Hannu HÃ¤kkinen

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/6491009/publications.pdf

Version: 2024-02-01

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	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
2	Selective Acrolein Hydrogenation over Ligand-Protected Gold Clusters: A Venus Flytrap Mechanism. ACS Catalysis, 2022, 12, 2365-2374.	5.5	6
3	Isomer dynamics of the [Au₆(NHC-S)₄]²⁺ nanocluster. Chemical Communications, 2022, 58, 3218-3221.	2.2	2
4	NHC-Stabilized Au₁₀ Nanoclusters and Their Conversion to Au₂₅ Nanoclusters. Jacs Au, 2022, 2, 875-885.	3.6	22
5	Regioselective hydrogenation of alkenes over atomically dispersed Pd sites on NHC-stabilized bimetallic nanoclusters. CheM, 2022, 8, 2380-2392.	5.8	19
6	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
7	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
8	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
9	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
10	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
11	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
12	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
13	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
14	Atomically Precise Gold Nanoclusters: Towards an Optimal Biocompatible System from a Theoreticalâ€“Experimental Strategy. Small, 2021, 17, e2005499.	5.2	28
15	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
16	Ag 44 (EBT) 26 (TPP) 4 Nanoclusters With Tailored Molecular and Electronic Structure. Angewandte Chemie, 2021, 133, 9120-9126.	1.6	6
17	Copper-hydride nanoclusters with enhanced stability by N-heterocyclic carbenes. Nano Research, 2021, 14, 3303-3308.	5.8	33
18	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

#	Article	IF	Citations
19	Ag₄₄(EBT)₂₆(TPP)₄ Nanoclusters With Tailored Molecular and Electronic Structure. Angewandte Chemie - International Edition, 2021, 60, 9038-9044.	7.2	33
20	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
21	Magnetically induced currents and aromaticity in ligand-stabilized Au and AuPt superatoms. Nature Communications, 2021, 12, 2477.	5.8	6
22	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
23	Prospects and challenges for computer simulations of monolayer-protected metal clusters. Nature Communications, 2021, 12, 2197.	5.8	20
24	Cubic aromaticity in ligand-stabilized doped Au superatoms. Journal of Chemical Physics, 2021, 154, 204303.	1.2	6
25	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
26	[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
27	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
28	Reversible isomerization of metal nanoclusters induced by intermolecular interaction. CheM, 2021, 7, 2227-2244.	5.8	38
29	Tertiary Chiral Nanostructures from Câ^'Hâ‹…â‹…â‹…F Directed Assembly of Chiroptical Superatoms. Angewandte Chemie, 2021, 133, 22585-22590.	1.6	1
30	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
31	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
32	[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
33	Analysis of the plasmonic excitations in assemblies of three-dimensional electron clusters. Physical Review B, 2020, 102, .	1.1	0
34	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
35	Solvent-mediated assembly of atom-precise goldâ€"silver nanoclusters to semiconducting one-dimensional materials. Nature Communications, 2020, 11, 2229.	5.8	91
36	Binding Behavior of Carbonmonoxide to Gold Atoms on Ag(001). Topics in Catalysis, 2020, 63, 1578-1584.	1.3	1

