Christine M Aikens

List of Publications by Year in Descending Order

128 papers	8,014 citations	41 h-index	88 g-index
142 ext. papers	8,876 ext. citations	6.5 avg, IF	6.78 L-index

#	Paper	IF	Citations
128	Plasmon-induced excitation energy transfer in silver nanoparticle dimers: A real-time TDDFTB investigation.. *Journal of Chemical Physics*, **2022**, 156, 154705	3.9	1
127	Excited-State Absorption in Silver Nanoclusters. *Journal of Physical Chemistry C*, **2021**, 125, 24996-25006	3.8	2
126	Theoretical Insights into Excitation-Induced Oxygen Activation on a Tetrahedral Ag Cluster. *Journal of Physical Chemistry A*, **2021**, 125, 9450-9458	2.8	1
125	Real-Time Electron Dynamics Study of Plasmon-Mediated Photocatalysis on an Icosahedral Al Nanocluster. *Journal of Physical Chemistry A*, **2021**, 125, 4847-4860	2.8	3
124	Understanding the Effect of Symmetry Breaking on Plasmon Coupling from TDDFT. *Journal of Physical Chemistry C*, **2021**, 125, 12198-12206	3.8	2
123	Nonradiative relaxation dynamics in the [AuAg(SH)] (n = 1, 12, 25) thiolate-protected nanoclusters. *Journal of Chemical Physics*, **2021**, 154, 184303	3.9	1
122	Impact of Ligands on Structural and Optical Properties of Ag Nanoclusters. *Journal of the American Chemical Society*, **2021**, 143, 9405-9414	16.4	13
121	A 34-Electron Superatom Ag Cluster with Regioselective Ternary Ligands Shells and Its 2D Rhombic Superlattice Assembly. *Angewandte Chemie - International Edition*, **2021**, 60, 4231-4237	16.4	27
120	Toward quantitative electronic structure in small gold nanoclusters. *Journal of Chemical Physics*, **2021**, 155, 014301	3.9	4
119	Deciphering the dual emission in the photoluminescence of AuCd(SR): A theoretical study using TDDFT and TDDFT + TB. *Journal of Chemical Physics*, **2021**, 155, 074302	3.9	1
118	Correction: Analysis and visualization of energy densities. I. Insights from real-time time-dependent density functional theory simulations. *Physical Chemistry Chemical Physics*, **2021**, 23, 8936	3.6	0
117	A 34-Electron Superatom Ag78 Cluster with Regioselective Ternary Ligands Shells and Its 2D Rhombic Superlattice Assembly. *Angewandte Chemie*, **2021**, 133, 4277-4283	3.6	6
116	A topological isomer of the Au(SR) nanocluster. *Chemical Communications*, **2020**, 56, 8087-8090	5.8	15
115	Polymorphism in Atomically Precise Cu Nanocluster Incorporating Tetrahedral [Cu] Kernel. *Journal of the American Chemical Society*, **2020**, 142, 5834-5841	16.4	41
114	Electronic relaxation dynamics in [Au(SR)] (R = CH, CH, CH, MPA, PET) thiolate-protected nanoclusters. *Physical Chemistry Chemical Physics*, **2020**, 22, 5272-5285	3.6	7
113	Theoretical Analysis of Optical Absorption Spectra of Parallel Nanowire Dimers and Dolmen Trimers. *Journal of Physical Chemistry C*, **2020**, 124, 13495-13507	3.8	2
112	TD-DFTB study of optical properties of silver nanoparticle homodimers and heterodimers. *Journal of Chemical Physics*, **2020**, 153, 144711	3.9	5

111	Analysis and visualization of energy densities. I. Insights from real-time time-dependent density functional theory simulations. *Physical Chemistry Chemical Physics*, **2020**, 22, 26838-26851	3.6	3
110	Analysis and visualization of energy densities. II. Insights from linear-response time-dependent density functional theory calculations. *Physical Chemistry Chemical Physics*, **2020**, 22, 26852-26864	3.6	4
109	Insights into the Metal-Exchange Synthesis of MAg24(SR)18 (M = Ni, Pd, Pt) Nanoclusters. *Chemistry of Materials*, **2020**, 32, 10216-10226	9.6	14
