Hannu Hkkinen

List of Publications by Citations

226 papers	20,511 citations	68 h-index	140 g-index
240 ext. papers	22,411 ext. citations	8.6 avg, IF	7.25 L-index

#	Paper	IF	Citations
226	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, 9157-62	11.5	1264
225	Charging effects on bonding and catalyzed oxidation of CO on Au8 clusters on MgO. *Science*, **2005**, 307, 403-7	33.3	1262
224	The gold-sulfur interface at the nanoscale. *Nature Chemistry*, **2012**, 4, 443-55	17.6	1216
223	On the structure of thiolate-protected Au25. *Journal of the American Chemical Society*, **2008**, 130, 3756-7	16.4	639
222	All-thiol-stabilized Ag44 and Au12Ag32 nanoparticles with single-crystal structures. *Nature Communications*, **2013**, 4, 2422	17.4	584
221	Self-passivating edge reconstructions of graphene. *Physical Review Letters*, **2008**, 101, 115502	7.4	583
220	Bonding in Cu, Ag, and Au clusters: relativistic effects, trends, and surprises. *Physical Review Letters*, **2002**, 89, 033401	7.4	580
219	On the Electronic and Atomic Structures of Small AuN- (N = 4−14) Clusters: A Photoelectron Spectroscopy and Density-Functional Study. *Journal of Physical Chemistry A*, **2003**, 107, 6168-6175	2.8	572
218	Atomic and electronic structure of gold clusters: understanding flakes, cages and superatoms from simple concepts. *Chemical Society Reviews*, **2008**, 37, 1847-59	58.5	556
217	Structural, electronic, and impurity-doping effects in nanoscale chemistry: supported gold nanoclusters. *Angewandte Chemie - International Edition*, **2003**, 42, 1297-300	16.4	502
216	Gold clusters (AuN, 2. *Physical Review B*, **2000**, 62, R2287-R2290	3.3	430
215	Divide and protect: capping gold nanoclusters with molecular gold-thiolate rings. *Journal of Physical Chemistry B*, **2006**, 110, 9927-31	3.4	370
214	Chirality and electronic structure of the thiolate-protected Au38 nanocluster. *Journal of the American Chemical Society*, **2010**, 132, 8210-8	16.4	367
213	Catalytic CO oxidation by free Au2-: experiment and theory. *Journal of the American Chemical Society*, **2003**, 125, 10437-45	16.4	367
212	Structure and Bonding in the Ubiquitous Icosahedral Metallic Gold Cluster Au144(SR)60. *Journal of Physical Chemistry C*, **2009**, 113, 5035-5038	3.8	363
211	Interaction of O2 with Gold Clusters: Molecular and Dissociative Adsorption. *Journal of Physical Chemistry A*, **2003**, 107, 4066-4071	2.8	330
210	A critical size for emergence of nonbulk electronic and geometric structures in dodecanethiolate-protected Au clusters. *Journal of the American Chemical Society*, **2015**, 137, 1206-12	16.4	271

209	Quantum size effects in ambient CO oxidation catalysed by ligand-protected gold clusters. *Nature Chemistry*, **2010**, 2, 329-34	17.6	266
208	Evidence for graphene edges beyond zigzag and armchair. *Physical Review B*, **2009**, 80,	3.3	250
207	Photoelectron spectra of aluminum cluster anions: Temperature effects and ab initio simulations. *Physical Review B*, **1999**, 60, R11297-R11300	3.3	247
206	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, 3278-81	16.4	246
205	Single crystal XRD structure and theoretical analysis of the chiral Au30S(S-t-Bu)18 cluster. *Journal of the American Chemical Society*, **2014**, 136, 5000-5	16.4	241
204	Nanoparticle imaging. Electron microscopy of gold nanoparticles at atomic resolution. *Science*, **2014**, 345, 909-12	33.3	234
203	Symmetry and electronic structure of noble-metal nanoparticles and the role of relativity. *Physical Review Letters*, **2004**, 93, 093401	7.4	225
202	Gas-phase catalytic oxidation of CO by Au(2-). *Journal of the American Chemical Society*, **2001**, 123, 9704-5	16.4	221
201	Birth of the localized surface plasmon resonance in monolayer-protected gold nanoclusters. *ACS Nano*, **2013**, 7, 10263-70	16.7	202
200	Plasmonic twinned silver nanoparticles with molecular precision. *Nature Communications*, **2016**, 7, 12809	17.4	191
199	Size-dependent structural evolution and chemical reactivity of gold clusters. *ChemPhysChem*, **2007**, 8, 157-61	3.2	187
198	Total Structure and Electronic Structure Analysis of Doped Thiolated Silver [MAg24(SR)18](2-) (M = Pd, Pt) Clusters. *Journal of the American Chemical Society*, **2015**, 137, 11880-3	16.4	186
197	N-heterocyclic carbene-functionalized magic-number gold nanoclusters. *Nature Chemistry*, **2019**, 11, 419-425	17.6	185
196	Structural, chemical, and dynamical trends in graphene grain boundaries. *Physical Review B*, **2010**, 81,	3.3	167
195	Structural and theoretical basis for ligand exchange on thiolate monolayer protected gold nanoclusters. *Journal of the American Chemical Society*, **2012**, 134, 13316-22	16.4	163
194	Time-dependent density-functional theory in the projector augmented-wave method. *Journal of Chemical Physics*, **2008**, 128, 244101	3.9	158
193	Asymmetric Synthesis of Chiral Bimetallic [AgCu(SR)] Nanoclusters via Ion Pairing. *Journal of the American Chemical Society*, **2016**, 138, 12751-12754	16.4	154
192	An intermetallic Au24Ag20 superatom nanocluster stabilized by labile ligands. *Journal of the American Chemical Society*, **2015**, 137, 4324-7	16.4	148