#	Article	IF	Citations
37	A topological isomer of the Au₂₅(SR)₁₈^{âˆ’}nanocluster. Chemical Communications, 2020, 56, 8087-8090.	2.2	30
38	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
39	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
40	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
41	Solubilityâ€Driven Isolation of a Metastable Nonagold Cluster with Bodyâ€Centered Cubic Structure. Chemistry - A European Journal, 2020, 26, 8465-8470.	1.7	17
42	Charge Transfer Plasmons in Dimeric Electron Clusters. Journal of Physical Chemistry C, 2020, 124, 12645-12654.	1.5	10
43	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
44	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
45	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
46	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
47	Highly Robust but Surfaceâ€Active: An Nâ€Heterocyclic Carbeneâ€Stabilized Au₂₅ Nanocluster. Angewandte Chemie - International Edition, 2019, 58, 17731-17735.	7.2	125
48	Highly Robust but Surfaceâ€Active: An Nâ€Heterocyclic Carbeneâ€Stabilized Au₂₅ Nanocluster. Angewandte Chemie, 2019, 131, 17895-17899.	1.6	39
49	A method for structure prediction of metal-ligand interfaces of hybrid nanoparticles. Nature Communications, 2019, 10, 3973.	5.8	37
50	Robust, Highly Luminescent Au₁₃ Superatoms Protected by N-Heterocyclic Carbenes. Journal of the American Chemical Society, 2019, 141, 14997-15002.	6.6	185
51	Ab initio molecular dynamics studies of Au38(SR)24 isomers under heating. European Physical Journal D, 2019, 73, 1.	0.6	8
52	Cd₁₂Ag₃₂(SePh)₃₆: Non-Noble Metal Doped Silver Nanoclusters. Journal of the American Chemical Society, 2019, 141, 8422-8425.	6.6	71
53	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
54	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

#	Article	IF	Citations
55	N-heterocyclic carbene-functionalized magic-number gold nanoclusters. Nature Chemistry, 2019, 11, 419-425.	6.6	333
56	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
57	Towards Controlled Synthesis of Water-Soluble Gold Nanoclusters: Synthesis and Analysis. Journal of Physical Chemistry C, 2019, 123, 2602-2612.	1.5	34
58	Connections Between Theory and Experiment for Gold and Silver Nanoclusters. Annual Review of Physical Chemistry, 2018, 69, 205-229.	4.8	80
59	Atomically Precise Nanocluster Assemblies Encapsulating Plasmonic Gold Nanorods. Angewandte Chemie, 2018, 130, 6632-6636.	1.6	10
60	Atomically Precise Nanocluster Assemblies Encapsulating Plasmonic Gold Nanorods. Angewandte Chemie - International Edition, 2018, 57, 6522-6526.	7.2	57
61	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
62	Ligand mediated evolution of size dependent magnetism in cobalt nanoclusters. Physical Chemistry Chemical Physics, 2018, 20, 4563-4570.	1.3	7
63	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
64	From Symmetry Breaking to Unraveling the Origin of the Chirality of Ligated Au₁₃Cu₂ Nanoclusters. Angewandte Chemie, 2018, 130, 3479-3483.	1.6	23
65	Thiol-stabilized atomically precise, superatomic silver nanoparticles for catalysing cycloisomerization of alkynyl amines. National Science Review, 2018, 5, 694-702.	4.6	63
66	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
67	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
68	Real-space imaging with pattern recognition of a ligand-protected Ag374 nanocluster at sub-molecular resolution. Nature Communications, 2018, 9, 2948.	5.8	26
69	Co-crystallization of atomically precise metal nanoparticles driven by magic atomic and electronic shells. Nature Communications, 2018, 9, 3357.	5.8	95
70	Stability, electronic structure, and optical properties of protected gold-doped silver Ag_{29âˆ’x}Au_x (x = 0â€“5) nanoclusters. Physical Chemistry Chemical Physics, 2017, 19, 13868-13874.	1.3	38
71	Reversible Supracolloidal Selfâ€Assembly of Cobalt Nanoparticles to Hollow Capsids and Their Superstructures. Angewandte Chemie - International Edition, 2017, 56, 6473-6477.	7.2	34
72	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

