(I) Edge Oxide at Flat Gold Nanoclusters on an Ultrathin MgO Film under Ambient Conditions. Angewandte Chemie - International Edition, 2010, 49, 7913-7916.	7.2	40
114	Role of the Central Gold Atom in Ligand-Protected Biicosahedral Au₂₄ and Au₂₅ Clusters. Journal of Physical Chemistry C, 2013, 117, 22079-22086.	1.5	39
115	Highly Robust but Surfaceâ€Active: An Nâ€Heterocyclic Carbeneâ€Stabilized Au₂₅ Nanocluster. Angewandte Chemie, 2019, 131, 17895-17899.	1.6	39
116	Stability, electronic structure, and optical properties of protected gold-doped silver Ag_{29â^'x}Au_x (x = 0â€"5) nanoclusters. Physical Chemistry Chemical Physics, 2017, 19, 13868-13874.	1.3	38
117	Reversible isomerization of metal nanoclusters induced by intermolecular interaction. CheM, 2021, 7, 2227-2244.	5.8	38
118	Dynamic Stabilization of the Ligandâ€"Metal Interface in Atomically Precise Gold Nanoclusters Au₆₈ and Au₁₄₄ Protected by <i>meta</i>-Mercaptobenzoic Acid. ACS Nano, 2017, 11, 11872-11879.	7.3	37
119	A method for structure prediction of metal-ligand interfaces of hybrid nanoparticles. Nature Communications, 2019, 10, 3973.	5.8	37
120	TDDFT Analysis of Optical Properties of Thiol Monolayer-Protected Gold and Intermetallic Silverâ€"Gold Au₁₄₄(SR)₆₀ and Au₈₄Ag₆₀(SR)₆₀ Clusters. Journal of Physical Chemistry C, 2014, 118, 20002-20008.	1.5	36
121	Electronic shell structures in bare and protected metal nanoclusters. Advances in Physics: X, 2016, 1, 467-491.	1.5	36
122	One-pot synthesis and characterization of subnanometre-size benzotriazolate protected copper clusters. Nanoscale, 2012, 4, 4095.	2.8	35
123	Electronic Structure and Optical Properties of the Intrinsically Chiral 16-Electron Superatom Complex [Au₂₀(PP₃)₄]⁴⁺. Journal of Physical Chemistry A, 2014, 118, 4214-4221.	1.1	35
124	Hydrophobic pocket targeting probes for enteroviruses. Nanoscale, 2015, 7, 17457-17467.	2.8	35
125	Mixed-Monolayer-Protected Au₂₅ Clusters with Bulky Calix[4]arene Functionalities. Journal of Physical Chemistry Letters, 2014, 5, 585-589.	2.1	34
126	Vibrational Perturbations and Ligandâ€"Layer Coupling in a Single Crystal of Au₁₄₄(SC₂H₄Ph)₆₀ Nanocluster. Journal of Physical Chemistry Letters, 2014, 5, 387-392.	2.1	34

#	Article	IF	Citations
127	Reversible Supracolloidal Selfâ€Assembly of Cobalt Nanoparticles to Hollow Capsids and Their Superstructures. Angewandte Chemie - International Edition, 2017, 56, 6473-6477.	7.2	34
128	Towards Controlled Synthesis of Water-Soluble Gold Nanoclusters: Synthesis and Analysis. Journal of Physical Chemistry C, 2019, 123, 2602-2612.	1.5	34
129	The Redox Chemistry of Gold with Highâ€Valence Doped Calcium Oxide. Angewandte Chemie - International Edition, 2013, 52, 1424-1427.	7.2	33
130	Dynamic Diglyme-Mediated Self-Assembly of Gold Nanoclusters. ACS Nano, 2015, 9, 11690-11698.	7.3	33
131	Monte Carlo Simulations of Au₃₈(SCH₃)₂₄ Nanocluster Using Distance-Based Machine Learning Methods. Journal of Physical Chemistry A, 2020, 124, 4827-4836.	1.1	33
132	Experimental Confirmation of a Topological Isomer of the Ubiquitous Au₂₅(SR)₁₈ Cluster in the Gas Phase. Journal of the American Chemical Society, 2021, 143, 1273-1277.	6.6	33