108	Ultrafast Nonradiative Decay of a Dipolar Plasmon-like State in Naphthalene. *Journal of Physical Chemistry A*, **2020**, 124, 9729-9737	2.8	3
107	Electronic Structure and Nonadiabatic Dynamics of Atomic Silver Nanowire$\mathbb{N}$2 Systems. *Journal of Physical Chemistry C*, **2020**, 124, 20834-20845	3.8	9
106	Ultrafast Nonlinear Plasmon Decay Processes in Silver Nanoclusters. *Journal of Physical Chemistry C*, **2020**, 124, 20477-20487	3.8	4
105	Theoretical investigation of relaxation dynamics in the Au(SH) thiolate-protected gold nanocluster. *Journal of Chemical Physics*, **2019**, 151, 094702	3.9	3
104	[Au(dppm)Cl]: a phosphine-protected gold nanocluster with rich charge states. *Dalton Transactions*, **2019**, 48, 3635-3640	4.3	24
103	Theoretical Investigation of Water Oxidation Mechanism on Pure Manganese and Ca-Doped Bimetal Oxide Complexes. *Journal of Physical Chemistry A*, **2019**, 123, 6152-6159	2.8	3
102	Real-Time TDDFT Investigation of Optical Absorption in Gold Nanowires. *Journal of Physical Chemistry C*, **2019**, 123, 14734-14745	3.8	18
101	Chiral Noble Metal Nanoparticles and Nanostructures. *Particle and Particle Systems Characterization* , **2019**, 36, 1900043	3.1	22
100	Understanding the Effect of Doping on Energetics and Electronic Structure for Au25, Ag25, and Au38Clusters. *Journal of Physical Chemistry C*, **2019**, 123, 9516-9527	3.8	27
99	Geometrical and Electronic Structure, Stability, and Optical Absorption Spectra Comparisons between Thiolate- and Chloride-Stabilized Gold Nanoclusters. *Journal of Physical Chemistry A*, **2019**, 123, 9712-9720	2.8	1
98	Luminescence and Electron Dynamics in Atomically Precise Nanoclusters with Eight Superatomic Electrons. *Journal of the American Chemical Society*, **2019**, 141, 18715-18726	16.4	35
97	[Ag(C?C Bu)(CrO)]: An Atomically Precise Silver Nanocluster Co-protected by Inorganic and Organic Ligands. *Journal of the American Chemical Society*, **2019**, 141, 4460-4467	16.4	101
96	Understanding plasmon coupling in nanoparticle dimers using molecular orbitals and configuration interaction. *Physical Chemistry Chemical Physics*, **2019**, 21, 23065-23075	3.6	6
95	Different Silver Nanoparticles in One Crystal: Ag210(iPrPhS)71(Ph3P)5Cl and Ag211(iPrPhS)71(Ph3P)6Cl. *Angewandte Chemie*, **2019**, 131, 201-205	3.6	28
94	Different Silver Nanoparticles in One Crystal: Ag (PrPhS) (Ph P) Cl and Ag (PrPhS) (Ph P) Cl. *Angewandte Chemie - International Edition*, **2019**, 58, 195-199	16.4	91

93	Connections Between Theory and Experiment for Gold and Silver Nanoclusters. *Annual Review of Physical Chemistry*, **2018**, 69, 205-229	15.7	60
92	Chiroptical Activity in BINAP- and DIOP-Stabilized Octa- and Undecagold Clusters. *Journal of Physical Chemistry C*, **2018**, 122, 11051-11065	3.8	14
91	Origin of Photoluminescence of Ag25(SR)18 Nanoparticles: Ligand and Doping Effect. *Journal of Physical Chemistry C*, **2018**, 122, 2440-2447	3.8	41
90	Anisotropic Polarizability-Induced Plasmon Transfer. *Journal of Physical Chemistry C*, **2018**, 122, 10621-10626	3.8	12
89	Theoretical Investigation of Relaxation Dynamics in Au38(SH)24 Thiolate-Protected Gold Nanoclusters. *Journal of Physical Chemistry C*, **2018**, 122, 16380-16388	3.8	19
88	Diphosphine-protected ultrasmall gold nanoclusters: opened icosahedral Au and heart-shaped Au clusters. *Chemical Science*, **2018**, 9, 1251-1258	9.4	60
