Vlasta BonaÄiÄ-KouteckÃ½

List of Publications by Year
in descending order

238 papers	10,406 citations	30070 54 h-index	45317 90 g-index
249 all docs	249 docs citations	249 times ranked	5226 citing authors

#	Article	IF	Citations
1	Quantum chemistry of small clusters of elements of groups Ia, Ib, and IIa: fundamental concepts, predictions, and interpretation of experiments. Chemical Reviews, 1991, 91, 1035-1108.	47.7	577
2	Neutral and Charged Biradicals, Zwitterions, Funnels in S1, and Proton Translocation: Their Role in Photochemistry, Photophysics, and Vision. Angewandte Chemie International Edition in English, 1987, 26, 170-189.	4.4	396
3	Density functional study of structural and electronic properties of bimetallic silverâ€“gold clusters: Comparison with pure gold and silver clusters. Journal of Chemical Physics, 2002, 117, 3120-3131.	3.0	305
4	Effective core potentialâ€configuration interaction study of electronic structure and geometry of small neutral and cationic Agnclusters: Predictions and interpretation of measured properties. Journal of Chemical Physics, 1993, 98, 7981-7994.	3.0	262
5	Photophysics of Internal Twisting. Advances in Chemical Physics, 2007, , 1-174.	0.3	203
6	Reactivity of Atomic Gold Anions toward Oxygen and the Oxidation of CO:Â Experiment and Theory. Journal of the American Chemical Society, 2004, 126, 2526-2535.	13.7	198
7	Ab initio study of the absorption spectra of Ag[sub n] (n=5â€“8) clusters. Journal of Chemical Physics, 2001, 115, 10450.	3.0	196
8	Theoretical and Experimental Consideration of the Reactions between VxOy+ and Ethylene. Journal of the American Chemical Society, 2003, 125, 6289-6299.	13.7	182
9	An accurate relativistic effective core potential for excited states of Ag atom: An application for studying the absorption spectra of Agn and Agn+ clusters. Journal of Chemical Physics, 1999, 110, 3876-3886.	3.0	167
10	Sudden Polarization in the Zwitterionic Z1Excited States of Organic Intermediates. Photochemical Implications. Angewandte Chemie International Edition in English, 1975, 14, 575-576.	4.4	161
11	Evolution of the electronic structure of lithium clusters between four and eight atoms. Journal of Chemical Physics, 1992, 96, 1793-1809.	3.0	160
12	Clusters as model systems for investigating nanoscale oxidation catalysis. Chemical Physics Letters, 2009, 475, 1-9.	2.6	160
13	Influence of Charge State on the Mechanism of CO Oxidation on Gold Clusters. Journal of the American Chemical Society, 2008, 130, 1694-1698.	13.7	147
14	Theoretical interpretation of the photoelectron detachment spectra of Naâ¯2â€“5 and of the absorption spectra of Na3, Na4, and Na8 clusters. Journal of Chemical Physics, 1990, 93, 3802-3825.	3.0	146
15	Nonadiabatic dynamics within the time dependent density functional theory: Ultrafast photodynamics in pyrazine. Chemical Physics, 2008, 349, 319-324.	1.9	137
16	Influence of Charge State on Catalytic Oxidation Reactions at Metal Oxide Clusters Containing Radical Oxygen Centers. Journal of the American Chemical Society, 2009, 131, 5460-5470.	13.7	135
17	Geometries of first triplet states of linear polyenes. Journal of the American Chemical Society, 1977, 99, 8134-8140.	13.7	130
18	Non-adiabatic dynamics of pyrrole: Dependence of deactivation mechanisms on the excitation energy. Chemical Physics, 2010, 375, 26-34.	1.9	124