191	[Ag(SPhMe)(PPh)]: Synthesis, Total Structure, and Optical Properties of a Large Box-Shaped Silver Nanocluster. *Journal of the American Chemical Society*, **2016**, 138, 14727-14732	16.4	138
190	Ligand-stabilized Au13Cu(x) (x = 2, 4, 8) bimetallic nanoclusters: ligand engineering to control the exposure of metal sites. *Journal of the American Chemical Society*, **2013**, 135, 9568-71	16.4	136
189	Structural evolution of atomically precise thiolated bimetallic [Au(12+n)Cu(SR)(30+n)]2 (n = 0, 2, 4, 6) nanoclusters. *Journal of the American Chemical Society*, **2014**, 136, 7197-200	16.4	128
188	Gold Nanowires and Their Chemical Modifications. *Journal of Physical Chemistry B*, **1999**, 103, 8814-8816	3.4	126
187	Gold thiolate Complexes Form a Unique c(4 2) Structure on Au(111). *Journal of Physical Chemistry C*, **2008**, 112, 15940-15942	3.8	122
186	Jahn-Teller effects in Au(SR). *Chemical Science*, **2016**, 7, 1882-1890	9.4	115
185	Theoretical characterization of cyclic thiolated gold clusters. *Journal of the American Chemical Society*, **2006**, 128, 10268-75	16.4	106
184	Aluminum cluster anions: Photoelectron spectroscopy and ab initio simulations. *Physical Review B*, **2000**, 62, 13216-13228	3.3	105
183	Effects of Silver Doping on the Geometric and Electronic Structure and Optical Absorption Spectra of the Au25 Agn(SH)18 (n = 1, 2, 4, 6, 8, 10, 12) Bimetallic Nanoclusters. *Journal of Physical Chemistry C*, **2012**, 116, 20617-20624	3.8	104
182	Nanowire Gold Chains: Formation Mechanisms and Conductance. *Journal of Physical Chemistry B*, **2000**, 104, 9063-9066	3.4	102
181	Chiral phase transfer and enantioenrichment of thiolate-protected Au clusters. *Journal of the American Chemical Society*, **2014**, 136, 4129-32	16.4	99
180	Thiolate-Protected Au25 Superatoms as Building Blocks: Dimers and Crystals *Journal of Physical Chemistry C*, **2010**, 114, 15986-15994	3.8	99
179	Au40(SR)24 cluster as a chiral dimer of 8-electron superatoms: structure and optical properties. *Journal of the American Chemical Society*, **2012**, 134, 19560-3	16.4	98
178	Bulky Surface Ligands Promote Surface Reactivities of [AgX(S-Adm)] (X = Cl, Br, I) Nanoclusters: Models for Multiple-Twinned Nanoparticles. *Journal of the American Chemical Society*, **2017**, 139, 13288-13291	16.4	97
177	Robust, Highly Luminescent Au Superatoms Protected by N-Heterocyclic Carbenes. *Journal of the American Chemical Society*, **2019**, 141, 14997-15002	16.4	95
176	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, 5407-11	3.6	94
175	A density functional investigation of thiolate-protected bimetal PdAu(24)(SR)(18)(z) clusters: doping the superatom complex. *Physical Chemistry Chemical Physics*, **2009**, 11, 7123-9	3.6	92
174	Gold in graphene: In-plane adsorption and diffusion. *Applied Physics Letters*, **2009**, 94, 043106	3.4	88