87	Electronic and Geometric Structure, Optical Properties, and Excited State Behavior in Atomically Precise Thiolate-Stabilized Noble Metal Nanoclusters. *Accounts of Chemical Research*, **2018**, 51, 3065-3073	24.3	135
86	Comparison and convergence of optical absorption spectra of noble metal nanoparticles computed using linear-response and real-time time-dependent density functional theories. *Computational and Theoretical Chemistry*, **2018**, 1146, 27-36	2	3
85	TD-DFT and TD-DFTB Investigation of the Optical Properties and Electronic Structure of Silver Nanorods and Nanorod Dimers. *Journal of Physical Chemistry C*, **2018**, 122, 23639-23650	3.8	29
84	Research Update: Density functional theory investigation of the interactions of silver nanoclusters with guanine. *APL Materials*, **2017**, 5, 053102	5.7	11
83	Relativistic DFT investigation of electronic structure effects arising from doping the Au nanocluster with transition metals. *Nanoscale*, **2017**, 9, 15825-15834	7.7	22
82	Optical Properties of Small Gold Clusters Au8L82+ (L = PH3, PPh3): Magnetic Circular Dichroism Spectra. *Journal of Physical Chemistry C*, **2017**, 121, 19478-19489	3.8	12
81	Molecular Vibration Induced Plasmon Decay. *Journal of Physical Chemistry C*, **2017**, 121, 15368-15374	3.8	20
80	Theoretical Investigation of Electron and Nuclear Dynamics in the [Au25(SH)18]1 Thiolate-Protected Gold Nanocluster. *Journal of Physical Chemistry C*, **2017**, 121, 10653-10662	3.8	39
79	Photoluminescence Origin of Au38(SR)24 and Au22(SR)18 Nanoparticles: A Theoretical Perspective. *Journal of Physical Chemistry C*, **2017**, 121, 15416-15423	3.8	43
78	Theoretical Investigation of Water Oxidation Catalysis by a Model Manganese Cubane Complex. *Journal of Physical Chemistry C*, **2016**, 120, 21148-21161	3.8	12
77	Theoretical Insights into the Origin of Photoluminescence of Au25(SR)18(-) Nanoparticles. *Journal of the American Chemical Society*, **2016**, 138, 11202-10	16.4	140
76	Deciphering the Ligand Exchange Process on Thiolate Monolayer Protected Au38(SR)24 Nanoclusters. *Journal of Physical Chemistry C*, **2016**, 120, 14948-14961	3.8	13

75	Insights from Theory and Experiment on the Photochromic spiro-Dihydropyrrolo-Pyridazine/Betaine System. *Journal of Physical Chemistry A*, **2016**, 120, 875-83	2.8	10
74	Time Dependent Density Functional Theory Study of Magnetic Circular Dichroism Spectra of Gold Clusters Au(PH) and Au(PPh). *Journal of Physical Chemistry A*, **2016**, 120, 9625-9635	2.8	18
73	Theoretical Investigation of Water Oxidation on Fully Saturated Mn2O3 and Mn2O4 Complexes. *Journal of Physical Chemistry A*, **2016**, 120, 2480-92	2.8	11
72	Effect of Aliphatic versus Aromatic Ligands on the Structure and Optical Absorption of Au20(SR)16. *Journal of Physical Chemistry C*, **2016**, 120, 8354-8363	3.8	18
71	Gold-doped silver nanocluster [AuAg(SCHPh)X] (X = Cl or Br). *Nanoscale*, **2016**, 8, 18905-18911	7.7	61
70	Time-Dependent Density Functional Theory Investigation of the Electronic Structure and Chiroptical Properties of Curved and Helical Silver Nanowires. *Journal of Physical Chemistry A*, **2015**, 119, 8163-73	2.8	17
69	Synthesis and Characterization of Gallium-Doped CdSe Quantum Dots. *Journal of Physical Chemistry C*, **2015**, 119, 10749-10757	3.8	12
68	Quantum Mechanical Studies of Large Metal, Metal Oxide, and Metal Chalcogenide Nanoparticles and Clusters. *Chemical Reviews*, **2015**, 115, 6112-216	68.1	268
67	Reaction Pathways for Water Oxidation to Molecular Oxygen Mediated by Model Cobalt Oxide Dimer and Cubane Catalysts. *Journal of Physical Chemistry C*, **2015**, 119, 11072-11085	3.8	38