133	Copper-hydride nanoclusters with enhanced stability by N-heterocyclic carbenes. Nano Research, 2021, 14, 3303-3308.	5.8	33
134	Ag₄₄(EBT)₂₆(TPP)₄ Nanoclusters With Tailored Molecular and Electronic Structure. Angewandte Chemie - International Edition, 2021, 60, 9038-9044.	7.2	33
135	Protected but Accessible: Oxygen Activation by a Calixarene-Stabilized Undecagold Cluster. Journal of the American Chemical Society, 2013, 135, 12944-12947.	6.6	32
136	Nonlinear Optical Properties of Thiolate-Protected Gold Clusters: A Theoretical Survey of the First Hyperpolarizabilities. Journal of Physical Chemistry C, 2015, 119, 27676-27682.	1.5	31
137	Symmetry breaking in ligand-protected gold clusters probed by nonlinear optics. Nanoscale, 2016, 8, 12123-12127.	2.8	31
138	First-principles simulations of hydrogen peroxide formation catalyzed by small neutral gold clusters. Physical Chemistry Chemical Physics, 2009, 11, 6359.	1.3	30
139	Divide and Protect: Passivating Cu(111) by Cu-(benzotriazole)₂. Journal of Physical Chemistry C, 2012, 116, 22346-22349.	1.5	30
140	A topological isomer of the Au₂₅(SR)₁₈^{â^’}nanocluster. Chemical Communications, 2020, 56, 8087-8090.	2.2	30
141	Photoelectron spectra from first principles: from the many-body to the single-particle picture. New Journal of Physics, 2008, 10, 043018.	1.2	29
142	Adsorption and activation of O2 at Au chains on MgO/Mo thin films. Physical Chemistry Chemical Physics, 2010, 12, 1483.	1.3	29
143	Optical absorption of magnesia-supported gold clusters and nanoscale catalysts: Effects due to the support, clusters, and adsorbants. Physical Review B, 2005, 72, .	1.1	28
144	Solvation chemistry of water-soluble thiol-protected gold nanocluster Au₁₀₂ from DOSY NMR spectroscopy and DFT calculations. Nanoscale, 2014, 6, 7823-7826.	2.8	28

#	Article	IF	Citations
145	Superatomic S² Silver Clusters Stabilized by a Thiolateâ€“Phosphine Monolayer: Insight into Electronic and Optical Properties of Ag₁₄(SC₆H₃F₂)₁₂(PPh₃)₈ and Ag₁₆(SC₆H₃F₂)₁₄(DPPE)₄. Journal of Physical Chemistry A, 2014, 118, 8351-8355.	1.1	28
146	The Role of the Anchor Atom in the Ligand of the Monolayer-Protected Au₂₅(XR)₁₈^{â€“} Nanocluster. Journal of Physical Chemistry C, 2015, 119, 9587-9594.	1.5	28
147	Atomically Precise Gold Nanoclusters: Towards an Optimal Biocompatible System from a Theoreticalâ€“Experimental Strategy. Small, 2021, 17, e2005499.	5.2	28
148	55-Atom clusters of silver and gold: Symmetry breaking by relativistic effects. Computational Materials Science, 2006, 35, 332-336.	1.4	27
149	Copper Induces a Core Plasmon in Intermetallic Au_{(144,145)â€“<i>x</i>}Cu_{<i>x</i>}(SR)₆₀ Nanoclusters. Journal of Physical Chemistry Letters, 2015, 6, 515-520.	2.1	27
150	Impacts of Copper Position on the Electronic Structure of [Au_{25-x}Cu_{<i>x</i>}(SH)₁₈]^{â^'} Nanoclusters. Journal of Physical Chemistry C, 2015, 119, 8290-8298.	1.5	27
151	Oxidation of small gas phase Pd clusters: A density functional study. Computational Materials Science, 2006, 35, 371-374.	1.4	26
