Christine M Aikens

List of Publications by Year
in descending order

138 papers	9,664 citations	50276 46 h-index	37204 96 g-index
142 all docs	142 docs citations	142 times ranked	6751 citing authors

#	Article	IF	Citations
1	Crystal Structure and Optical Properties of a Chiral Mixed Thiolate/Stibine-Protected Au₁₈ Cluster. Journal of the American Chemical Society, 2022, 144, 478-484.	13.7	19
2	Plasmon-induced excitation energy transfer in silver nanoparticle dimers: A real-time TDDFTB investigation. Journal of Chemical Physics, 2022, 156, 154705.	3.0	7
3	Timeâ€dependent density functional theory study of the optical properties of tetrahedral aluminum nanoparticles. Journal of Computational Chemistry, 2022, 43, 1033-1041.	3.3	2
4	From atom-precise nanoclusters to superatom materials. Journal of Chemical Physics, 2022, 156, 170401.	3.0	11
5	An Ultrastable 155â€Nuclei Silver Nanocluster Protected by Thiacalix[4]arene and Cyclohexanethiol for Photothermal Conversion. Angewandte Chemie - International Edition, 2022, 61, .	13.8	29
6	An Ultrastable 155â€Nuclei Silver Nanocluster Protected by Thiacalix[4]arene and Cyclohexanethiol for Photothermal Conversion. Angewandte Chemie, 2022, 134, .	2.0	4
7	An ultrastable thiolate/diglyme ligated cluster: Au₂₀(PET)₁₅(DG)₂. Nanoscale, 2022, 14, 9134-9141.	5.6	2
8	A 34â€Electron Superatom Ag₇₈ Cluster with Regioselective Ternary Ligands Shells and Its 2D Rhombic Superlattice Assembly. Angewandte Chemie - International Edition, 2021, 60, 4231-4237.	13.8	50
9	Real-Time Electron Dynamics Study of Plasmon-Mediated Photocatalysis on an Icosahedral Al₁₃^{â€“1} Nanocluster. Journal of Physical Chemistry A, 2021, 125, 4847-4860.	2.5	13
10	Understanding the Effect of Symmetry Breaking on Plasmon Coupling from TDDFT. Journal of Physical Chemistry C, 2021, 125, 12198-12206.	3.1	4
11	Nonradiative relaxation dynamics in the [Au25-nAgn(SH)18]â^'1 (n = 1, 12, 25) thiolate-protected nanoclusters. Journal of Chemical Physics, 2021, 154, 184303.	3.0	3
12	Impact of Ligands on Structural and Optical Properties of Ag₂₉ Nanoclusters. Journal of the American Chemical Society, 2021, 143, 9405-9414.	13.7	60
13	Toward quantitative electronic structure in small gold nanoclusters. Journal of Chemical Physics, 2021, 155, 014301.	3.0	9
14	Deciphering the dual emission in the photoluminescence of Au14Cd(SR)12: A theoretical study using TDDFT and TDDFT + TB. Journal of Chemical Physics, 2021, 155, 074302.	3.0	10
15	Correction: Analysis and visualization of energy densities. I. Insights from real-time time-dependent density functional theory simulations. Physical Chemistry Chemical Physics, 2021, 23, 8936-8936.	2.8	1
16	A 34â€Electron Superatom Ag 78 Cluster with Regioselective Ternary Ligands Shells and Its 2D Rhombic Superlattice Assembly. Angewandte Chemie, 2021, 133, 4277-4283.	2.0	10
17	Theoretical Insights into Excitation-Induced Oxygen Activation on a Tetrahedral Ag₈ Cluster. Journal of Physical Chemistry A, 2021, 125, 9450-9458.	2.5	5
18	Excited-State Absorption in Silver Nanoclusters. Journal of Physical Chemistry C, 2021, 125, 24996-25006.	3.1	9

#	Article	IF	Citations
19	TD-DFTB study of optical properties of silver nanoparticle homodimers and heterodimers. Journal of Chemical Physics, 2020, 153, 144711.	3.0	12
20	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.	2.8	9
21	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.	2.8	12