#	ARTICLE	IF	CITATIONS
19	Effective core potentialâ€configuration interaction study of electronic structure and geometry of small anionic Agn clusters: Predictions and interpretation of photodetachment spectra. Journal of Chemical Physics, 1994, 100, 490-506.	3.0	120
20	Stoichiometric Zirconium Oxide Cations as Potential Building Blocks for Cluster Assembled Catalysts. Journal of the American Chemical Society, 2008, 130, 13912-13920.	13.7	120
21	Theoretical Exploration of Ultrafast Dynamics in Atomic Clusters:â€‰ Analysis and Control. Chemical Reviews, 2005, 105, 11-66.	47.7	110
22	Cooperative Effects in the Activation of Molecular Oxygen by Anionic Silver Clusters. Journal of the American Chemical Society, 2004, 126, 3442-3443.	13.7	105
23	Oxygen Adsorption on Hydrated Gold Cluster Anions:â€‰ Experiment and Theory. Journal of the American Chemical Society, 2003, 125, 8408-8414.	13.7	100
24	Nonadiabatic dynamics and simulation of time resolved photoelectron spectra within time-dependent density functional theory: Ultrafast photoswitching in benzylideneaniline. Journal of Chemical Physics, 2008, 129, 164118.	3.0	100
25	Laser-field-induced surface-hopping method for the simulation and control of ultrafast photodynamics. Physical Review A, 2009, 79, .	2.5	99
26	On a possible mechanism of the multiple fluorescence of p-N, N-dimethylaminobenzonitrile and related compounds. Chemical Physics Letters, 1979, 62, 115-120.	2.6	95
27	Prediction of structural and environmental effects on the S1î—¸S0 energy gap and jump probability in double-bond cisâ€”trans photoisomeriz. Chemical Physics Letters, 1984, 104, 440-443.	2.6	88
28	Nonadiabatic Dynamics within Time-Dependent Density Functional Tight Binding Method. Journal of Physical Chemistry A, 2009, 113, 12700-12705.	2.5	88
29	Ab initio predictions of structural and optical response properties of Na+n clusters: Interpretation of depletion spectra at low temperature. Journal of Chemical Physics, 1996, 104, 1427-1440.	3.0	87
30	Synthesis, characterization and optical properties of low nuclearity liganded silver clusters: Ag31(SG)19 and Ag15(SG)11. Nanoscale, 2013, 5, 5637.	5.6	83
31	A theory of free radical reactions. Journal of the American Chemical Society, 1977, 99, 842-850.	13.7	80
32	Charge-transfer-biradical excited states: relation to anomalous fluorescence. "Negative" S1-T1 splitting in twisted aminoborane. Journal of the American Chemical Society, 1985, 107, 1765-1766.	13.7	79
33	Isomer-specific spectroscopy of metal clusters trapped in a matrix:Ag9. Physical Review A, 2004, 70, .	2.5	77
34	Tuning Ag₂₉ nanocluster light emission from red to blue with one and two-photon excitation. Nanoscale, 2016, 8, 2892-2898.	5.6	75
35	Ab initio configuration interaction study of the electronic and geometric structures of small sodium cationic clusters. Journal of Chemical Physics, 1988, 89, 4861-4866.	3.0	74
36	Probing the Electronic Structure and Chemical Bonding of Gold Oxides and Sulfides in AuO_n^{â^’} and AuS_n^{â^’} (n = 1, 2). Journal of the American Chemical Society, 2008, 130, 9156-9167.	13.7	72

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37	An ab initio configuration interaction study of the excited states of the Na4 cluster: Assignment of the absorption spectrum. Chemical Physics Letters, 1990, 166, 32-38.	2.6	71
38	Critically heterosymmetric biradicaloid geometries of of protonated Schiff bases. Theoretica Chimica Acta, 1987, 72, 459-474.	0.8	70
39	Ultrafast photodynamics of furan. Journal of Chemical Physics, 2010, 133, 234303.	3.0	69
40	Generation of Oxygen Radical Centers in Binary Neutral Metal Oxide Clusters for Catalytic Oxidation Reactions. Angewandte Chemie - International Edition, 2010, 49, 407-410.	13.8	68
41	Theoretical exploration of femtosecond multi-state nuclear dynamics of small clusters. Journal of Chemical Physics, 1998, 108, 3096-3113.	3.0	67
42	Ligand-induced substrate steering and reshaping of [Ag2(H)]+ scaffold for selective CO2 extrusion from formic acid. Nature Communications, 2016, 7, 11746.	12.8	66
43	Interpretation of the absorption spectrum of Na8. Chemical Physics Letters, 1990, 170, 26-34.	2.6	65
44	Competition between planar and nonplanar structure in alkali hexamers: The example ofLi6. Physical Review Letters, 1991, 67, 2638-2641.	7.8	65
45	Ab initio CI study of the electronic structure and geometry of neutral and cationic hydrogenated lithium clusters. Predictions and interpretation of measured properties. Chemical Physics Letters, 1993, 206, 528-539.	2.6	62
46	Quantum molecular interpretation of the absorption spectra of Na5, Na6, and Na7 clusters. Journal of Chemical Physics, 1992, 96, 7938-7958.	3.0	58
47	Ab initio configurationâ€interaction study of the photoelectron spectra of small sodium cluster anions. Journal of Chemical Physics, 1989, 91, 3794-3795.	3.0	57
48	The Structures of Vanadium Oxide Clusterâ^'Ethene Complexes. A Combined IR Multiple Photon Dissociation Spectroscopy and DFT Calculation Study. Journal of the American Chemical Society, 2003, 125, 15716-15717.	13.7	57
49	How Shaped Light Discriminates Nearly Identical Biochromophores. Physical Review Letters, 2010, 105, 073003.	7.8	57
50	Ab initio Hartreeâ€"Fock selfâ€consistentâ€field molecular dynamics study of structure and dynamics of Li8. Journal of Chemical Physics, 1994, 101, 10092-10100.	3.0	56
51	Ab initio study of structural and optical response properties of excess-electron lithium-hydride and sodium-fluoride clusters. Chemical Physics, 1996, 210, 313-341.	1.9	56
52	Biradicals and biradicaloids: a unified view. Tetrahedron, 1988, 44, 7559-7585.	1.9	55
53	Time-dependent density functional theory excited state nonadiabatic dynamics combined with quantum mechanical/molecular mechanical approach: Photodynamics of indole in water. Journal of Chemical Physics, 2011, 135, 054105.	3.0	55
54	Sudden polarization in zwitterionic excited states of organic intermediates in photochemical reactions. On a possible mechanism for bicyclo[3.1.0]hex-2-ene formation. Journal of the American Chemical Society, 1978, 100, 396-402.	13.7	54