173	Supramolecular functionalization and concomitant enhancement in properties of Au(25) clusters. *ACS Nano*, **2014**, 8, 139-52	16.7	81
172	Atomistic Simulations of Functional Au144(SR)60 Gold Nanoparticles in Aqueous Environment. *Journal of Physical Chemistry C*, **2012**, 116, 9805-9815	3.8	80
171	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, 1277-81	11.5	79
170	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	16.4	78
169	Conformation and dynamics of the ligand shell of a water-soluble Au102 nanoparticle. *Nature Communications*, **2016**, 7, 10401	17.4	77
168	Atomically Precise, Thiolated Copper-Hydride Nanoclusters as Single-Site Hydrogenation Catalysts for Ketones in Mild Conditions. *ACS Nano*, **2019**, 13, 5975-5986	16.7	75
167	Highly Robust but Surface-Active: An N-Heterocyclic Carbene-Stabilized Au Nanocluster. *Angewandte Chemie - International Edition*, **2019**, 58, 17731-17735	16.4	75
166	Electronic and vibrational signatures of the Au102(p-MBA)44 cluster. *Journal of the American Chemical Society*, **2011**, 133, 3752-5	16.4	74
165	Charging of atoms, clusters, and molecules on metal-supported oxides: A general and long-ranged phenomenon. *Physical Review B*, **2008**, 78,	3.3	72
164	Au Adsorption on Regular and Defected Thin MgO(100) Films Supported by Mo. *Journal of Physical Chemistry C*, **2007**, 111, 4319-4327	3.8	72
163	Carbon dioxide activation and reaction induced by electron transfer at an oxide-metal interface. *Angewandte Chemie - International Edition*, **2015**, 54, 12484-7	16.4	71
162	Polymerization at the alkylthiolate-Au(111) interface. *Journal of Physical Chemistry B*, **2007**, 111, 3325-7	3.4	71
161	Electronic Structure and Bonding of Icosahedral Core□Shell Gold□Silver Nanoalloy Clusters Au144□Agx(SR)60. *Journal of Physical Chemistry Letters*, **2011**, 2, 2316-2321	6.4	70
160	Co-crystallization of atomically precise metal nanoparticles driven by magic atomic and electronic shells. *Nature Communications*, **2018**, 9, 3357	17.4	69
159	Ag44(SeR)30: A Hollow Cage Silver Cluster with Selenolate Protection. *Journal of Physical Chemistry Letters*, **2013**, 4, 3351-5	6.4	68
158	From Symmetry Breaking to Unraveling the Origin of the Chirality of Ligated Au Cu Nanoclusters. *Angewandte Chemie - International Edition*, **2018**, 57, 3421-3425	16.4	66
157	Trapping of 27 bp□8 kbp DNA and immobilization of thiol-modified DNA using dielectrophoresis. *Nanotechnology*, **2007**, 18, 295204	3.4	66
156	Template-Free Supracolloidal Self-Assembly of Atomically Precise Gold Nanoclusters: From 2D Colloidal Crystals to Spherical Capsids. *Angewandte Chemie - International Edition*, **2016**, 55, 16035-16038	16.4	64

155	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,	3.3	64
154	Hydrogen Welding and Hydrogen Switches in a Monatomic Gold Nanowire. *Nano Letters*, **2004**, 4, 1845-1853	13.3	64
153	Molecule-like photodynamics of Au102(pMBA)44 nanocluster. *ACS Nano*, **2015**, 9, 2328-35	16.7	61
152	Connections Between Theory and Experiment for Gold and Silver Nanoclusters. *Annual Review of Physical Chemistry*, **2018**, 69, 205-229	15.7	60
151	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	3.8	60
150	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	3.8	59
149	Liquid-liquid phase coexistence in gold clusters: 2D or not 2D?. *Physical Review Letters*, **2007**, 98, 015701	7.4	58
148	Electronic structure and optical properties of the thiolate-protected Au28(SMe)20 cluster. *Journal of Physical Chemistry A*, **2013**, 117, 10526-33	2.8	53
147	Adsorption of gold clusters on metal-supported MgO: Correlation to electron affinity of gold. *Physical Review B*, **2007**, 76,	3.3	52
146	Oxidation of magnesia-supported Pd-clusters leads to the ultimate limit of epitaxy with a catalytic function. *Nature Materials*, **2006**, 5, 44-7	27	52
145	Nondestructive size determination of thiol-stabilized gold nanoclusters in solution by diffusion ordered NMR spectroscopy. *Analytical Chemistry*, **2013**, 85, 3489-92	7.8	50
144	Chiral Inversion of Thiolate-Protected Gold Nanoclusters via Core Reconstruction without Breaking a Au-S Bond. *Journal of the American Chemical Society*, **2019**, 141, 6006-6012	16.4	49
143	Covalently linked multimers of gold nanoclusters Au(p-MBA) and Au(p-MBA). *Nanoscale*, **2016**, 8, 18665-18674	7.8	48
142	CdAg(SePh): Non-Noble Metal Doped Silver Nanoclusters. *Journal of the American Chemical Society*, **2019**, 141, 8422-8425	16.4	47
141	Solvent-mediated assembly of atom-precise gold-silver nanoclusters to semiconducting one-dimensional materials. *Nature Communications*, **2020**, 11, 2229	17.4	47
140	Site Preference in Multimetallic Nanoclusters: Incorporation of Alkali Metal Ions or Copper Atoms into the Alkynyl-Protected Body-Centered Cubic Cluster [Au Ag (C?C Bu)]. *Angewandte Chemie - International Edition*, **2016**, 55, 15152-15156	16.4	47
139	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	3.8	46
138	Theoretical Characterization of Cyclic Thiolated Copper, Silver, and Gold Clusters. *Journal of Physical Chemistry C*, **2010**, 114, 13571-13576	3.8	46