66	Real-Time TDDFT Studies of Exciton Decay and Transfer in Silver Nanowire Arrays. *Journal of Physical Chemistry C*, **2015**, 119, 6421-6427	3.8	40
65	Time-Dependent Density Functional Theory Studies of Optical Properties of Au Nanoparticles: Octahedra, Truncated Octahedra, and Icosahedra. *Journal of Physical Chemistry C*, **2015**, 119, 23127-23137	3.8	24
64	Strong Tunable Visible Absorption Predicted for Polysilo-acenes Using TDDFT Calculations. *Journal of Physical Chemistry Letters*, **2015**, 6, 3341-5	6.4	4
63	Cu2S3 complex on Cu(111) as a candidate for mass transport enhancement. *Physical Review B*, **2015**, 91,	3.3	26
62	Water Splitting Processes on Mn4O4 and CaMn3O4 Model Cubane Systems. *Journal of Physical Chemistry A*, **2015**, 119, 9325-37	2.8	9
61	Ligand Exchange Mechanism on Thiolate Monolayer Protected Au25(SR)18 Nanoclusters. *Journal of Physical Chemistry C*, **2015**, 119, 20179-20187	3.8	54
60	Theoretical examination of solvent and R group dependence in gold thiolate nanoparticle synthesis. *Physical Chemistry Chemical Physics*, **2015**, 17, 7676-80	3.6	6
59	Refined Insights in the Photochromic spiro-Dihydroindolizine/Betaine System. *Journal of Physical Chemistry A*, **2015**, 119, 9621-9	2.8	10
58	Ab initio electronic structure study of a model water splitting dimer complex. *Physical Chemistry Chemical Physics*, **2015**, 17, 32443-54	3.6	9

57	Optical Properties and Chirality. *Frontiers of Nanoscience*, **2015**, 9, 223-261	0.7	4
56	Time-dependent density functional theory study of the luminescence properties of gold phosphine thiolate complexes. *Journal of Physical Chemistry A*, **2015**, 119, 3337-47	2.8	13
55	Prediction of nonradical Au(0)-containing precursors in nanoparticle growth processes. *Journal of Physical Chemistry A*, **2015**, 119, 889-95	2.8	12
54	Theoretical investigation of water oxidation processes on small Mn(x)Ti(2-x)O4 (x = 0-2) complexes. *Journal of Physical Chemistry A*, **2014**, 118, 8204-21	2.8	8
53	X-ray Crystal Structure and Theoretical Analysis of Au25-xAgx(SCH2CH2Ph)18(-) Alloy. *Journal of Physical Chemistry Letters*, **2014**, 5, 461-6	6.4	184
52	Water adsorption and dissociation processes on small Mn-doped TiO2 complexes. *Journal of Physical Chemistry A*, **2014**, 118, 598-605	2.8	14
51	Quantum mechanical origin of the plasmon: from molecular systems to nanoparticles. *Nanoscale*, **2014**, 6, 11512-27	7.7	84
50	Chiral electronic transitions in fluorescent silver clusters stabilized by DNA. *ACS Nano*, **2014**, 8, 6883-92	16.7	70
49	Plasmon resonance analysis with configuration interaction. *Physical Chemistry Chemical Physics*, **2014**, 16, 15501-9	3.6	21
48	Au36(SPh)24 nanomolecules: X-ray crystal structure, optical spectroscopy, electrochemistry, and theoretical analysis. *Journal of Physical Chemistry B*, **2014**, 118, 14157-67	3.4	68
47	Quantum coherent plasmon in silver nanowires: a real-time TDDFT study. *Journal of Chemical Physics*, **2014**, 140, 244705	3.9	50
46	Origin and TDDFT Benchmarking of the Plasmon Resonance in Acenes. *Journal of Physical Chemistry C*, **2013**, 117, 21466-21475	3.8	51
45	Improved ReaxFF force field parameters for Au-S-C-H systems. *Journal of Physical Chemistry A*, **2013** , 117, 10438-46	2.8	24
44	Oxidation of gold clusters by thiols. *Journal of Physical Chemistry A*, **2013**, 117, 5377-84	2.8	18
43	Diameter Dependence of the Excitation Spectra of Silver and Gold Nanorods. *Journal of Physical Chemistry C*, **2013**, 117, 12325-12336	3.8	55