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55	An ab initio configuration interaction investigation of the excited states of the Li4 cluster. Chemical Physics Letters, 1988, 146, 518-523.	2.6	54
56	Measured and calculated absolute total cross-sections for the single ionization of CFx and NFx by electron impact. International Journal of Mass Spectrometry and Ion Processes, 1994, 137, 77-91.	1.8	54
57	Kinetic Analysis of the Reaction between (V2O5)n=1,2+ and Ethylene. Journal of Physical Chemistry B, 2006, 110, 3015-3022.	2.6	54
58	Enhanced two-photon absorption of ligated silver and gold nanoclusters: theoretical and experimental assessments. Nanoscale, 2019, 11, 12436-12448.	5.6	54
59	Photochemicalsyn-anti isomerization of a Schiff base: A two-dimensional description of a conical intersection in formaldimine. Theoretica Chimica Acta, 1985, 68, 45-55.	0.8	53
60	Joint experimental and theoretical investigations of the reactivity of Au2Onâ¯ and Au3Onâ¯ (n=1â€“5) with carbon monoxide. Journal of Chemical Physics, 2006, 125, 204311.	3.0	53
61	PlÃ¶tzliche Polarisation im zwitterionischen angeregten Zustand Z₁ organischer Zwischenstufen â€” Photochemische Auswirkungen. Angewandte Chemie, 1975, 87, 599-601.	2.0	52
62	Time-Resolved Femtosecond Photoelectron Spectroscopy by Field-Induced Surface Hopping. Journal of Physical Chemistry A, 2011, 115, 3755-3765.	2.5	52
63	Ab Initio Adiabatic Dynamics Combined with Wigner Distribution Approach to Femtosecond Pumpâ¯Probe Negative Ion to Neutral to Positive Ion (NeNePo) Spectroscopy of Ag2Au, Ag4, and Au4Clusters. Journal of Physical Chemistry A, 2001, 105, 8892-8905.	2.5	51
64	Silver clusterâ€“biomolecule hybrids: from basics towards sensors. Physical Chemistry Chemical Physics, 2012, 14, 9282.	2.8	51
65	Ab initio configuration interaction study of mixed BeLik clusters (k=1â€“9). Journal of Chemical Physics, 1988, 89, 5794-5802.	3.0	50
66	Absorption Enhancement and Conformational Control of Peptides by Small Silver Clusters. Physical Review Letters, 2008, 101, 213001.	7.8	50
67	Structure and stability of lithium (Li4 and Li6) clusters. The Journal of Physical Chemistry, 1983, 87, 1096-1097.	2.9	49
68	Au10(SG)10: A Chiral Gold Catenane Nanocluster with Zero Confined Electrons. Optical Properties and First-Principles Theoretical Analysis. Journal of Physical Chemistry Letters, 2017, 8, 1979-1985.	4.6	49
69	Optimal Control of Ionization Processes in NaK:â€‰ Comparison between Theory and Experiment. Journal of Physical Chemistry A, 2004, 108, 4175-4179.	2.5	48
70	Simulation of time resolved photoelectron spectra with Stieltjes imaging illustrated on ultrafast internal conversion in pyrazine. Journal of Chemical Physics, 2010, 132, 174301.	3.0	48
71	Ab initio CI study of chemical reactions of singlet and triplet imidogen (NH) radicals. Journal of the American Chemical Society, 1983, 105, 5547-5557.	13.7	46
72	Ab initio configuration interaction study of the electronic and geometric structure of small, mixed neutral and cationic MgNak and MgLik (k=2â€“8) clusters. Journal of Chemical Physics, 1989, 91, 4229-4241.	3.0	46