137	Electronic structure of MgO-supported Au clusters: quantum dots probed by scanning tunneling microscopy. *Physical Review Letters*, **2007**, 99, 096102	7.4	46
136	A Unified AMBER-Compatible Molecular Mechanics Force Field for Thiolate-Protected Gold Nanoclusters. *Journal of Chemical Theory and Computation*, **2016**, 12, 1342-50	6.4	45
135	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, 3076-80	6.4	45
134	Einfluss der geometrischen und elektronischen Struktur sowie der elementaren Zusammensetzung von Clustern auf chemische Prozesse in der Nanometerskala. *Angewandte Chemie*, **2003**, 115, 1335-1338	3.6	45
133	Thiol-stabilized atomically precise, superatomic silver nanoparticles for catalysing cycloisomerization of alkynyl amines. *National Science Review*, **2018**, 5, 694-702	10.8	42
132	Combinatorial Identification of Hydrides in a Ligated Ag Nanocluster with Noncompact Metal Core. *Journal of the American Chemical Society*, **2019**, 141, 11905-11911	16.4	41
131	A 58-electron superatom-complex model for the magic phosphine-protected gold clusters (Schmid-gold, Nanogold) of 1.4-nm dimension. *Chemical Science*, **2011**, 2, 1583	9.4	41
130	Oligomeric Gold thiolate Units Define the Properties of the Molecular Junction between Gold and Benzene Dithiols. *Journal of Physical Chemistry Letters*, **2010**, 1, 1528-1532	6.4	40
129	Evidence of superatom electronic shells in ligand-stabilized aluminum clusters. *Journal of Chemical Physics*, **2011**, 135, 094701	3.9	40
128	The Al50Cp*12 Cluster A 138-Electron Closed Shell (L = 6) Superatom. *European Journal of Inorganic Chemistry*, **2011**, 2011, 2649-2652	2.3	39
127	Formation of gold(I) edge oxide at flat gold nanoclusters on an ultrathin MgO film under ambient conditions. *Angewandte Chemie - International Edition*, **2010**, 49, 7913-6	16.4	39
126	Density functional study of gold atoms and clusters on a graphite (0001) surface with defects. *Physical Review B*, **2006**, 74,	3.3	38
125	Pd2Au36(SR)24 cluster: structure studies. *Nanoscale*, **2015**, 7, 17012-9	7.7	37
124	Atomically Precise Nanocluster Assemblies Encapsulating Plasmonic Gold Nanorods. *Angewandte Chemie - International Edition*, **2018**, 57, 6522-6526	16.4	37
123	AuS(PPh): an intermediate sized metalloid gold cluster stabilized by the AuS ring motif and Au-PPh groups. *Chemical Communications*, **2018**, 54, 248-251	5.8	37
122	[Cu(PET)HCl](PPh): A Copper Hydride Nanocluster with a Bisquare Antiprismatic Core. *Journal of the American Chemical Society*, **2020**, 142, 13974-13981	16.4	36
121	AcidBase Properties and Surface Charge Distribution of the Water-Soluble Au102(pMBA)44 Nanocluster. *Journal of Physical Chemistry C*, **2016**, 120, 10041-10050	3.8	36
120	Role of the Central Gold Atom in Ligand-Protected Biicosahedral Au24 and Au25 Clusters. *Journal of Physical Chemistry C*, **2013**, 117, 22079-22086	3.8	34