#	Article	IF	Citations
73	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
74	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
75	Exploring Strategies for Labeling Viruses with Gold Nanoclusters through Non-equilibrium Molecular Dynamics Simulations. Bioconjugate Chemistry, 2017, 28, 2327-2339.	1.8	9
76	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
77	Structural characterization of site-modified nanocapsid with monodispersed gold clusters. Scientific Reports, 2017, 7, 17048.	1.6	13
78	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
79	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
80	Exploring the atomic structure of 1.8 nm monolayer-protected gold clusters with aberration-corrected STEM. Ultramicroscopy, 2017, 176, 146-150.	0.8	8
81	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
82	Patterning of supported gold monolayers via chemical lift-off lithography. Beilstein Journal of Nanotechnology, 2017, 8, 2648-2661.	1.5	16
83	Reversible Supracolloidal Selfâ€Assembly of Cobalt Nanoparticles to Hollow Capsids and Their Superstructures. Angewandte Chemie, 2017, 129, 6573-6577.	1.6	18
84	Au102(p-MBA)44 nanocluster, a superatom suitable for bio-applications. , 2016, , .		0
85	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
86	Surface Chemistry Controls Magnetism in Cobalt Nanoclusters. Journal of Physical Chemistry C, 2016, 120, 20822-20827.	1.5	10
87	Symmetry breaking in ligand-protected gold clusters probed by nonlinear optics. Nanoscale, 2016, 8, 12123-12127.	2.8	31
88	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
89	Jahnâ€“Teller effects in Au₂₅(SR)₁₈. Chemical Science, 2016, 7, 1882-1890.	3.7	149
90	Gold/Isophorone Interaction Driven by Keto/Enol Tautomerization. Journal of Physical Chemistry C, 2016, 120, 21962-21966.	1.5	5

#	Article	IF	Citations
91	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
92	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
93	Covalently linked multimers of gold nanoclusters Au₁₀₂(p-MBA)₄₄and Au_{â^¼250}(p-MBA)_n. Nanoscale, 2016, 8, 18665-18674.	2.8	59
94	[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
95	Electronic shell structures in bare and protected metal nanoclusters. Advances in Physics: X, 2016, 1, 467-491.	1.5	36
96	Plasmonic twinned silver nanoparticles with molecular precision. Nature Communications, 2016, 7, 12809.	5.8	235
97	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
98	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
99	Conformation and dynamics of the ligand shell of a water-soluble Au102 nanoparticle. Nature Communications, 2016, 7, 10401.	5.8	91
100	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
101	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
102	Gold assisted oxygen dissociation on a molybdenum-doped CaO(001) surface. Catalysis Science and Technology, 2016, 6, 6784-6793.	2.1	3
103	How many gold atoms make gold metal?. Europhysics News, 2015, 46, 23-26.	0.1	7
104	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
105	Electronic Structure. Frontiers of Nanoscience, 2015, 9, 189-222.	0.3	12
106	Theoretical Analysis of the M₁₂Ag₃₂(SR)₄₀^{4â€“} and X@M₁₂Ag₃₂(SR)₃₀^{4â€“} Nanoclusters (M = Au, Ag; X = H,) Tj ETQq0 0 0 rgBT /Ove	1.5	19
107	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
108	Silver Sulfide Nanoclusters and the Superatom Model. Journal of Physical Chemistry C, 2015, 119, 1583-1590.	1.5	10