22	Insights into the Metal-Exchange Synthesis of MAg₂₄(SR)₁₈ (M = Ni, Pd, Pt) Nanoclusters. Chemistry of Materials, 2020, 32, 10216-10226.	6.7	35
23	Ultrafast Nonradiative Decay of a Dipolar Plasmon-like State in Naphthalene. Journal of Physical Chemistry A, 2020, 124, 9729-9737.	2.5	4
24	Electronic Structure and Nonadiabatic Dynamics of Atomic Silver Nanowireâ€“N₂ Systems. Journal of Physical Chemistry C, 2020, 124, 20834-20845.	3.1	15
25	Ultrafast Nonlinear Plasmon Decay Processes in Silver Nanoclusters. Journal of Physical Chemistry C, 2020, 124, 20477-20487.	3.1	9
26	A topological isomer of the Au₂₅(SR)₁₈^{â^'}nanocluster. Chemical Communications, 2020, 56, 8087-8090.	4.1	30
27	Polymorphism in Atomically Precise Cu₂₃ Nanocluster Incorporating Tetrahedral [Cu₄]⁰ Kernel. Journal of the American Chemical Society, 2020, 142, 5834-5841.	13.7	103
28	Electronic relaxation dynamics in [Au₂₅(SR)₁₈]^{â^'1} (R =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 3 thiolate-protected nanoclusters. Physical Chemistry Chemical Physics, 2020, 22, 5272-5285.	2.8	14
29	Theoretical Analysis of Optical Absorption Spectra of Parallel Nanowire Dimers and Dolmen Trimers. Journal of Physical Chemistry C, 2020, 124, 13495-13507.	3.1	3
30	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.	2.5	5
31	Luminescence and Electron Dynamics in Atomically Precise Nanoclusters with Eight Superatomic Electrons. Journal of the American Chemical Society, 2019, 141, 18715-18726.	13.7	59
32	Theoretical investigation of relaxation dynamics in the Au18(SH)14 thiolate-protected gold nanocluster. Journal of Chemical Physics, 2019, 151, 094702.	3.0	5
33	[Au18(dppm)6Cl4]4+: a phosphine-protected gold nanocluster with rich charge states. Dalton Transactions, 2019, 48, 3635-3640.	3.3	28
34	Theoretical Investigation of Water Oxidation Mechanism on Pure Manganese and Ca-Doped Bimetal Oxide Complexes. Journal of Physical Chemistry A, 2019, 123, 6152-6159.	2.5	4
35	Real-Time TDDFT Investigation of Optical Absorption in Gold Nanowires. Journal of Physical Chemistry C, 2019, 123, 14734-14745.	3.1	31
36	Chiral Noble Metal Nanoparticles and Nanostructures. Particle and Particle Systems Characterization, 2019, 36, 1900043.	2.3	29

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37	Understanding the Effect of Doping on Energetics and Electronic Structure for Au₂₅, Ag₂₅, and Au₃₈ Clusters. Journal of Physical Chemistry C, 2019, 123, 9516-9527.	3.1	44
38	[Ag₄₈(Câ‰¡C^tBu)₂₀(CrO₄)₇]: An Atomically Precise Silver Nanocluster Co-protected by Inorganic and Organic Ligands. Journal of the American Chemical Society, 2019, 141, 4460-4467.	13.7	139
39	Understanding plasmon coupling in nanoparticle dimers using molecular orbitals and configuration interaction. Physical Chemistry Chemical Physics, 2019, 21, 23065-23075.	2.8	10
40	Different Silver Nanoparticles in One Crystal: Ag₂₁₀(ⁱPrPhS)₇₁(Ph₃P)₅Cl and Ag₂₁₁(ⁱPrPhS)₇₁(Ph₃P)₆Cl. Angewandte Chemie, 2019, 131, 201-205.	2.0	34
41	Different Silver Nanoparticles in One Crystal: Ag₂₁₀(ⁱPrPhS)₇₁(Ph₃P)₅Cl and Ag₂₁₁(ⁱPrPhS)₇₁(Ph₃P)₆Cl. Angewandte Chemie - International Edition, 2019, 58, 195-199.	13.8	118
42	Connections Between Theory and Experiment for Gold and Silver Nanoclusters. Annual Review of Physical Chemistry, 2018, 69, 205-229.	10.8	80
43	Chiroptical Activity in BINAP- and DIOP-Stabilized Octa- and Undecagold Clusters. Journal of Physical Chemistry C, 2018, 122, 11051-11065.	3.1	20
