

Christine M Aikens

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128
papers

8,014
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41
h-index

88
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142
ext. papers

8,876
ext. citations

6.5
avg, IF

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L-index

#	Paper	IF	Citations
128	Correlating the crystal structure of a thiol-protected Au ₂₅ cluster and optical properties. <i>Journal of the American Chemical Society</i> , 2008 , 130, 5883-5	16.4	1752
127	Electronic structure methods for studying surface-enhanced Raman scattering. <i>Chemical Society Reviews</i> , 2008 , 37, 1061-73	58.5	465
126	Reversible switching of magnetism in thiolate-protected Au ₂₅ superatoms. <i>Journal of the American Chemical Society</i> , 2009 , 131, 2490-2	16.4	371
125	Chirality and electronic structure of the thiolate-protected Au ₃₈ nanocluster. <i>Journal of the American Chemical Society</i> , 2010 , 132, 8210-8	16.4	367
124	Quantum Mechanical Studies of Large Metal, Metal Oxide, and Metal Chalcogenide Nanoparticles and Clusters. <i>Chemical Reviews</i> , 2015 , 115, 6112-216	68.1	268
123	Electronic Structure of Ligand-Passivated Gold and Silver Nanoclusters. <i>Journal of Physical Chemistry Letters</i> , 2011 , 2, 99-104	6.4	268
122	Silver nanoparticles with broad multiband linear optical absorption. <i>Angewandte Chemie - International Edition</i> , 2009 , 48, 5921-6	16.4	223
121	From Discrete Electronic States to Plasmons: TDDFT Optical Absorption Properties of Ag _n (n = 10, 20, 35, 56, 84, 120) Tetrahedral Clusters. <i>Journal of Physical Chemistry C</i> , 2008 , 112, 11272-11279	3.8	223
120	Origin of Discrete Optical Absorption Spectra of M ₂₅ (SH) ₁₈ Nanoparticles (M = Au, Ag). <i>Journal of Physical Chemistry C</i> , 2008 , 112, 19797-19800	3.8	204
119	X-ray Crystal Structure and Theoretical Analysis of Au _{25-x} Ag _x (SCH ₂ CH ₂ Ph) ₁₈ (-) Alloy. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 461-6	6.4	184
118	Incremental solvation of nonionized and zwitterionic glycine. <i>Journal of the American Chemical Society</i> , 2006 , 128, 12835-50	16.4	165
117	TDDFT studies of absorption and SERS spectra of pyridine interacting with Au ₂₀ . <i>Journal of Physical Chemistry A</i> , 2006 , 110, 13317-24	2.8	150
116	Theoretical Insights into the Origin of Photoluminescence of Au ₂₅ (SR) ₁₈ (-) Nanoparticles. <i>Journal of the American Chemical Society</i> , 2016 , 138, 11202-10	16.4	140
115	Electronic and Geometric Structure, Optical Properties, and Excited State Behavior in Atomically Precise Thiolate-Stabilized Noble Metal Nanoclusters. <i>Accounts of Chemical Research</i> , 2018 , 51, 3065-3073	24.3	135
114	A derivation of the frozen-orbital unrestricted open-shell and restricted closed-shell second-order perturbation theory analytic gradient expressions. <i>Theoretical Chemistry Accounts</i> , 2003 , 110, 233-253	1.9	134
113	Effects of core distances, solvent, ligand, and level of theory on the TDDFT optical absorption spectrum of the thiolate-protected Au(25) nanoparticle. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 10811-7	2.8	127
112	Effects of Silver Doping on the Geometric and Electronic Structure and Optical Absorption Spectra of the Au ₂₅ Ag _n (SH) ₁₈ (n = 1, 2, 4, 6, 8, 10, 12) Bimetallic Nanoclusters. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 20617-20624	3.8	104