152	Raman spectra of single-walled carbon nanotubes with vacancies. Physical Review B, 2008, 77, .	1.1	26
153	Modeling thiolate-protected gold clusters with density-functional tight-binding. European Physical Journal D, 2013, 67, 1.	0.6	26
154	Electron quantization in arbitrarily shaped gold islands on MgO thin films. Physical Review B, 2013, 88, .	1.1	26
155	Real-space imaging with pattern recognition of a ligand-protected Ag374 nanocluster at sub-molecular resolution. Nature Communications, 2018, 9, 2948.	5.8	26
156	Towards Atomically Precise Supported Catalysts from Monolayerâ€Protected Clusters: The Critical Role of the Support. Chemistry - A European Journal, 2020, 26, 7051-7058.	1.7	25
157	A DFT Study of Linear Goldâ€“Thiolate Superclusters Absorbing in the Therapeutic NIR Window. Journal of Physical Chemistry Letters, 2014, 5, 1329-1334.	2.1	24
158	Tertiary Chiral Nanostructures from Câ^'Hâ‹…â‹…â‹…F Directed Assembly of Chiroptical Superatoms. Angewandte Chemie - International Edition, 2021, 60, 22411-22416.	7.2	24
159	From Symmetry Breaking to Unraveling the Origin of the Chirality of Ligated Au₁₃Cu₂ Nanoclusters. Angewandte Chemie, 2018, 130, 3479-3483.	1.6	23
160	Atomic Layer Deposition of Aluminum Oxide on TiO2 and Its Impact on N3 Dye Adsorption from First Principles. Journal of Physical Chemistry C, 2011, 115, 9250-9259.	1.5	22
161	Optical and electronic properties of graphene nanoribbons upon adsorption of ligand-protected aluminum clusters. Physical Chemistry Chemical Physics, 2014, 16, 3558.	1.3	22
162	NHC-Stabilized Au₁₀ Nanoclusters and Their Conversion to Au₂₅ Nanoclusters. Jacs Au, 2022, 2, 875-885.	3.6	22

#	Article	IF	Citations
163	Effect of bending on Raman-active vibration modes of carbon nanotubes. Physical Review B, 2008, 78, .	1.1	21
164	Role of Nanocrystal Symmetry in the Crossover Region from Molecular to Metallic Gold Nanoparticles. Journal of Physical Chemistry C, 2019, 123, 20655-20663.	1.5	21
165	Electronic structure and thermal behavior of a magicNa59+cluster. Physical Review A, 2004, 70, .	1.0	20
166	The electronic structure of Ge9[Si(SiMe3)3]3â˜': a superantiatom complex. Physical Chemistry Chemical Physics, 2012, 14, 9311.	1.3	20
167	Photodynamics of a Molecular Water-Soluble Nanocluster Identified as Au₁₃₀(<i>p</i>MBA)₅₀. Journal of Physical Chemistry C, 2015, 119, 20224-20229.	1.5	20
168	Electron Binding in a Superatom with a Repulsive Coulomb Barrier: The Case of [Ag₄₄(SC₆H₃F₂)₃₀]^{4â€"} in the Gas Phase. Journal of Physical Chemistry Letters, 2020, 11, 3069-3074.	2.1	20
169	Prospects and challenges for computer simulations of monolayer-protected metal clusters. Nature Communications, 2021, 12, 2197.	5.8	20
170	A small spherical liquid: A DFT molecular dynamics study of WAu12. Physical Chemistry Chemical Physics, 2005, 7, 2208.	1.3	19
171	Theoretical Analysis of the M₁₂Ag₃₂(SR)₄₀^{4â€"} and X@M₁₂Ag₃₂(SR)₃₀^{4â€"} Nanoclusters (M = Au, Ag; X = H,) Tj ETQq1 1 0.784314	1.5	19
172	Templateâ€Free Supracolloidal Selfâ€Assembly of Atomically Precise Gold Nanoclusters: From 2D Colloidal Crystals to Spherical Capsids. Angewandte Chemie, 2016, 128, 16269-16272.	1.6	19