42	Effects of Mn doping on (TiO2)n (n=2–8) complexes. *Computational and Theoretical Chemistry*, **2013**, 1013, 32-45	2	15
41	Theoretical investigation of surface reactions of lactic acid on MgO clusters. *Journal of Physical Chemistry A*, **2013**, 117, 765-70	2.8	2
40	Helical Oxidovanadium(IV) Salen-Type Complexes: Synthesis, Characterisation and Catalytic Behaviour. *European Journal of Inorganic Chemistry*, **2013**, 2013, 5708-5717	2.3	9

39	Binding of carboxylates to gold nanoparticles: A theoretical study of the adsorption of formate on Au20. *Computational and Theoretical Chemistry*, **2012**, 987, 16-21	2	15
38	Development of a charge-perturbed particle-in-a-sphere model for nanoparticle electronic structure. *Physical Chemistry Chemical Physics*, **2012**, 14, 4287-95	3.6	12
37	The golden pathway to thiolate-stabilized nanoparticles: following the formation of gold(I) thiolate from gold(III) chloride. *Journal of the American Chemical Society*, **2012**, 134, 12590-5	16.4	41
36	TDDFT and CIS studies of optical properties of dimers of silver tetrahedra. *Journal of Physical Chemistry A*, **2012**, 116, 8260-9	2.8	47
35	Formyloxyl radical-gold nanoparticle binding: a theoretical study. *Journal of Physical Chemistry A*, **2012**, 116, 5445-52	2.8	8
34	Effects of Silver Doping on the Geometric and Electronic Structure and Optical Absorption Spectra of the Au25−nAgn(SH)18− (n = 1, 2, 4, 6, 8, 10, 12) Bimetallic Nanoclusters. *Journal of Physical Chemistry C*, **2012**, 116, 20617-20624	3.8	104
33	Time-Dependent Density Functional Theory Studies of Optical Properties of Ag Nanoparticles: Octahedra, Truncated Octahedra, and Icosahedra. *Journal of Physical Chemistry C*, **2012**, 116, 10356-10367	3.8	84
32	Modelling small gold and silver nanoparticles with electronic structure methods. *Molecular Simulation*, **2012**, 38, 607-614	2	18
31	Theoretical investigation of the electrochemical mechanism of water splitting on a titanium oxide cluster model. *Journal of Physical Chemistry A*, **2012**, 116, 526-35	2.8	17
30	Theoretical analysis of the optical excitation spectra of silver and gold nanowires. *Nanoscale*, **2012**, 4, 4190-8	7.7	73
29	Northwestern University Initiative for Teaching NanoSciences (NUITNS): An Approach for Teaching Computational Chemistry to Engineering Undergraduate Students. *Journal of Chemical Education*, **2011**, 88, 1079-1084	2.4	8
28	Structure and stability of (TiO2)n, (SiO2)n, and mixed Ti(m)Si(n-m)O(2n) [n = 2-5, m = 1 to (n - 1)] clusters. *Journal of Physical Chemistry A*, **2011**, 115, 868-79	2.8	29
27	Electronic Structure of Ligand-Passivated Gold and Silver Nanoclusters. *Journal of Physical Chemistry Letters*, **2011**, 2, 99-104	6.4	268
26	Density functional analysis of geometries and electronic structures of gold-phosphine clusters. The case of Au4(PR3)42+ and A(u4−I)2(PR3)4. *Journal of Physical Chemistry A*, **2011**, 115, 8017-31	2.8	46
25	Initial Growth Mechanisms of Gold-Phosphine Clusters. *Journal of Physical Chemistry C*, **2011**, 115, 6305-6316	3.8	22
24	Incremental binding energies of gold(I) and silver(I) thiolate clusters. *Journal of Physical Chemistry A* , **2011**, 115, 11818-23	2.8	42
23	Electron and Hydride Addition to Gold(I) Thiolate Oligomers: Implications for Gold−Thiolate Nanoparticle Growth Mechanisms. *Journal of Physical Chemistry Letters*, **2011**, 2, 990-994	6.4	43
22	Thiolate Ligand Exchange Mechanisms of Au1 and Subnanometer Gold Particle Au11. *Journal of Physical Chemistry C*, **2010**, 114, 18134-18138	3.8	16