44	Origin of Photoluminescence of Ag₂₅(SR)₁₈^{â€“} Nanoparticles: Ligand and Doping Effect. Journal of Physical Chemistry C, 2018, 122, 2440-2447.	3.1	57
45	Anisotropic Polarizability-Induced Plasmon Transfer. Journal of Physical Chemistry C, 2018, 122, 10621-10626.	3.1	22
46	Diphosphine-protected ultrasmall gold nanoclusters: opened icosahedral Au₁₃and heart-shaped Au₈clusters. Chemical Science, 2018, 9, 1251-1258.	7.4	86
47	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.	15.6	209
48	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.	2.5	3
49	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.	3.1	44
50	Theoretical Investigation of Relaxation Dynamics in Au₃₈(SH)₂₄ Thiolate-Protected Gold Nanoclusters. Journal of Physical Chemistry C, 2018, 122, 16380-16388.	3.1	27
51	Preface: Mark S. Gordon. Journal of Physical Chemistry A, 2017, 121, 2715-2718.	2.5	0
52	Research Update: Density functional theory investigation of the interactions of silver nanoclusters with guanine. APL Materials, 2017, 5, .	5.1	16
53	Relativistic DFT investigation of electronic structure effects arising from doping the Au₂₅ nanocluster with transition metals. Nanoscale, 2017, 9, 15825-15834.	5.6	28
54	Optical Properties of Small Gold Clusters Au8L82+ (L = PH3, PPh3): Magnetic Circular Dichroism Spectra. Journal of Physical Chemistry C, 2017, 121, 19478-19489.	3.1	15

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55	Molecular Vibration Induced Plasmon Decay. Journal of Physical Chemistry C, 2017, 121, 15368-15374.	3.1	24
56	Theoretical Investigation of Electron and Nuclear Dynamics in the [Au₂₅(SH)₁₈]^{â^'1} Thiolate-Protected Gold Nanocluster. Journal of Physical Chemistry C, 2017, 121, 10653-10662.	3.1	48
57	Photoluminescence Origin of Au38(SR)24 and Au22(SR)18 Nanoparticles: A Theoretical Perspective. Journal of Physical Chemistry C, 2017, 121, 15416-15423.	3.1	53
58	Time Dependent Density Functional Theory Study of Magnetic Circular Dichroism Spectra of Gold Clusters Au₉(PH₃)₈³⁺ and Au₉(PPh₃)₈³⁺. Journal of Physical Chemistry A, 2016, 120, 9625-9635.	2.5	20
59	Theoretical Investigation of Water Oxidation on Fully Saturated Mn₂O₃ and Mn₂O₄ Complexes. Journal of Physical Chemistry A, 2016, 120, 2480-2492.	2.5	11
60	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.	3.1	21
61	Gold-doped silver nanocluster [Au₃Ag₃₈(SCH₂Ph)₂₄X₅]^{2â^'}(X) Tj ET Q q 1 0 0 [illegible]	[illegible]	[illegible]
62	Theoretical Investigation of Water Oxidation Catalysis by a Model Manganese Cubane Complex. Journal of Physical Chemistry C, 2016, 120, 21148-21161.	3.1	15
63	Theoretical Insights into the Origin of Photoluminescence of Au₂₅(SR)₁₈^{â€“} Nanoparticles. Journal of the American Chemical Society, 2016, 138, 11202-11210.	13.7	194
64	Deciphering the Ligand Exchange Process on Thiolate Monolayer Protected Au₃₈(SR)₂₄ Nanoclusters. Journal of Physical Chemistry C, 2016, 120, 14948-14961.	3.1	15
65	Insights from Theory and Experiment on the Photochromic spiro-Dihydropyrroloâ€“Pyridazine/Betaine System. Journal of Physical Chemistry A, 2016, 120, 875-883.	2.5	11
66	Optical Properties and Chirality. Frontiers of Nanoscience, 2015, 9, 223-261.	0.6	5
67	Time-Dependent Density Functional Theory Study of the Luminescence Properties of Gold Phosphine Thiolate Complexes. Journal of Physical Chemistry A, 2015, 119, 3337-3347.	2.5	14
68	Prediction of Nonradical Au(0)-Containing Precursors in Nanoparticle Growth Processes. Journal of Physical Chemistry A, 2015, 119, 889-895.	2.5	13