173	Point Group Symmetry Analysis of the Electronic Structure of Bare and Protected Metal Nanocrystals. Journal of Physical Chemistry A, 2018, 122, 8576-8584.	1.1	19
174	Synthesis and properties of an Au₆ cluster supported by a mixed N-heterocyclic carbeneâ€"thiolate ligand. Chemical Communications, 2020, 56, 6102-6105.	2.2	19
175	Regioselective hydrogenation of alkenes over atomically dispersed Pd sites on NHC-stabilized bimetallic nanoclusters. CheM, 2022, 8, 2380-2392.	5.8	19
176	Crystal Structures and Density Functional Theory Calculations of <i>o</i>- and <i>p</i>-Nitroaniline Derivatives: Combined Effect of Hydrogen Bonding and Aromatic Interactions on Dimerization Energy. Crystal Growth and Design, 2013, 13, 3603-3612.	1.4	18
177	Analysis of Localized Surface Plasmon Resonances in Spherical Jellium Clusters and Their Assemblies. Journal of Physical Chemistry C, 2017, 121, 27036-27052.	1.5	18
178	Reversible Supracolloidal Selfâ€Assembly of Cobalt Nanoparticles to Hollow Capsids and Their Superstructures. Angewandte Chemie, 2017, 129, 6573-6577.	1.6	18
179	Characterization of Ironâ˜'Carbonyl-Protected Gold Clusters. Journal of the American Chemical Society, 2009, 131, 12573-12575.	6.6	17
180	Solubilityâ€Driven Isolation of a Metastable Nonagold Cluster with Bodyâ€Centered Cubic Structure. Chemistry - A European Journal, 2020, 26, 8465-8470.	1.7	17

#	Article	IF	Citations
181	Patterning of supported gold monolayers via chemical lift-off lithography. Beilstein Journal of Nanotechnology, 2017, 8, 2648-2661.	1.5	16
182	Role of Donor and Acceptor Substituents on the Nonlinear Optical Properties of Gold Nanoclusters. Journal of Physical Chemistry C, 2018, 122, 4019-4028.	1.5	15
183	Surface Coordination of Multiple Ligands Endows Nâ€Heterocyclic Carbeneâ€Stabilized Gold Nanoclusters with High Robustness and Surface Reactivity. Angewandte Chemie, 2021, 133, 3796-3802.	1.6	14
184	Solvent driven formation of silver embedded resorcinarene nanorods. CrystEngComm, 2012, 14, 347-350.	1.3	13
185	Structural characterization of site-modified nanocapsid with monodispersed gold clusters. Scientific Reports, 2017, 7, 17048.	1.6	13
186	Atomically Precise Alkynyl- and Halide-Protected AuAg Nanoclusters Au78Ag66(Câ‰¡CPh)48Cl8 and Au74Ag60(Câ‰¡CPh)40Br12: The Ligation Effects of Halides. Inorganic Chemistry, 2021, 60, 3529-3533.	1.9	13
187	Photo-Induced Cluster-to-Cluster Transformation of [Au_{37â€“<i>x</i>}Ag_{<i>x</i>}(PPh₃)₁₃Cl₁₀]³⁺ into [Au_{25â€“<i>y</i>}Ag_{<i>y</i>}(PPh₃)₁₀Cl₈]⁺: Fragmentation of a Trimer of 8-Electron Superatoms by Light. Journal of Physical Chemistry Letters, 2021, 12, 10920-10926.	2.1	13
188	Electronic Structure. Frontiers of Nanoscience, 2015, 9, 189-222.	0.3	12
189	Site Preference in Multimetallic Nanoclusters: Incorporation of Alkali Metal Ions or Copper Atoms into the Alkynylâ€Protected Bodyâ€Centered Cubic Cluster [Au₇Ag₈(Câ‰¡C^{<i>t</i>}Bu)₁₂]⁺. Angewandte Chemie, 2016, 128, 15376-15380.	1.6	11
190	Analysis of the Electronic Structure of Non-Spherical Ligand-Protected Metal Nanoclusters: The Case of a Box-Like Ag₆₇. Journal of Physical Chemistry C, 2017, 121, 10698-10705.	1.5	11