119	Stability, electronic structure, and optical properties of protected gold-doped silver AgAu (x = 0-5) nanoclusters. *Physical Chemistry Chemical Physics*, **2017**, 19, 13868-13874	3.6	33
118	TDDFT Analysis of Optical Properties of Thiol Monolayer-Protected Gold and Intermetallic Silver□old Au144(SR)60 and Au84Ag60(SR)60 Clusters. *Journal of Physical Chemistry C*, **2014**, 118, 20002-20008	3.8	33
117	Vibrational Perturbations and Ligand-Layer Coupling in a Single Crystal of Au144(SC2H4Ph)60 Nanocluster. *Journal of Physical Chemistry Letters*, **2014**, 5, 387-92	6.4	32
116	The redox chemistry of gold with high-valence doped calcium oxide. *Angewandte Chemie - International Edition*, **2013**, 52, 1424-7	16.4	32
115	Surface Coordination of Multiple Ligands Endows N-Heterocyclic Carbene-Stabilized Gold Nanoclusters with High Robustness and Surface Reactivity. *Angewandte Chemie - International Edition*, **2021**, 60, 3752-3758	16.4	31
114	Electronic shell structures in bare and protected metal nanoclusters. *Advances in Physics: X*, **2016**, 1, 467-491	3.1	29
113	Mixed-Monolayer-Protected Au25 Clusters with Bulky Calix[4]arene Functionalities. *Journal of Physical Chemistry Letters*, **2014**, 5, 585-9	6.4	29
112	Electronic structure and optical properties of the intrinsically chiral 16-electron superatom complex [Au20(PP3)4](4+). *Journal of Physical Chemistry A*, **2014**, 118, 4214-21	2.8	29
111	Dynamic Stabilization of the Ligand-Metal Interface in Atomically Precise Gold Nanoclusters Au and Au Protected by meta-Mercaptobenzoic Acid. *ACS Nano*, **2017**, 11, 11872-11879	16.7	29
110	One-pot synthesis and characterization of subnanometre-size benzotriazolate protected copper clusters. *Nanoscale*, **2012**, 4, 4095-8	7.7	29
109	Adsorption and activation of O(2) at Au chains on MgO/Mo thin films. *Physical Chemistry Chemical Physics*, **2010**, 12, 1483-92	3.6	29
108	First-principles simulations of hydrogen peroxide formation catalyzed by small neutral gold clusters. *Physical Chemistry Chemical Physics*, **2009**, 11, 6359-64	3.6	29
107	Photoelectron spectra from first principles: from the many-body to the single-particle picture. *New Journal of Physics*, **2008**, 10, 043018	2.9	29
106	Reversible Supracolloidal Self-Assembly of Cobalt Nanoparticles to Hollow Capsids and Their Superstructures. *Angewandte Chemie - International Edition*, **2017**, 56, 6473-6477	16.4	28
105	Dynamic Diglyme-Mediated Self-Assembly of Gold Nanoclusters. *ACS Nano*, **2015**, 9, 11690-8	16.7	28
104	Nonlinear Optical Properties of Thiolate-Protected Gold Clusters: A Theoretical Survey of the First Hyperpolarizabilities. *Journal of Physical Chemistry C*, **2015**, 119, 27676-27682	3.8	28
103	Optical absorption of magnesia-supported gold clusters and nanoscale catalysts: Effects due to the support, clusters, and adsorbants. *Physical Review B*, **2005**, 72,	3.3	28
102	Symmetry breaking in ligand-protected gold clusters probed by nonlinear optics. *Nanoscale*, **2016**, 8, 12123-7	7.7	27

101	The Role of the Anchor Atom in the Ligand of the Monolayer-Protected Au25(XR)18 Nanocluster. *Journal of Physical Chemistry C*, **2015**, 119, 9587-9594	3.8	26
100	Copper Induces a Core Plasmon in Intermetallic Au(144,145)-xCux(SR)60 Nanoclusters. *Journal of Physical Chemistry Letters*, **2015**, 6, 515-20	6.4	26
99	Divide and Protect: Passivating Cu(111) by Cu-(benzotriazole)2. *Journal of Physical Chemistry C*, **2012**, 116, 22346-22349	3.8	26
98	55-Atom clusters of silver and gold: Symmetry breaking by relativistic effects. *Computational Materials Science*, **2006**, 35, 332-336	3.2	26
97	Highly Robust but Surface-Active: An N-Heterocyclic Carbene-Stabilized Au25 Nanocluster. *Angewandte Chemie*, **2019**, 131, 17895-17899	3.6	25
96	Electron quantization in arbitrarily shaped gold islands on MgO thin films. *Physical Review B*, **2013**, 88,	3.3	25
95	Raman spectra of single-walled carbon nanotubes with vacancies. *Physical Review B*, **2008**, 77,	3.3	25
94	Impacts of Copper Position on the Electronic Structure of [Au25-xCux(SH)18] Nanoclusters. *Journal of Physical Chemistry C*, **2015**, 119, 8290-8298	3.8	24
93	Hydrophobic pocket targeting probes for enteroviruses. *Nanoscale*, **2015**, 7, 17457-67	7.7	24
92	Superatomic S(2) silver clusters stabilized by a thiolate-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, 8351-5	2.8	24
91	Modeling thiolate-protected gold clusters with density-functional tight-binding. *European Physical Journal D*, **2013**, 67, 1	1.3	23
90	Oxidation of small gas phase Pd clusters: A density functional study. *Computational Materials Science*, **2006**, 35, 371-374	3.2	23
89	Solvation chemistry of water-soluble thiol-protected gold nanocluster Au from DOSY NMR spectroscopy and DFT calculations. *Nanoscale*, **2014**, 6, 7823-6	7.7	22
88	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	3.8	22
87	A DFT Study of Linear Gold-Thiolate Superclusters Absorbing in the Therapeutic NIR Window. *Journal of Physical Chemistry Letters*, **2014**, 5, 1329-34	6.4	21
86	Protected but accessible: oxygen activation by a calixarene-stabilized undecagold cluster. *Journal of the American Chemical Society*, **2013**, 135, 12944-7	16.4	21
85	Towards Controlled Synthesis of Water-Soluble Gold Nanoclusters: Synthesis and Analysis. *Journal of Physical Chemistry C*, **2019**, 123, 2602-2612	3.8	21
84	From Symmetry Breaking to Unraveling the Origin of the Chirality of Ligated Au13Cu2 Nanoclusters. *Angewandte Chemie*, **2018**, 130, 3479-3483	3.6	19