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73	Ab initiononadiabatic dynamics involving conical intersection combined with Wigner distribution approach to ultrafast spectroscopy illustrated on Na3F2 cluster. Journal of Chemical Physics, 2001, 114, 2123-2136.	3.0	45
74	Semiclassical calculations of the cross section for electron-impact ionization of. Journal of Physics B: Atomic, Molecular and Optical Physics, 1996, 29, 5175-5181.	1.5	43
75	Stereochemical effects in the quenching of Na*(3â€‰2P) by CO: Crossed beam experiment and ab initio CI potential energy surfaces. Journal of Chemical Physics, 1982, 77, 1908-1920.	3.0	42
76	Experimental and theoretical approach to the pseudorotating sodium cluster (Na3(B)). The Journal of Physical Chemistry, 1993, 97, 12509-12515.	2.9	42
77	Ab initio nonadiabatic dynamics study of ultrafast radiationless decay over conical intersections illustrated on the Na3F cluster. Journal of Chemical Physics, 2006, 125, 024303.	3.0	40
78	Ligand-core NLO-phores: a combined experimental and theoretical approach to the two-photon absorption and two-photon excited emission properties of small-ligated silver nanoclusters. Nanoscale, 2017, 9, 1221-1228.	5.6	40
79	Electronic states of cyclobutadiene heteroanalogs. Critical biradicaloids. Journal of the American Chemical Society, 1989, 111, 6140-6146.	13.7	39
80	Reactivity of stoichiometric titanium oxide cations. Physical Chemistry Chemical Physics, 2011, 13, 4243.	2.8	39
81	pH-Induced transformation of ligated Au₂₅ to brighter Au₂₃ nanoclusters. Nanoscale, 2018, 10, 11335-11341.	5.6	39
82	Nonadiabatic coupling between low lying singlet states of geometrically relaxed olefines: Ethylene and propylene. Journal of Chemical Physics, 1982, 76, 6018-6030.	3.0	38
83	Tuning Cluster Reactivity by Charge State and Composition: Experimental and Theoretical Investigation of CO Binding Energies to Ag_nAu_m^{+/â^’} (n +) Tj ETQq1 1 0.784314 rgBT /O	12.1	38
84	Doubly Charged Silver Clusters Stabilized by Tryptophan: Ag₄²⁺ as an Optical Marker for Monitoring Particle Growth. Angewandte Chemie - International Edition, 2011, 50, 878-881.	13.8	38
85	Predicting fluorescence quantum yields for molecules in solution: A critical assessment of the harmonic approximation and the choice of the lineshape function. Journal of Chemical Physics, 2020, 152, 054107.	3.0	35
86	A theoretical study of PdCONa and 6PdCONa9+ complexes as a simple model of a promoted catalyst. Journal of Catalysis, 1988, 111, 409-417.	6.2	34
87	Ab initio Hartree-Fock molecular dynamics with parallel processing: application to small neutral and charged Lin clusters. Chemical Physics Letters, 1996, 250, 47-58.	2.6	34
88	Ab initio molecular dynamics study of solid- to liquidlike transitions in Li9+, Li10, and Li11+ clusters. Journal of Chemical Physics, 1997, 107, 6321-6334.	3.0	34
89	Ab initio gradient corrected density functional molecular dynamics: investigation of structural and dynamical properties of the Li8 cluster. Chemical Physics Letters, 1997, 279, 129-139.	2.6	34
90	New Strategy for Optimal Control of Femtosecond Pumpâ^’Dump Processes. Journal of Physical Chemistry A, 2002, 106, 10477-10481.	2.5	34