69	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, 8163-8173.	2.5	20
70	Synthesis and Characterization of Gallium-Doped CdSe Quantum Dots. Journal of Physical Chemistry C, 2015, 119, 10749-10757.	3.1	17
71	Quantum Mechanical Studies of Large Metal, Metal Oxide, and Metal Chalcogenide Nanoparticles and Clusters. Chemical Reviews, 2015, 115, 6112-6216.	47.7	329
72	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.	3.1	40

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73	Real-Time TDDFT Studies of Exciton Decay and Transfer in Silver Nanowire Arrays. Journal of Physical Chemistry C, 2015, 119, 6421-6427.	3.1	46
74	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.	3.1	29
75	Strong Tunable Visible Absorption Predicted for Polysilo-acenes Using TDDFT Calculations. Journal of Physical Chemistry Letters, 2015, 6, 3341-3345.	4.6	5
76	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi mathvariant="normal">Cu</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mrow><mml:mi mathvariant="normal">S</mml:mi></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:math>complex on Cu(111) as a candidate for mass transport enhancement. Physical Review B, 2015, 91, .	3.2	30
77	Water Splitting Processes on Mn4O4 and CaMn3O4 Model Cubane Systems. Journal of Physical Chemistry A, 2015, 119, 9325-9337.	2.5	9
78	Ligand Exchange Mechanism on Thiolate Monolayer Protected Au₂₅(SR)₁₈ Nanoclusters. Journal of Physical Chemistry C, 2015, 119, 20179-20187.	3.1	67
79	Theoretical examination of solvent and R group dependence in gold thiolate nanoparticle synthesis. Physical Chemistry Chemical Physics, 2015, 17, 7676-7680.	2.8	6
80	Refined Insights in the Photochromic spiro-Dihydroindolizine/Betaine System. Journal of Physical Chemistry A, 2015, 119, 9621-9629.	2.5	11
81	Ab initio electronic structure study of a model water splitting dimer complex. Physical Chemistry Chemical Physics, 2015, 17, 32443-32454.	2.8	9
82	Au₃₆(SPh)₂₄ Nanomolecules: X-ray Crystal Structure, Optical Spectroscopy, Electrochemistry, and Theoretical Analysis. Journal of Physical Chemistry B, 2014, 118, 14157-14167.	2.6	74
83	Quantum coherent plasmon in silver nanowires: A real-time TDDFT study. Journal of Chemical Physics, 2014, 140, 244705.	3.0	57
84	Theoretical Investigation of Water Oxidation Processes on Small MnxTi2â€“xO4 (x = 0â€“2) Complexes. Journal of Physical Chemistry A, 2014, 118, 8204-8221.	2.5	8
85	X-ray Crystal Structure and Theoretical Analysis of Au_{25â€“x}Ag_x(SCH₂CH₂Ph)₁₈^{1â€“} Alloy. Journal of Physical Chemistry Letters, 2014, 5, 461-466.	4.6	215
86	Water Adsorption and Dissociation Processes on Small Mn-Doped TiO₂ Complexes. Journal of Physical Chemistry A, 2014, 118, 598-605.	2.5	17
87	Quantum mechanical origin of the plasmon: from molecular systems to nanoparticles. Nanoscale, 2014, 6, 11512-11527.	5.6	97
88	Chiral Electronic Transitions in Fluorescent Silver Clusters Stabilized by DNA. ACS Nano, 2014, 8, 6883-6892.	14.6	80
89	Plasmon resonance analysis with configuration interaction. Physical Chemistry Chemical Physics, 2014, 16, 15501.	2.8	24
90	Origin and TDDFT Benchmarking of the Plasmon Resonance in Acenes. Journal of Physical Chemistry C, 2013, 117, 21466-21475.	3.1	58

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91	Improved ReaxFF Force Field Parameters for Auâ€“Sâ€“Câ€“H Systems. Journal of Physical Chemistry A, 2013, 117, 10438-10446.	2.5	31