#	Article	IF	Citations
109	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
110	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
111	Impacts of Copper Position on the Electronic Structure of [Au_{25-x}Cu_{<i>x</i>}(SH)₁₈]^{âˆ’} Nanoclusters. Journal of Physical Chemistry C, 2015, 119, 8290-8298.	1.5	27
112	Molecule-like Photodynamics of Au₁₀₂(<i>p</i>MBA)₄₄ Nanocluster. ACS Nano, 2015, 9, 2328-2335.	7.3	66
113	An Intermetallic Au₂₄Ag₂₀ Superatom Nanocluster Stabilized by Labile Ligands. Journal of the American Chemical Society, 2015, 137, 4324-4327.	6.6	175
114	Pd₂Au₃₆(SR)₂₄cluster: structure studies. Nanoscale, 2015, 7, 17012-17019.	2.8	46
115	Dynamic Diglyme-Mediated Self-Assembly of Gold Nanoclusters. ACS Nano, 2015, 9, 11690-11698.	7.3	33
116	Hydrophobic pocket targeting probes for enteroviruses. Nanoscale, 2015, 7, 17457-17467.	2.8	35
117	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
118	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
119	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
120	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
121	Supramolecular Functionalization and Concomitant Enhancement in Properties of Au₂₅ Clusters. ACS Nano, 2014, 8, 139-152.	7.3	94
122	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
123	Mixed-Monolayer-Protected Au₂₅ Clusters with Bulky Calix[4]arene Functionalities. Journal of Physical Chemistry Letters, 2014, 5, 585-589.	2.1	34
124	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
125	Optical and electronic properties of graphene nanoribbons upon adsorption of ligand-protected aluminum clusters. Physical Chemistry Chemical Physics, 2014, 16, 3558.	1.3	22
126	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
127	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
128	Structural Evolution of Atomically Precise Thiolated Bimetallic [Au_{12+<i>n</i>}Cu₃₂(SR)_{30+<i>n</i>}]^{4â€“} (<i>n</i> = 0,) Tj ET Q q 0 0 0 rg BT /Over	6.6	145
129	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
130	Electron microscopy of gold nanoparticles at atomic resolution. Science, 2014, 345, 909-912.	6.0	269
131	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
132	Chiral Phase Transfer and Enantioenrichment of Thiolate-Protected Au₁₀₂ Clusters. Journal of the American Chemical Society, 2014, 136, 4129-4132.	6.6	125
133	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
134	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
135	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
136	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
137	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
138	Protected but Accessible: Oxygen Activation by a Calixarene-Stabilized Undecagold Cluster. Journal of the American Chemical Society, 2013, 135, 12944-12947.	6.6	32
139	All-thiol-stabilized Ag44 and Au12Ag32 nanoparticles with single-crystal structures. Nature Communications, 2013, 4, 2422.	5.8	675
140	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
141	Birth of the Localized Surface Plasmon Resonance in Monolayer-Protected Gold Nanoclusters. ACS Nano, 2013, 7, 10263-10270.	7.3	240
142	Ag₄₄(SeR)₃₀: A Hollow Cage Silver Cluster with Selenolate Protection. Journal of Physical Chemistry Letters, 2013, 4, 3351-3355.	2.1	78
143	Modeling thiolate-protected gold clusters with density-functional tight-binding. European Physical Journal D, 2013, 67, 1.	0.6	26
144	The Redox Chemistry of Gold with Highâ€Valence Doped Calcium Oxide. Angewandte Chemie - International Edition, 2013, 52, 1424-1427.	7.2	33

#	Article	IF	Citations
145	Nondestructive Size Determination of Thiol-Stabilized Gold Nanoclusters in Solution by Diffusion Ordered NMR Spectroscopy. Analytical Chemistry, 2013, 85, 3489-3492.	3.2	57
146	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
147	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
148	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
149	Electron quantization in arbitrarily shaped gold islands on MgO thin films. Physical Review B, 2013, 88, .	1.1	26
150	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
151	One-pot synthesis and characterization of subnanometre-size benzotriazolate protected copper clusters. Nanoscale, 2012, 4, 4095.	2.8	35
152	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
153	Solvent driven formation of silver embedded resorcinarene nanorods. CrystEngComm, 2012, 14, 347-350.	1.3	13
154	The electronic structure of Ge9[Si(SiMe3)3]3â^': a superantiatom complex. Physical Chemistry Chemical Physics, 2012, 14, 9311.	1.3	20
155	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
156	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
157	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 ET Q q1 1 0.78431	1.5	10
158	The goldâ€“sulfur interface at the nanoscale. Nature Chemistry, 2012, 4, 443-455.	6.6	1,418
159	Theoretical Studies of Gold Nanoclusters in Various Chemical Environments: When the Size Matters. , 2012, , 233-272.		6
160	Ligand-Protected Gold Nanoclusters as Superatomsâ€"Insights from Theory and Computations. Frontiers of Nanoscience, 2012, 3, 129-157.	0.3	7
161	Divide and Protect: Passivating Cu(111) by Cu-(benzotriazole)₂. Journal of Physical Chemistry C, 2012, 116, 22346-22349.	1.5	30
162	Atomistic Simulations of Functional Au₁₄₄(SR)₆₀ Gold Nanoparticles in Aqueous Environment. Journal of Physical Chemistry C, 2012, 116, 9805-9815.	1.5	94