21	Origin of intense chiroptical effects in undecagold subnanometer particles. *Journal of the American Chemical Society*, **2010**, 132, 1302-10	16.4	66
20	Geometric and Electronic Structure of Au25(SPhX)18 (X = H, F, Cl, Br, CH3, and OCH3). *Journal of Physical Chemistry Letters*, **2010**, 1, 2594-2599	6.4	97
19	Chirality and electronic structure of the thiolate-protected Au38 nanocluster. *Journal of the American Chemical Society*, **2010**, 132, 8210-8	16.4	367
18	TDDFT investigation of surface-enhanced Raman scattering of HCN and CN(-) on Ag(20). *Journal of Physical Chemistry A*, **2010**, 114, 8858-63	2.8	18
17	Electronic structure and TDDFT optical absorption spectra of silver nanorods. *Journal of Physical Chemistry A*, **2009**, 113, 4445-50	2.8	89
16	Silver nanoparticles with broad multiband linear optical absorption. *Angewandte Chemie - International Edition*, **2009**, 48, 5921-6	16.4	223
15	Effects of core distances, solvent, ligand, and level of theory on the TDDFT optical absorption spectrum of the thiolate-protected Au(25) nanoparticle. *Journal of Physical Chemistry A*, **2009**, 113, 10811-7	2.8	127
14	Reversible switching of magnetism in thiolate-protected Au25 superatoms. *Journal of the American Chemical Society*, **2009**, 131, 2490-2	16.4	371
13	Quantum Mechanical Examination of Optical Absorption Spectra of Silver Nanorod Dimers. *Progress in Theoretical Chemistry and Physics*, **2009**, 253-264	0.6	7
12	Correlating the crystal structure of a thiol-protected Au25 cluster and optical properties. *Journal of the American Chemical Society*, **2008**, 130, 5883-5	16.4	1752
11	Electronic structure methods for studying surface-enhanced Raman scattering. *Chemical Society Reviews*, **2008**, 37, 1061-73	58.5	465
10	From Discrete Electronic States to Plasmons: TDDFT Optical Absorption Properties of Ag n (n = 10, 20, 35, 56, 84, 120) Tetrahedral Clusters. *Journal of Physical Chemistry C*, **2008**, 112, 11272-11279	3.8	223
9	Origin of Discrete Optical Absorption Spectra of M25(SH)18 Nanoparticles (M = Au, Ag). *Journal of Physical Chemistry C*, **2008**, 112, 19797-19800	3.8	204
8	Time-Dependent Density Functional Theory Examination of the Effects of Ligand Adsorption on Metal Nanoparticles. *ACS Symposium Series*, **2008**, 108-121	0.4	1
7	Scalable implementation of analytic gradients for second-order Z-averaged perturbation theory using the distributed data interface. *Journal of Chemical Physics*, **2006**, 124, 14107	3.9	22
6	Incremental solvation of nonionized and zwitterionic glycine. *Journal of the American Chemical Society*, **2006**, 128, 12835-50	16.4	165
5	TDDFT studies of absorption and SERS spectra of pyridine interacting with Au20. *Journal of Physical Chemistry A*, **2006**, 110, 13317-24	2.8	150
4	Influence of multi-atom bridging ligands on the electronic structure and magnetic properties of homodinuclear titanium molecules. *Journal of Physical Chemistry A*, **2005**, 109, 11885-901	2.8	4

3	Parallel Unrestricted MP2 Analytic Gradients Using the Distributed Data Interface. *Journal of Physical Chemistry A*, **2004**, 108, 3103-3110	2.8	20
2	Electronic Structure and Magnetic Properties of Y2Ti(μX)2TiY2 (X, YH, F, Cl, Br) Isomers. *Journal of Physical Chemistry A*, **2003**, 107, 104-114	2.8	7
1	A derivation of the frozen-orbital unrestricted open-shell and restricted closed-shell second-order perturbation theory analytic gradient expressions. *Theoretical Chemistry Accounts*, **2003**, 110, 233-253	1.9	134