111	[Ag(C ₇ C Bu)(CrO)]: An Atomically Precise Silver Nanocluster Co-protected by Inorganic and Organic Ligands. <i>Journal of the American Chemical Society</i> , 2019 , 141, 4460-4467	16.4	101
110	Geometric and Electronic Structure of Au ₂₅ (SPhX) ₁₈ [X = H, F, Cl, Br, CH ₃ , and OCH ₃). <i>Journal of Physical Chemistry Letters</i> , 2010 , 1, 2594-2599	6.4	97
109	Different Silver Nanoparticles in One Crystal: Ag (PrPhS) (Ph P) Cl and Ag (PrPhS) (Ph P) Cl. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 195-199	16.4	91
108	Electronic structure and TDDFT optical absorption spectra of silver nanorods. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 4445-50	2.8	89
107	Quantum mechanical origin of the plasmon: from molecular systems to nanoparticles. <i>Nanoscale</i> , 2014 , 6, 11512-27	7.7	84
106	Time-Dependent Density Functional Theory Studies of Optical Properties of Ag Nanoparticles: Octahedra, Truncated Octahedra, and Icosahedra. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 10356-10367 ²⁸	7.8	84
105	Theoretical analysis of the optical excitation spectra of silver and gold nanowires. <i>Nanoscale</i> , 2012 , 4, 4190-8	7.7	73
104	Chiral electronic transitions in fluorescent silver clusters stabilized by DNA. <i>ACS Nano</i> , 2014 , 8, 6883-92	16.7	70
103	Au ₃₆ (SPh) ₂₄ nanomolecules: X-ray crystal structure, optical spectroscopy, electrochemistry, and theoretical analysis. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 14157-67	3.4	68
102	Origin of intense chiroptical effects in undecagold subnanometer particles. <i>Journal of the American Chemical Society</i> , 2010 , 132, 1302-10	16.4	66
101	Gold-doped silver nanocluster [AuAg(SCHPh)X] (X = Cl or Br). <i>Nanoscale</i> , 2016 , 8, 18905-18911	7.7	61
100	Connections Between Theory and Experiment for Gold and Silver Nanoclusters. <i>Annual Review of Physical Chemistry</i> , 2018 , 69, 205-229	15.7	60
99	Diphosphine-protected ultrasmall gold nanoclusters: opened icosahedral Au and heart-shaped Au clusters. <i>Chemical Science</i> , 2018 , 9, 1251-1258	9.4	60
98	Diameter Dependence of the Excitation Spectra of Silver and Gold Nanorods. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 12325-12336	3.8	55
97	Ligand Exchange Mechanism on Thiolate Monolayer Protected Au ₂₅ (SR) ₁₈ Nanoclusters. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 20179-20187	3.8	54
96	Origin and TDDFT Benchmarking of the Plasmon Resonance in Acenes. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 21466-21475	3.8	51
95	Quantum coherent plasmon in silver nanowires: a real-time TDDFT study. <i>Journal of Chemical Physics</i> , 2014 , 140, 244705	3.9	50
94	TDDFT and CIS studies of optical properties of dimers of silver tetrahedra. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 8260-9	2.8	47