#	Article	IF	Citations
163	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
164	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
165	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
166	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
167	The Al50Cp*12 Cluster - A 138-Electron Closed Shell (L = 6) Superatom. European Journal of Inorganic Chemistry, 2011, 2011, 2649-2652.	1.0	41
168	Evidence of superatom electronic shells in ligand-stabilized aluminum clusters. Journal of Chemical Physics, 2011, 135, 094701.	1.2	42
169	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
170	Quantum size effects in ambient CO oxidation catalysed by ligand-protected gold clusters. Nature Chemistry, 2010, 2, 329-334.	6.6	295
171	Structural, chemical, and dynamical trends in graphene grain boundaries. Physical Review B, 2010, 81, .	1.1	184
172	Theoretical Characterization of Cyclic Thiolated Copper, Silver, and Gold Clusters. Journal of Physical Chemistry C, 2010, 114, 13571-13576.	1.5	51
173	Thiolate-Protected Au₂₅ Superatoms as Building Blocks: Dimers and Crystals. Journal of Physical Chemistry C, 2010, 114, 15986-15994.	1.5	109
174	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
175	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
176	Chirality and Electronic Structure of the Thiolate-Protected Au₃₈ Nanocluster. Journal of the American Chemical Society, 2010, 132, 8210-8218.	6.6	401
177	Protected Metallic Clusters, Quantum Wells and Metal-Nanocrystal Molecules. Journal of Physical Chemistry C, 2010, 114, 15877-15878.	1.5	6
178	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
179	Adsorption and activation of O2 at Au chains on MgO/Mo thin films. Physical Chemistry Chemical Physics, 2010, 12, 1483.	1.3	29
180	Characterization of Ironâˆ'Carbonyl-Protected Gold Clusters. Journal of the American Chemical Society, 2009, 131, 12573-12575.	6.6	17

#	Article	IF	Citations
181	First-principles simulations of hydrogen peroxide formation catalyzed by small neutral gold clusters. Physical Chemistry Chemical Physics, 2009, 11, 6359.	1.3	30
182	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
183	Evidence for graphene edges beyond zigzag and armchair. Physical Review B, 2009, 80, .	1.1	274
184	Gold in graphene: In-plane adsorption and diffusion. Applied Physics Letters, 2009, 94, .	1.5	93
185	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
186	Atomic and electronic structure of gold clusters: understanding flakes, cages and superatoms from simple concepts. Chemical Society Reviews, 2008, 37, 1847.	18.7	639
187	Goldâˆ’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
188	On the Structure of Thiolate-Protected Au₂₅. Journal of the American Chemical Society, 2008, 130, 3756-3757.	6.6	682
189	Self-Passivating Edge Reconstructions of Graphene. Physical Review Letters, 2008, 101, 115502.	2.9	674
190	Time-dependent density-functional theory in the projector augmented-wave method. Journal of Chemical Physics, 2008, 128, 244101.	1.2	187
191	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
192	Raman spectra of single-walled carbon nanotubes with vacancies. Physical Review B, 2008, 77, .	1.1	26
193	Photoelectron spectra from first principles: from the many-body to the single-particle picture. New Journal of Physics, 2008, 10, 043018.	1.2	29
194	Effect of bending on Raman-active vibration modes of carbon nanotubes. Physical Review B, 2008, 78, .	1.1	21
195	Charging of atoms, clusters, and molecules on metal-supported oxides: A general and long-ranged phenomenon. Physical Review B, 2008, 78, .	1.1	74
196	Trapping of 27 bpâ€“8 kbp DNA and immobilization of thiol-modified DNA using dielectrophoresis. Nanotechnology, 2007, 18, 295204.	1.3	68
197	Liquid-Liquid Phase Coexistence in Gold Clusters: 2D or Not 2D?. Physical Review Letters, 2007, 98, 015701.	2.9	62
198	Electronic Structure of MgO-Supported Au Clusters: Quantum Dots Probed by Scanning Tunneling Microscopy. Physical Review Letters, 2007, 99, 096102.	2.9	49