83	Optical and electronic properties of graphene nanoribbons upon adsorption of ligand-protected aluminum clusters. *Physical Chemistry Chemical Physics*, **2014**, 16, 3558-65	3.6	19
82	Effect of bending on Raman-active vibration modes of carbon nanotubes. *Physical Review B*, **2008**, 78,	3.3	19
81	Electronic structure and thermal behavior of a magic Na59+ cluster. *Physical Review A*, **2004**, 70,	2.6	19
80	A method for structure prediction of metal-ligand interfaces of hybrid nanoparticles. *Nature Communications*, **2019**, 10, 3973	17.4	18
79	Monte Carlo Simulations of Au(SCH) Nanocluster Using Distance-Based Machine Learning Methods. *Journal of Physical Chemistry A*, **2020**, 124, 4827-4836	2.8	18
78	Photodynamics of a Molecular Water-Soluble Nanocluster Identified as Au130(pMBA)50. *Journal of Physical Chemistry C*, **2015**, 119, 20224-20229	3.8	17
77	Electron Binding in a Superatom with a Repulsive Coulomb Barrier: The Case of [Ag(SCHF)] in the Gas Phase. *Journal of Physical Chemistry Letters*, **2020**, 11, 3069-3074	6.4	17
76	Theoretical Analysis of the M12Ag32(SR)404 and 12Ag32(SR)304 Nanoclusters (M = Au, Ag; X = H, Mn). *Journal of Physical Chemistry C*, **2015**, 119, 10943-10948	3.8	17
75	Characterization of iron-carbonyl-protected gold clusters. *Journal of the American Chemical Society*, **2009**, 131, 12573-5	16.4	17
74	Real-space imaging with pattern recognition of a ligand-protected Ag nanocluster at sub-molecular resolution. *Nature Communications*, **2018**, 9, 2948	17.4	16
73	The electronic structure of Ge9[Si(SiMe3)3]3-: a superantiatom complex. *Physical Chemistry Chemical Physics*, **2012**, 14, 9311-6	3.6	16
72	Template-Free Supracolloidal Self-Assembly of Atomically Precise Gold Nanoclusters: From 2D Colloidal Crystals to Spherical Capsids. *Angewandte Chemie*, **2016**, 128, 16269-16272	3.6	16
71	A topological isomer of the Au(SR) nanocluster. *Chemical Communications*, **2020**, 56, 8087-8090	5.8	15
70	Patterning of supported gold monolayers via chemical lift-off lithography. *Beilstein Journal of Nanotechnology*, **2017**, 8, 2648-2661	3	15
69	Crystal Structures and Density Functional Theory Calculations of o- and p-Nitroaniline Derivatives: Combined Effect of Hydrogen Bonding and Aromatic Interactions on Dimerization Energy. *Crystal Growth and Design*, **2013**, 13, 3603-3612	3.5	15
68	A small spherical liquid: a DFT molecular dynamics study of WAu12. *Physical Chemistry Chemical Physics*, **2005**, 7, 2208-11	3.6	15
67	A Homoleptic Alkynyl-Ligated [Au Ag L] Cluster as a Catalytically Active Eight-Electron Superatom. *Angewandte Chemie - International Edition*, **2021**, 60, 970-975	16.4	15
66	Experimental Confirmation of a Topological Isomer of the Ubiquitous Au(SR) Cluster in the Gas Phase. *Journal of the American Chemical Society*, **2021**, 143, 1273-1277	16.4	15