93	Density functional analysis of geometries and electronic structures of gold-phosphine clusters. The case of Au ₄ (PR ₃) ₄ ²⁺ and Au ₄ (I) ₂ (PR ₃) ₄ . <i>Journal of Physical Chemistry A</i> , 2011 , 115, 8017-31	2.8	46
92	Electron and Hydride Addition to Gold(I) Thiolate Oligomers: Implications for Gold Thiolate Nanoparticle Growth Mechanisms. <i>Journal of Physical Chemistry Letters</i> , 2011 , 2, 990-994	6.4	43
91	Photoluminescence Origin of Au ₃₈ (SR) ₂₄ and Au ₂₂ (SR) ₁₈ Nanoparticles: A Theoretical Perspective. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 15416-15423	3.8	43
90	Incremental binding energies of gold(I) and silver(I) thiolate clusters. <i>Journal of Physical Chemistry A</i> , 2011 , 115, 11818-23	2.8	42
89	Polymorphism in Atomically Precise Cu Nanocluster Incorporating Tetrahedral [Cu] Kernel. <i>Journal of the American Chemical Society</i> , 2020 , 142, 5834-5841	16.4	41
88	Origin of Photoluminescence of Ag ₂₅ (SR) ₁₈ Nanoparticles: Ligand and Doping Effect. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 2440-2447	3.8	41
87	The golden pathway to thiolate-stabilized nanoparticles: following the formation of gold(I) thiolate from gold(III) chloride. <i>Journal of the American Chemical Society</i> , 2012 , 134, 12590-5	16.4	41
86	Real-Time TDDFT Studies of Exciton Decay and Transfer in Silver Nanowire Arrays. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 6421-6427	3.8	40
85	Theoretical Investigation of Electron and Nuclear Dynamics in the [Au ₂₅ (SH) ₁₈] Thiolate-Protected Gold Nanocluster. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 10653-10662	3.8	39
84	Reaction Pathways for Water Oxidation to Molecular Oxygen Mediated by Model Cobalt Oxide Dimer and Cubane Catalysts. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 11072-11085	3.8	38
83	Luminescence and Electron Dynamics in Atomically Precise Nanoclusters with Eight Superatomic Electrons. <i>Journal of the American Chemical Society</i> , 2019 , 141, 18715-18726	16.4	35
82	Structure and stability of (TiO ₂) _n , (SiO ₂) _n , and mixed Ti(m)Si(n-m)O(2n) [n = 2-5, m = 1 to (n - 1)] clusters. <i>Journal of Physical Chemistry A</i> , 2011 , 115, 868-79	2.8	29
81	TD-DFT and TD-DFTB Investigation of the Optical Properties and Electronic Structure of Silver Nanorods and Nanorod Dimers. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 23639-23650	3.8	29
80	Different Silver Nanoparticles in One Crystal: Ag ₂₁₀ (iPrPhS) ₇₁ (Ph ₃ P) ₅ Cl and Ag ₂₁₁ (iPrPhS) ₇₁ (Ph ₃ P) ₆ Cl. <i>Angewandte Chemie</i> , 2019 , 131, 201-205	3.6	28
79	Understanding the Effect of Doping on Energetics and Electronic Structure for Au ₂₅ , Ag ₂₅ , and Au ₃₈ Clusters. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 9516-9527	3.8	27
78	A 34-Electron Superatom Ag Cluster with Regioselective Ternary Ligands Shells and Its 2D Rhombic Superlattice Assembly. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 4231-4237	16.4	27
77	Cu ₂ S ₃ complex on Cu(111) as a candidate for mass transport enhancement. <i>Physical Review B</i> , 2015 , 91,	3.3	26
76	[Au(dppm)Cl]: a phosphine-protected gold nanocluster with rich charge states. <i>Dalton Transactions</i> , 2019 , 48, 3635-3640	4.3	24