92	Oxidation of Gold Clusters by Thiols. Journal of Physical Chemistry A, 2013, 117, 5377-5384.	2.5	22
93	Diameter Dependence of the Excitation Spectra of Silver and Gold Nanorods. Journal of Physical Chemistry C, 2013, 117, 12325-12336.	3.1	64
94	The effect of field gradient on SERS. Nature Photonics, 2013, 7, 508-510.	31.4	59
95	Effects of Mn doping on (TiO2)n (n=2â€“5) complexes. Computational and Theoretical Chemistry, 2013, 1013, 32-45.	2.5	15
96	Theoretical Investigation of Surface Reactions of Lactic Acid on MgO Clusters. Journal of Physical Chemistry A, 2013, 117, 765-770.	2.5	2
97	Helical Oxidovanadium(IV) Salenâ€Type Complexes: Synthesis, Characterisation and Catalytic Behaviour. European Journal of Inorganic Chemistry, 2013, 2013, 5708-5717.	2.0	11
98	Binding of carboxylates to gold nanoparticles: A theoretical study of the adsorption of formate on Au20. Computational and Theoretical Chemistry, 2012, 987, 16-21.	2.5	18
99	Development of a charge-perturbed particle-in-a-sphere model for nanoparticle electronic structure. Physical Chemistry Chemical Physics, 2012, 14, 4287.	2.8	12
100	Correction to â€œTime-Dependent Density Functional Theory Studies of Optical Properties of Ag Nanoparticles: Octahedra, Truncated Octahedra, and Icosahedraâ€• Journal of Physical Chemistry C, 2012, 116, 21646-21646.	3.1	0
101	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, 12590-12595.	13.7	47
102	TDDFT and CIS Studies of Optical Properties of Dimers of Silver Tetrahedra. Journal of Physical Chemistry A, 2012, 116, 8260-8269.	2.5	48
103	Formyloxyl Radicalâ€“Gold Nanoparticle Binding: A Theoretical Study. Journal of Physical Chemistry A, 2012, 116, 5445-5452.	2.5	9
104	Effects of Silver Doping on the Geometric and Electronic Structure and Optical Absorption Spectra of the Au_{25â€“n}Ag_n(SH)₁₈^{â€“} (n = 1,) TJETQq0 0 0 rgBT /Ov	3	0
105	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.	3.1	94
106	Modelling small gold and silver nanoparticles with electronic structure methods. Molecular Simulation, 2012, 38, 607-614.	2.0	20
107	Theoretical Investigation of the Electrochemical Mechanism of Water Splitting on a Titanium Oxide Cluster Model. Journal of Physical Chemistry A, 2012, 116, 526-535.	2.5	19
108	Theoretical analysis of the optical excitation spectra of silver and gold nanowires. Nanoscale, 2012, 4, 4190.	5.6	81

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109	Density Functional Analysis of Geometries and Electronic Structures of Gold-Phosphine Clusters. The Case of Au₄(PR₃)₄²⁺ and Au₄(Î¼₂-I)₂(PR₃)₄.. Journal of Physical Chemistry A, 2011, 115, 8017-8031.	2.5	51
110	Initial Growth Mechanisms of Gold-Phosphine Clusters. Journal of Physical Chemistry C, 2011, 115, 6305-6316.	3.1	23
111	Incremental Binding Energies of Gold(I) and Silver(I) Thiolate Clusters. Journal of Physical Chemistry A, 2011, 115, 11818-11823.	2.5	52
112	Electron and Hydride Addition to Gold(I) Thiolate Oligomers: Implications for Goldâ€“Thiolate Nanoparticle Growth Mechanisms. Journal of Physical Chemistry Letters, 2011, 2, 990-994.	4.6	43
113	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.	2.3	8
114	Structure and Stability of (TiO₂)_n, (SiO₂)_n, and Mixed Ti_mSi_{nâ^'m}O_{2n} [n = 2â^'5, m = 1 to (n â^' 1)] Clusters. Journal of Physical Chemistry A, 2011, 115, 868-879.	2.5	32
115	Electronic Structure of Ligand-Passivated Gold and Silver Nanoclusters. Journal of Physical Chemistry Letters, 2011, 2, 99-104.	4.6	296