191	Nonmagnetic and magnetic thiolate-protected Au<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>25</mml:mn></mml:msub></mml:math>superatoms on Cu(111), Ag(111), and Au(111) surfaces. Physical Review B, 2012, 85, .	1.1	10
192	Silver Sulfide Nanoclusters and the Superatom Model. Journal of Physical Chemistry C, 2015, 119, 1583-1590.	1.5	10
193	Surface Chemistry Controls Magnetism in Cobalt Nanoclusters. Journal of Physical Chemistry C, 2016, 120, 20822-20827.	1.5	10
194	Atomically Precise Nanocluster Assemblies Encapsulating Plasmonic Gold Nanorods. Angewandte Chemie, 2018, 130, 6632-6636.	1.6	10
195	Chiral footprint of the ligand layer in the all-alkynyl-protected gold nanocluster Au144(CCPhF)60. Chemical Communications, 2019, 55, 9460-9462.	2.2	10
196	Charge Transfer Plasmons in Dimeric Electron Clusters. Journal of Physical Chemistry C, 2020, 124, 12645-12654.	1.5	10
197	Symmetry-induced long-lived excited state in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msubsup><mml:mi mathvariant="normal">Au</mml:mi><mml:mn>6</mml:mn><mml:mo>â^’</mml:mo></mml:msubsup></mml:math>. Physical Review B, 2007, 76, .	1.1	9
198	Exploring Strategies for Labeling Viruses with Gold Nanoclusters through Non-equilibrium Molecular Dynamics Simulations. Bioconjugate Chemistry, 2017, 28, 2327-2339.	1.8	9

#	Article	IF	Citations
199	Exploring the atomic structure of 1.8 nm monolayer-protected gold clusters with aberration-corrected STEM. Ultramicroscopy, 2017, 176, 146-150.	0.8	8
200	Ab initio molecular dynamics studies of Au38(SR)24 isomers under heating. European Physical Journal D, 2019, 73, 1.	0.6	8
201	Ab initio simulation of <mml:math altimg="si14.gif" overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" xmlns:sb="http://www.elsevier.com/xml/common/struct-bib/dtd" xmlns:ce="http://www.elsevier.com/x	1.4	7
202	Ligand-Protected Gold Nanoclusters as Superatomsâ€”Insights from Theory and Computations. Frontiers of Nanoscience, 2012, 3, 129-157.	0.3	7
203	How many gold atoms make gold metal?. Europhysics News, 2015, 46, 23-26.	0.1	7
204	Ligand mediated evolution of size dependent magnetism in cobalt nanoclusters. Physical Chemistry Chemical Physics, 2018, 20, 4563-4570.	1.3	7
205	Covalent and non-covalent coupling of a Au₁₀₂ nanocluster with a fluorophore: energy transfer, quenching and intracellular pH sensing. Nanoscale Advances, 2021, 3, 6649-6658.	2.2	7
206	Ligand Ratio Plays a Critical Role in the Design of Optimal Multifunctional Gold Nanoclusters for Targeted Gastric Cancer Therapy. ACS Nanoscience Au, 2021, 1, 47-60.	2.0	7
207	Protected Metallic Clusters, Quantum Wells and Metal-Nanocrystal Molecules. Journal of Physical Chemistry C, 2010, 114, 15877-15878.	1.5	6
208	Theoretical Studies of Gold Nanoclusters in Various Chemical Environments: When the Size Matters. , 2012, , 233-272.		6
209	Solid state halogen bonded networks vs. dynamic assemblies in solution: explaining Nâ‹¯X interactions of multivalent building blocks. CrystEngComm, 2015, 17, 8231-8241.	1.3	6