75	Time-Dependent Density Functional Theory Studies of Optical Properties of Au Nanoparticles: Octahedra, Truncated Octahedra, and Icosahedra. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 23127-23137	3.8	24
74	Improved ReaxFF force field parameters for Au-S-C-H systems. <i>Journal of Physical Chemistry A</i> , 2013 , 117, 10438-46	2.8	24
73	Relativistic DFT investigation of electronic structure effects arising from doping the Au nanocluster with transition metals. <i>Nanoscale</i> , 2017 , 9, 15825-15834	7.7	22
72	Chiral Noble Metal Nanoparticles and Nanostructures. <i>Particle and Particle Systems Characterization</i> , 2019 , 36, 1900043	3.1	22
71	Initial Growth Mechanisms of Gold-Phosphine Clusters. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 6305-6316	3.1	22
70	Scalable implementation of analytic gradients for second-order Z-averaged perturbation theory using the distributed data interface. <i>Journal of Chemical Physics</i> , 2006 , 124, 14107	3.9	22
69	Plasmon resonance analysis with configuration interaction. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 15501-9	3.6	21
68	Molecular Vibration Induced Plasmon Decay. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 15368-15374	3.8	20
67	Parallel Unrestricted MP2 Analytic Gradients Using the Distributed Data Interface. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 3103-3110	2.8	20
66	Theoretical Investigation of Relaxation Dynamics in Au ₃₈ (SH) ₂₄ Thiolate-Protected Gold Nanoclusters. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 16380-16388	3.8	19
65	Real-Time TDDFT Investigation of Optical Absorption in Gold Nanowires. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 14734-14745	3.8	18
64	Modelling small gold and silver nanoparticles with electronic structure methods. <i>Molecular Simulation</i> , 2012 , 38, 607-614	2	18
63	Oxidation of gold clusters by thiols. <i>Journal of Physical Chemistry A</i> , 2013 , 117, 5377-84	2.8	18
62	TDDFT investigation of surface-enhanced Raman scattering of HCN and CN(-) on Ag(20). <i>Journal of Physical Chemistry A</i> , 2010 , 114, 8858-63	2.8	18
61	Time Dependent Density Functional Theory Study of Magnetic Circular Dichroism Spectra of Gold Clusters Au(PH) and Au(PPh). <i>Journal of Physical Chemistry A</i> , 2016 , 120, 9625-9635	2.8	18
60	Effect of Aliphatic versus Aromatic Ligands on the Structure and Optical Absorption of Au ₂₀ (SR) ₁₆ . <i>Journal of Physical Chemistry C</i> , 2016 , 120, 8354-8363	3.8	18
59	Time-Dependent Density Functional Theory Investigation of the Electronic Structure and Chiroptical Properties of Curved and Helical Silver Nanowires. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 8163-73	2.8	17
58	Theoretical investigation of the electrochemical mechanism of water splitting on a titanium oxide cluster model. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 526-35	2.8	17

57	Thiolate Ligand Exchange Mechanisms of Au ₁ and Subnanometer Gold Particle Au ₁₁ . <i>Journal of Physical Chemistry C</i> , 2010 , 114, 18134-18138	3.8	16
56	A topological isomer of the Au(SR) nanocluster. <i>Chemical Communications</i> , 2020 , 56, 8087-8090	5.8	15
55	Binding of carboxylates to gold nanoparticles: A theoretical study of the adsorption of formate on Au ₂₀ . <i>Computational and Theoretical Chemistry</i> , 2012 , 987, 16-21	2	15
54	Effects of Mn doping on (TiO ₂) _n (n=2B) complexes. <i>Computational and Theoretical Chemistry</i> , 2013 , 1013, 32-45	2	15
53	Chiroptical Activity in BINAP- and DIOP-Stabilized Octa- and Undecagold Clusters. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 11051-11065	3.8	14
52	Water adsorption and dissociation processes on small Mn-doped TiO ₂ complexes. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 598-605	2.8	14
51	Insights into the Metal-Exchange Synthesis of MAg ₂₄ (SR) ₁₈ (M = Ni, Pd, Pt) Nanoclusters. <i>Chemistry of Materials</i> , 2020 , 32, 10216-10226	9.6	14
50	Deciphering the Ligand Exchange Process on Thiolate Monolayer Protected Au ₃₈ (SR) ₂₄ Nanoclusters. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 14948-14961	3.8	13
49	Time-dependent density functional theory study of the luminescence properties of gold phosphine thiolate complexes. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 3337-47	2.8	13
48	Impact of Ligands on Structural and Optical Properties of Ag Nanoclusters. <i>Journal of the American Chemical Society</i> , 2021 , 143, 9405-9414	16.4	13
47	Synthesis and Characterization of Gallium-Doped CdSe Quantum Dots. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 10749-10757	3.8	12
46	Anisotropic Polarizability-Induced Plasmon Transfer. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 10621-10626	3.8	12
45	Theoretical Investigation of Water Oxidation Catalysis by a Model Manganese Cubane Complex. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 21148-21161	3.8	12
44	Optical Properties of Small Gold Clusters Au ₈ L ₈₂₊ (L = PH ₃ , PPh ₃): Magnetic Circular Dichroism Spectra. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 19478-19489	3.8	12
43	Prediction of nonradical Au(0)-containing precursors in nanoparticle growth processes. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 889-95	2.8	12
42	Development of a charge-perturbed particle-in-a-sphere model for nanoparticle electronic structure. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 4287-95	3.6	12
41	Research Update: Density functional theory investigation of the interactions of silver nanoclusters with guanine. <i>APL Materials</i> , 2017 , 5, 053102	5.7	11
40	Theoretical Investigation of Water Oxidation on Fully Saturated Mn ₂ O ₃ and Mn ₂ O ₄ Complexes. <i>Journal of Physical Chemistry A</i> , 2016 , 120, 2480-92	2.8	11