116	Thiolate Ligand Exchange Mechanisms of Au₁ and Subnanometer Gold Particle Au₁₁. Journal of Physical Chemistry C, 2010, 114, 18134-18138.	3.1	18
117	Origin of Intense Chiroptical Effects in Undecagold Subnanometer Particles. Journal of the American Chemical Society, 2010, 132, 1302-1310.	13.7	73
118	Geometric and Electronic Structure of Au₂₅(SPhX)₁₈^{â^'} (X = H, F,) Tj ETQq0 0 0 rgBT /Overlock 1 2594-2599.	4.6	111
119	Chirality and Electronic Structure of the Thiolate-Protected Au₃₈ Nanocluster. Journal of the American Chemical Society, 2010, 132, 8210-8218.	13.7	401
120	TDDFT Investigation of Surface-Enhanced Raman Scattering of HCN and CN^{â^'}on Ag₂₀^{â€}. Journal of Physical Chemistry A, 2010, 114, 8858-8863.	2.5	23
121	Electronic Structure and TDDFT Optical Absorption Spectra of Silver Nanorods. Journal of Physical Chemistry A, 2009, 113, 4445-4450.	2.5	99
122	Silver Nanoparticles with Broad Multiband Linear Optical Absorption. Angewandte Chemie - International Edition, 2009, 48, 5921-5926.	13.8	235
123	Effects of Core Distances, Solvent, Ligand, and Level of Theory on the TDDFT Optical Absorption Spectrum of the Thiolate-Protected Au₂₅ Nanoparticle. Journal of Physical Chemistry A, 2009, 113, 10811-10817.	2.5	139
124	Reversible Switching of Magnetism in Thiolate-Protected Au₂₅ Superatoms. Journal of the American Chemical Society, 2009, 131, 2490-2492.	13.7	414
125	Quantum Mechanical Examination of Optical Absorption Spectra of Silver Nanorod Dimers. Progress in Theoretical Chemistry and Physics, 2009, , 253-264.	0.2	7
126	Correlating the Crystal Structure of A Thiol-Protected Au₂₅ Cluster and Optical Properties. Journal of the American Chemical Society, 2008, 130, 5883-5885.	13.7	2,014

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127	Electronic structure methods for studying surface-enhanced Raman scattering. Chemical Society Reviews, 2008, 37, 1061.	38.1	568
128	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.	3.1	252
129	Origin of Discrete Optical Absorption Spectra of M₂₅(SH)₁₈^{â^'} Nanoparticles (M = Au, Ag). Journal of Physical Chemistry C, 2008, 112, 19797-19800.	3.1	221
130	Time-Dependent Density Functional Theory Examination of the Effects of Ligand Adsorption on Metal Nanoparticles. ACS Symposium Series, 2008, , 108-121.	0.5	1
131	Incremental Solvation of Nonionized and Zwitterionic Glycine. Journal of the American Chemical Society, 2006, 128, 12835-12850.	13.7	183
132	TDDFT Studies of Absorption and SERS Spectra of Pyridine Interacting with Au20. Journal of Physical Chemistry A, 2006, 110, 13317-13324.	2.5	169
133	Scalable implementation of analytic gradients for second-order Z-averaged perturbation theory using the distributed data interface. Journal of Chemical Physics, 2006, 124, 014107.	3.0	23
134	Influence of Multi-atom Bridging Ligands on the Electronic Structure and Magnetic Properties of Homodinuclear Titanium Molecules. Journal of Physical Chemistry A, 2005, 109, 11885-11901.	2.5	4
135	Parallel Unrestricted MP2 Analytic Gradients Using the Distributed Data Interfaceâ€. Journal of Physical Chemistry A, 2004, 108, 3103-3110.	2.5	22
136	Electronic Structure and Magnetic Properties of Y2Ti(Ì¼-X)2TiY2 (X, YH, F, Cl, Br) Isomers. Journal of Physical Chemistry A, 2003, 107, 104-114.	2.5	8
137	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.	1.4	142
138	Electronic Structure and Magnetic Properties of Y2Ti(Ì¼-X)2TiY2 (X, Y: H, F, Cl, Br) Isomers.. ChemInform, 2003, 34, no.	0.0	0