65	Solvent driven formation of silver embedded resorcinarene nanorods. *CrystEngComm*, **2012**, 14, 347-350	3.3	13
64	Towards Atomically Precise Supported Catalysts from Monolayer-Protected Clusters: The Critical Role of the Support. *Chemistry - A European Journal*, **2020**, 26, 7051-7058	4.8	13
63	Point Group Symmetry Analysis of the Electronic Structure of Bare and Protected Metal Nanocrystals. *Journal of Physical Chemistry A*, **2018**, 122, 8576-8584	2.8	13
62	Role of Donor and Acceptor Substituents on the Nonlinear Optical Properties of Gold Nanoclusters. *Journal of Physical Chemistry C*, **2018**, 122, 4019-4028	3.8	12
61	Solubility-Driven Isolation of a Metastable Nonagold Cluster with Body-Centered Cubic Structure. *Chemistry - A European Journal*, **2020**, 26, 8465-8470	4.8	11
60	Reversible Supracolloidal Self-Assembly of Cobalt Nanoparticles to Hollow Capsids and Their Superstructures. *Angewandte Chemie*, **2017**, 129, 6573-6577	3.6	11
59	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	3.8	10
58	Nonmagnetic and magnetic thiolate-protected Au25 superatoms on Cu(111), Ag(111), and Au(111) surfaces. *Physical Review B*, **2012**, 85,	3.3	10
57	Ag (EBT) (TPP) Nanoclusters With Tailored Molecular and Electronic Structure. *Angewandte Chemie - International Edition*, **2021**, 60, 9038-9044	16.4	10
56	Site Preference in Multimetallic Nanoclusters: Incorporation of Alkali Metal Ions or Copper Atoms into the Alkynyl-Protected Body-Centered Cubic Cluster [Au7Ag8(C?CtBu)12]+. *Angewandte Chemie* , **2016**, 128, 15376-15380	3.6	9
55	Role of Nanocrystal Symmetry in the Crossover Region from Molecular to Metallic Gold Nanoparticles. *Journal of Physical Chemistry C*, **2019**, 123, 20655-20663	3.8	9
54	Structural characterization of site-modified nanocapsid with monodispersed gold clusters. *Scientific Reports*, **2017**, 7, 17048	4.9	9
53	Analysis of Localized Surface Plasmon Resonances in Spherical Jellium Clusters and Their Assemblies. *Journal of Physical Chemistry C*, **2017**, 121, 27036-27052	3.8	9
52	Electronic Structure: Shell Structure and the Superatom Concept. *Frontiers of Nanoscience*, **2015**, 9, 189-222	2.7	9
51	Symmetry-induced long-lived excited state in Au6 *Physical Review B*, **2007**, 76,	3.3	9
50	Enhanced Surface Ligands Reactivity of Metal Clusters by Bulky Ligands for Controlling Optical and Chiral Properties. *Angewandte Chemie - International Edition*, **2021**, 60, 12897-12903	16.4	9
49	Surface Chemistry Controls Magnetism in Cobalt Nanoclusters. *Journal of Physical Chemistry C*, **2016**, 120, 20822-20827	3.8	9
48	Atomically Precise Gold Nanoclusters: Towards an Optimal Biocompatible System from a Theoretical-Experimental Strategy. *Small*, **2021**, 17, e2005499	11	9

47	Reversible isomerization of metal nanoclusters induced by intermolecular interaction. *CheM*, **2021**, 7, 2227-2244	16.2	9
46	Exploring the atomic structure of 1.8nm monolayer-protected gold clusters with aberration-corrected STEM. *Ultramicroscopy*, **2017**, 176, 146-150	3.1	8
45	Silver Sulfide Nanoclusters and the Superatom Model. *Journal of Physical Chemistry C*, **2015**, 119, 1583-1588	3.3	8
44	Synthesis and Characterization of Enantiopure Chiral Bis NHC-Stabilized Edge-Shared Au Nanocluster with Unique Prolate Shape.. *Journal of the American Chemical Society*, **2022**,	16.4	8
43	Synthesis and properties of an Au cluster supported by a mixed N-heterocyclic carbene-thiolate ligand. *Chemical Communications*, **2020**, 56, 6102-6105	5.8	7
42	How many gold atoms make gold metal?. *Europhysics News*, **2015**, 46, 23-26	0.2	7
41	Ligand-Protected Gold Nanoclusters as Superatoms: Insights from Theory and Computations. *Frontiers of Nanoscience*, **2012**, 3, 129-157	0.7	7
40	Ab initio simulation of Na59+ and Na93+. *Computational Materials Science*, **2006**, 35, 158-162	3.2	7
39	Tertiary Chiral Nanostructures from C-H???F Directed Assembly of Chiroptical Superatoms. *Angewandte Chemie - International Edition*, **2021**, 60, 22411-22416	16.4	7
38	Ab initio molecular dynamics studies of Au38(SR)24 isomers under heating. *European Physical Journal D*, **2019**, 73, 1	1.3	6
37	Solid state halogen bonded networks vs. dynamic assemblies in solution: explaining N?X interactions of multivalent building blocks. *CrystEngComm*, **2015**, 17, 8231-8241	3.3	6
36	Atomically Precise Nanocluster Assemblies Encapsulating Plasmonic Gold Nanorods. *Angewandte Chemie*, **2018**, 130, 6632-6636	3.6	6
35	Ligand mediated evolution of size dependent magnetism in cobalt nanoclusters. *Physical Chemistry Chemical Physics*, **2018**, 20, 4563-4570	3.6	6
34	Exploring Strategies for Labeling Viruses with Gold Nanoclusters through Non-equilibrium Molecular Dynamics Simulations. *Bioconjugate Chemistry*, **2017**, 28, 2327-2339	6.3	6
33	Copper-hydride nanoclusters with enhanced stability by N-heterocyclic carbenes. *Nano Research*, **2021**, 14, 3303-3308	10	6
32	Chiral footprint of the ligand layer in the all-alkynyl-protected gold nanocluster Au(CCPhF). *Chemical Communications*, **2019**, 55, 9460-9462	5.8	5
31	The Redox Chemistry of Gold with High-Valence Doped Calcium Oxide. *Angewandte Chemie*, **2013**, 125, 1464-1467	3.6	5
30	Theoretical Studies of Gold Nanoclusters in Various Chemical Environments: When the Size Matters **2012**, 233-272		5