39	Refined Insights in the Photochromic spiro-Dihydroindolizine/Betaine System. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 9621-9	2.8	10
38	Insights from Theory and Experiment on the Photochromic spiro-Dihydropyrrolo-Pyridazine/Betaine System. <i>Journal of Physical Chemistry A</i> , 2016 , 120, 875-83	2.8	10
37	Water Splitting Processes on Mn ₄ O ₄ and CaMn ₃ O ₄ Model Cubane Systems. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 9325-37	2.8	9
36	Ab initio electronic structure study of a model water splitting dimer complex. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 32443-54	3.6	9
35	Helical Oxidovanadium(IV) Salen-Type Complexes: Synthesis, Characterisation and Catalytic Behaviour. <i>European Journal of Inorganic Chemistry</i> , 2013 , 2013, 5708-5717	2.3	9
34	Electronic Structure and Nonadiabatic Dynamics of Atomic Silver Nanowire-N ₂ Systems. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 20834-20845	3.8	9
33	Theoretical investigation of water oxidation processes on small Mn(x)Ti(2-x)O ₄ (x = 0-2) complexes. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 8204-21	2.8	8
32	Formyloxyl radical-gold nanoparticle binding: a theoretical study. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 5445-52	2.8	8
31	Northwestern University Initiative for Teaching NanoSciences (NUITNS): An Approach for Teaching Computational Chemistry to Engineering Undergraduate Students. <i>Journal of Chemical Education</i> , 2011 , 88, 1079-1084	2.4	8
30	Electronic relaxation dynamics in [Au(SR)] (R = CH ₃ , CH ₂ , CH, MPA, PET) thiolate-protected nanoclusters. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 5272-5285	3.6	7
29	Electronic Structure and Magnetic Properties of Y ₂ Ti(X)Z ₂ TiY ₂ (X, YH, F, Cl, Br) Isomers. <i>Journal of Physical Chemistry A</i> , 2003 , 107, 104-114	2.8	7
28	Quantum Mechanical Examination of Optical Absorption Spectra of Silver Nanorod Dimers. <i>Progress in Theoretical Chemistry and Physics</i> , 2009 , 253-264	0.6	7
27	Theoretical examination of solvent and R group dependence in gold thiolate nanoparticle synthesis. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 7676-80	3.6	6
26	Understanding plasmon coupling in nanoparticle dimers using molecular orbitals and configuration interaction. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 23065-23075	3.6	6
25	A 34-Electron Superatom Ag ₇₈ Cluster with Regioselective Ternary Ligands Shells and Its 2D Rhombic Superlattice Assembly. <i>Angewandte Chemie</i> , 2021 , 133, 4277-4283	3.6	6
24	TD-DFTB study of optical properties of silver nanoparticle homodimers and heterodimers. <i>Journal of Chemical Physics</i> , 2020 , 153, 144711	3.9	5
23	Strong Tunable Visible Absorption Predicted for Polysilo-acenes Using TDDFT Calculations. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 3341-5	6.4	4
22	Optical Properties and Chirality. <i>Frontiers of Nanoscience</i> , 2015 , 9, 223-261	0.7	4