210	A Homoleptic Alkynylâ€Ligated [Au 13 Ag 16 L 24] 3âˆ’ Cluster as a Catalytically Active Eightâ€Electron Superatom. Angewandte Chemie, 2021, 133, 983-988.	1.6	6
211	Ag 44 (EBT) 26 (TPP) 4 Nanoclusters With Tailored Molecular and Electronic Structure. Angewandte Chemie, 2021, 133, 9120-9126.	1.6	6
212	Magnetically induced currents and aromaticity in ligand-stabilized Au and AuPt superatoms. Nature Communications, 2021, 12, 2477.	5.8	6
213	Cubic aromaticity in ligand-stabilized doped Au superatoms. Journal of Chemical Physics, 2021, 154, 204303.	1.2	6
214	Dynamics of weak interactions in the ligand layer of <i>meta</i>-mercaptobenzoic acid protected gold nanoclusters Au₆₈(<i>m</i>-MBA)₃₂ and Au₁₄₄(<i>m</i>-MBA)₄₀. Nanoscale, 2020, 12, 23859-23868.	2.8	6
215	Selective Acrolein Hydrogenation over Ligand-Protected Gold Clusters: A Venus Flytrap Mechanism. ACS Catalysis, 2022, 12, 2365-2374.	5.5	6
216	Gold/Isophorone Interaction Driven by Keto/Enol Tautomerization. Journal of Physical Chemistry C, 2016, 120, 21962-21966.	1.5	5

#	Article	IF	Citations
217	Anomalous binding sequence of CO ligands to an anionic triplatinum carbonyl complex. Chemical Physics Letters, 2005, 406, 44-48.	1.2	4
218	Computational Study of Adsorption of CO2, SO2, and H2CO on Free-Standing and Molybdenum-Supported CaO Films. Journal of Physical Chemistry C, 2019, 123, 7758-7765.	1.5	4
219	Enhanced Surface Ligands Reactivity of Metal Clusters by Bulky Ligands for Controlling Optical and Chiral Properties. Angewandte Chemie, 2021, 133, 13007-13013.	1.6	4
220	Polymorphic and solvate structures of ethyl ester and carboxylic acid derivatives of WIN 61893 analogue and their stability in solution. CrystEngComm, 2014, 16, 9001-9009.	1.3	3
221	Gold assisted oxygen dissociation on a molybdenum-doped CaO(001) surface. Catalysis Science and Technology, 2016, 6, 6784-6793.	2.1	3
222	Gold Nanoclusters: Atomically Precise Gold Nanoclusters: Towards an Optimal Biocompatible System from a Theoreticalâ€“Experimental Strategy (Small 27/2021). Small, 2021, 17, 2170140.	5.2	3
223	Structure and dynamics of CaO films: A computational study of an effect of external static electric field. Physical Review B, 2017, 95, .	1.1	2
224	The Journal of Physical Chemistry C Virtual Special Issue on Metal Clusters, Nanoparticles, and the Physical Chemistry of Catalysis. Journal of Physical Chemistry C, 2021, 125, 4927-4929.	1.5	2
225	Isomer dynamics of the [Au₆(NHC-S)₄]²⁺ nanocluster. Chemical Communications, 2022, 58, 3218-3221.	2.2	2
226	Binding Behavior of Carbonmonoxide to Gold Atoms on Ag(001). Topics in Catalysis, 2020, 63, 1578-1584.	1.3	1
227	Tertiary Chiral Nanostructures from Câˆ’Hâ‹…â‹…â‹…F Directed Assembly of Chiroptical Superatoms. Angewandte Chemie, 2021, 133, 22585-22590.	1.6	1
228	Au102(p-MBA)44 nanocluster, a superatom suitable for bio-applications. , 2016, , .		0
229	Preface to the Special Issue â€œISSPIC XVIII: International Symposium on Small Particles and Inorganic Clusters 2016â€• Journal of Physical Chemistry C, 2017, 121, 10629-10631.	1.5	0
230	Analysis of the plasmonic excitations in assemblies of three-dimensional electron clusters. Physical Review B, 2020, 102, .	1.1	0