29	Protected Metallic Clusters, Quantum Wells and Metal-Nanocrystal Molecules. *Journal of Physical Chemistry C*, **2010**, 114, 15877-15878	3.8	5
28	Charge Transfer Plasmons in Dimeric Electron Clusters. *Journal of Physical Chemistry C*, **2020**, 124, 12645-12654	3.8	5
27	Surface Coordination of Multiple Ligands Endows N-Heterocyclic Carbene-Stabilized Gold Nanoclusters with High Robustness and Surface Reactivity. *Angewandte Chemie*, **2021**, 133, 3796-3802	3.6	5
26	[PtCu(PET)Cl]: An Atomically Precise, 10-Electron PtCu Bimetal Nanocluster with a Direct Pt-Pt Bond. *Journal of the American Chemical Society*, **2021**, 143, 12100-12107	16.4	5
25	Formation of Gold(I) Edge Oxide at Flat Gold Nanoclusters on an Ultrathin MgO Film under Ambient Conditions. *Angewandte Chemie*, **2010**, 122, 8085-8088	3.6	4
24	Anomalous binding sequence of CO ligands to an anionic triplatinum carbonyl complex. *Chemical Physics Letters*, **2005**, 406, 44-48	2.5	4
23	Gold/Isophorone Interaction Driven by Keto/Enol Tautomerization. *Journal of Physical Chemistry C*, **2016**, 120, 21962-21966	3.8	4
22	Atomically Precise Alkynyl- and Halide-Protected AuAg Nanoclusters AuAg(C?CPh)Cl and AuAg(C?CPh)Br: The Ligation Effects of Halides. *Inorganic Chemistry*, **2021**, 60, 3529-3533	5.1	4
21	Gold assisted oxygen dissociation on a molybdenum-doped CaO(001) surface. *Catalysis Science and Technology*, **2016**, 6, 6784-6793	5.5	3
20	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	3.3	3
19	Photo-Induced Cluster-to-Cluster Transformation of [AuAg(PPh)Cl] into [AuAg(PPh)Cl]: Fragmentation of a Trimer of 8-Electron Superatoms by Light. *Journal of Physical Chemistry Letters*, **2021**, 12, 10920-10926	6.4	3
18	Prospects and challenges for computer simulations of monolayer-protected metal clusters. *Nature Communications*, **2021**, 12, 2197	17.4	3
17	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	3.8	3
16	A Homoleptic Alkynyl-Ligated [Au13Ag16L24]3□Cluster as a Catalytically Active Eight-Electron Superatom. *Angewandte Chemie*, **2021**, 133, 983-988	3.6	3
15	Structure and dynamics of CaO films: A computational study of an effect of external static electric field. *Physical Review B*, **2017**, 95,	3.3	2
14	Dynamics of weak interactions in the ligand layer of -mercaptobenzoic acid protected gold nanoclusters Au(-MBA) and Au(-MBA). *Nanoscale*, **2020**, 12, 23859-23868	7.7	2
13	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	3.8	2
12	Magnetically induced currents and aromaticity in ligand-stabilized Au and AuPt superatoms. *Nature Communications*, **2021**, 12, 2477	17.4	2

11	Cubic aromaticity in ligand-stabilized doped Au superatoms. *Journal of Chemical Physics*, **2021**, 154, 204303	3.9	2
10	Ag44(EBT)26(TPP)4 Nanoclusters With Tailored Molecular and Electronic Structure. *Angewandte Chemie*, **2021**, 133, 9120-9126	3.6	2
9	Ligand Ratio Plays a Critical Role in the Design of Optimal Multifunctional Gold Nanoclusters for Targeted Gastric Cancer Therapy. *ACS Nanoscience Au*,		2
8	NHC-Stabilized Au Nanoclusters and Their Conversion to Au Nanoclusters.. *Jacs Au*, **2022**, 2, 875-885		2
7	Selective Acrolein Hydrogenation over Ligand-Protected Gold Clusters: A Venus Flytrap Mechanism. *ACS Catalysis*,2365-2374	13.1	1
6	Enhanced Surface Ligands Reactivity of Metal Clusters by Bulky Ligands for Controlling Optical and Chiral Properties. *Angewandte Chemie*, **2021**, 133, 13007-13013	3.6	0
5	Gold Nanoclusters: Atomically Precise Gold Nanoclusters: Towards an Optimal Biocompatible System from a TheoreticalEExperimental Strategy (Small 27/2021). *Small*, **2021**, 17, 2170140	11	0
4	Tertiary Chiral Nanostructures from CH???F Directed Assembly of Chiroptical Superatoms. *Angewandte Chemie*, **2021**, 133, 22585-22590	3.6	0
3	Binding Behavior of Carbonmonoxide to Gold Atoms on Ag(001). *Topics in Catalysis*, **2020**, 63, 1578-1584	2.3	
2	Preface to the Special Issue ISSPIC XVIII: International Symposium on Small Particles and Inorganic Clusters 2016 *Journal of Physical Chemistry C*, **2017**, 121, 10629-10631	3.8	
1	Atomically Precise Noble Metals in the Nanoscale, Stabilized by Ligands **2021**, 183-208		