21	Influence of multi-atom bridging ligands on the electronic structure and magnetic properties of homodinuclear titanium molecules. <i>Journal of Physical Chemistry A</i> , 2005 , 109, 11885-901	2.8	4
20	Analysis and visualization of energy densities. II. Insights from linear-response time-dependent density functional theory calculations. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 26852-26864	3.6	4
19	Ultrafast Nonlinear Plasmon Decay Processes in Silver Nanoclusters. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 20477-20487	3.8	4
18	Toward quantitative electronic structure in small gold nanoclusters. <i>Journal of Chemical Physics</i> , 2021 , 155, 014301	3.9	4
17	Theoretical investigation of relaxation dynamics in the Au(SH) thiolate-protected gold nanocluster. <i>Journal of Chemical Physics</i> , 2019 , 151, 094702	3.9	3
16	Theoretical Investigation of Water Oxidation Mechanism on Pure Manganese and Ca-Doped Bimetal Oxide Complexes. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 6152-6159	2.8	3
15	Analysis and visualization of energy densities. I. Insights from real-time time-dependent density functional theory simulations. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 26838-26851	3.6	3
14	Ultrafast Nonradiative Decay of a Dipolar Plasmon-like State in Naphthalene. <i>Journal of Physical Chemistry A</i> , 2020 , 124, 9729-9737	2.8	3
13	Real-Time Electron Dynamics Study of Plasmon-Mediated Photocatalysis on an Icosahedral Al Nanocluster. <i>Journal of Physical Chemistry A</i> , 2021 , 125, 4847-4860	2.8	3
12	Comparison and convergence of optical absorption spectra of noble metal nanoparticles computed using linear-response and real-time time-dependent density functional theories. <i>Computational and Theoretical Chemistry</i> , 2018 , 1146, 27-36	2	3
11	Theoretical investigation of surface reactions of lactic acid on MgO clusters. <i>Journal of Physical Chemistry A</i> , 2013 , 117, 765-70	2.8	2
10	Excited-State Absorption in Silver Nanoclusters. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 24996-25006	3.8	2
9	Theoretical Analysis of Optical Absorption Spectra of Parallel Nanowire Dimers and Dolmen Trimers. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 13495-13507	3.8	2
8	Understanding the Effect of Symmetry Breaking on Plasmon Coupling from TDDFT. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 12198-12206	3.8	2
7	Geometrical and Electronic Structure, Stability, and Optical Absorption Spectra Comparisons between Thiolate- and Chloride-Stabilized Gold Nanoclusters. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 9712-9720	2.8	1
6	Time-Dependent Density Functional Theory Examination of the Effects of Ligand Adsorption on Metal Nanoparticles. <i>ACS Symposium Series</i> , 2008 , 108-121	0.4	1
5	Theoretical Insights into Excitation-Induced Oxygen Activation on a Tetrahedral Ag Cluster. <i>Journal of Physical Chemistry A</i> , 2021 , 125, 9450-9458	2.8	1
4	Nonradiative relaxation dynamics in the [AuAg(SH)] (n = 1, 12, 25) thiolate-protected nanoclusters. <i>Journal of Chemical Physics</i> , 2021 , 154, 184303	3.9	1

3	Deciphering the dual emission in the photoluminescence of AuCd(SR): A theoretical study using TDDFT and TDDFT + TB. <i>Journal of Chemical Physics</i> , 2021 , 155, 074302	3.9	1
2	Plasmon-induced excitation energy transfer in silver nanoparticle dimers: A real-time TDDFTB investigation.. <i>Journal of Chemical Physics</i> , 2022 , 156, 154705	3.9	1
1	Correction: Analysis and visualization of energy densities. I. Insights from real-time time-dependent density functional theory simulations. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 8936	3.6	0