#	Article	IF	Citations
199	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
200	Polymerization at the Alkylthiolateâ^'Au(111) Interface. Journal of Physical Chemistry B, 2007, 111, 3325-3327.	1.2	73
201	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
202	Size-Dependent Structural Evolution and Chemical Reactivity of Gold Clusters. ChemPhysChem, 2007, 8, 157-161.	1.0	197
203	Adsorption of gold clusters on metal-supported MgO: Correlation to electron affinity of gold. Physical Review B, 2007, 76, .	1.1	53
204	Density functional study of gold atoms and clusters on a graphite (0001) surface with defects. Physical Review B, 2006, 74, .	1.1	41
205	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
206	Divide and Protect:Â Capping Gold Nanoclusters with Molecular Goldâ^'Thiolate Rings. Journal of Physical Chemistry B, 2006, 110, 9927-9931.	1.2	405
207	Theoretical Characterization of Cyclic Thiolated Gold Clusters. Journal of the American Chemical Society, 2006, 128, 10268-10275.	6.6	118
208	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
209	55-Atom clusters of silver and gold: Symmetry breaking by relativistic effects. Computational Materials Science, 2006, 35, 332-336.	1.4	27
210	Oxidation of small gas phase Pd clusters: A density functional study. Computational Materials Science, 2006, 35, 371-374.	1.4	26
211	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
212	Anomalous binding sequence of CO ligands to an anionic triplatinum carbonyl complex. Chemical Physics Letters, 2005, 406, 44-48.	1.2	4
213	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
214	Charging Effects on Bonding and Catalyzed Oxidation of CO on Au8 Clusters on MgO. Science, 2005, 307, 403-407.	6.0	1,358
215	A small spherical liquid: A DFT molecular dynamics study of WAu12. Physical Chemistry Chemical Physics, 2005, 7, 2208.	1.3	19
216	Electronic structure and thermal behavior of a magicNa59+cluster. Physical Review A, 2004, 70, .	1.0	20

#	Article	IF	Citations
217	Symmetry and Electronic Structure of Noble-Metal Nanoparticles and the Role of Relativity. Physical Review Letters, 2004, 93, 093401.	2.9	241
218	Hydrogen Welding and Hydrogen Switches in a Monatomic Gold Nanowire. Nano Letters, 2004, 4, 1845-1852.	4.5	66
219	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
220	Structural, Electronic, and Impurity-Doping Effects in Nanoscale Chemistry: Supported Gold Nanoclusters. Angewandte Chemie - International Edition, 2003, 42, 1297-1300.	7.2	547
221	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
222	Catalytic CO Oxidation by Free Au2-:Â Experiment and Theory. Journal of the American Chemical Society, 2003, 125, 10437-10445.	6.6	386
223	Interaction of O2 with Gold Clusters:â€‰ Molecular and Dissociative Adsorption. Journal of Physical Chemistry A, 2003, 107, 4066-4071.	1.1	349
224	Bonding in Cu, Ag, and Au Clusters: Relativistic Effects, Trends, and Surprises. Physical Review Letters, 2002, 89, 033401.	2.9	611
225	Gas-Phase Catalytic Oxidation of CO by Au2-. Journal of the American Chemical Society, 2001, 123, 9704-9705.	6.6	230
226	Aluminum cluster anions: Photoelectron spectroscopy andab initiosimulations. Physical Review B, 2000, 62, 13216-13228.	1.1	111
227	Gold clusters(AuN,2<~N<~10)and their anions. Physical Review B, 2000, 62, R2287-R2290.	1.1	454
228	Nanowire Gold Chains:Â Formation Mechanisms and Conductance. Journal of Physical Chemistry B, 2000, 104, 9063-9066.	1.2	106
229	Photoelectron spectra of aluminum cluster anions: Temperature effects andab initiosimulations. Physical Review B, 1999, 60, R11297-R11300.	1.1	289
230	Gold Nanowires and Their Chemical Modifications. Journal of Physical Chemistry B, 1999, 103, 8814-8816.	1.2	135