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91	Spectroscopy of isolated, mass-selected tryptophan-Ag3 complexes: A model for photoabsorption enhancement in nanoparticle-biomolecule hybrid systems. Journal of Chemical Physics, 2006, 125, 164326.	3.0	34
92	Structural and Optical Properties of Isolated Noble Metalâ€“Glutathione Complexes: Insight into the Chemistry of Liganded Nanoclusters. Journal of Physical Chemistry C, 2011, 115, 24549-24554.	3.1	34
93	Tuning Structural and Optical Properties of Thiolate-Protected Silver Clusters by Formation of a Silver Core with Confined Electrons. Journal of Physical Chemistry C, 2013, 117, 14824-14831.	3.1	34
94	Use of configuration selection methods to study the sudden polarization effect. Journal of the American Chemical Society, 1979, 101, 5917-5922.	13.7	33
95	Femtosecond Time-Resolved Geometry Relaxation and Ultrafast Intramolecular Energy Redistribution in Ag2Au. ChemPhysChem, 2005, 6, 243-253.	2.1	33
96	UV Photodissociation of Proline-containing Peptide Ions: Insights from Molecular Dynamics. Journal of the American Society for Mass Spectrometry, 2015, 26, 432-443.	2.8	33
97	Selectivity Effects in Bimetallic Catalysis: Role of the Metal Sites in the Decomposition of Formic Acid into H₂ and CO₂ by the Coinage Metal Binuclear Complexes [dppmMMâ€²(H)]⁺. ChemCatChem, 2017, 9, 1298-1302.	3.7	33
98	A Mixed Quantumâ€“Classical Description of Excitation Energy Transfer in Supramolecular Complexes: FÃ¶rster Theory and beyond. ChemPhysChem, 2011, 12, 645-656.	2.1	32
99	Ab initio adiabatic dynamics involving excited states combined with Wigner distribution approach to ultrafast spectroscopy illustrated on alkali halide clusters. Journal of Chemical Physics, 2001, 114, 2106-2122.	3.0	31
100	Photoabsorption and photofragmentation of isolated cationic silver clusterâ€“tryptophan hybrid systems. Journal of Chemical Physics, 2007, 127, 134301.	3.0	31
101	Experimental and theoretical study of the absorption properties of thiolated diamondoids. Journal of Chemical Physics, 2010, 132, 144305.	3.0	31
102	Two-photon absorption of ligand-protected Ag₁₅ nanoclusters. Towards a new class of nonlinear optics nanomaterials. Physical Chemistry Chemical Physics, 2016, 18, 12404-12408.	2.8	31
103	Ultrafast Dynamics of Small Clusters on the Time Scale of Nuclear Motion. Journal of Physical Chemistry A, 1998, 102, 4069-4074.	2.5	30
104	Multiple pathways in the photodynamics of a polar Ï€-bond: A case study of silaethylene. Chemical Physics Letters, 2006, 418, 377-382.	2.6	30
105	The Origin of the Selectivity and Activity of Rutheniumâ€Cluster Catalysts for Fuelâ€Cell Feedâ€Gas Purification: A Gasâ€Phase Approach. Angewandte Chemie - International Edition, 2014, 53, 5467-5471.	13.8	30
106	General properties of the electronic structure of alkali metal clusters and Ia-IIa mixed clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1989, 12, 307-314.	1.0	29
107	Optical Properties of Gas-Phase Tryptophan-Silver Cations: Charge Transfer from the Indole Ring to the Silver Atom. ChemPhysChem, 2006, 7, 524-528.	2.1	29
108	Optical and Structural Properties of Copperâ”Oxytocin Dications in the Gas Phase. Journal of Physical Chemistry B, 2009, 113, 11293-11300.	2.6	29

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109	Geometrical relaxation in the excited singlet states of propylene. Tetrahedron, 1982, 38, 741-751.	1.9	28
110	Compact formulation of multiconfigurational response theory. Applications to small alkali metal clusters. Journal of Chemical Physics, 1993, 98, 3121-3140.	3.0	28
111	Composition dependent adsorption of multiple CO molecules on binary silverâ€“gold clusters AgnAum+ (n + m = 5): theory and experiment. Physical Chemistry Chemical Physics, 2010, 12, 7865.	2.8	28
112	Field-induced surface hopping method for probing transition state nonadiabatic dynamics of Ag3. Physical Chemistry Chemical Physics, 2011, 13, 8690.	2.8	28
113	Binding motifs of silver in prion octarepeat model peptides: a joint ion mobility, IR and UV spectroscopies, and theoretical approach. Physical Chemistry Chemical Physics, 2012, 14, 11433.	2.8	28
114	CO₂ Methanation on Cu-Cluster Decorated Zirconia Supports with Different Morphology: A Combined Experimental In Situ GIXANES/GISAXS, Ex Situ XPS and Theoretical DFT Study. ACS Catalysis, 2021, 11, 6210-6224.	11.2	28
115	Approximate calculations of correlation energy using oneâ€electron densityâ€functional procedures: Application to Lin and Nan clusters. Journal of Chemical Physics, 1990, 92, 6645-6654.	3.0	27
116	Total electron impact ionization cross sections of free molecular radicals: the failure of the additivity rule revisited. International Journal of Mass Spectrometry and Ion Processes, 1993, 129, 43-48.	1.8	27
117	Theoretical Study of the Reactivity of Bismuth Oxide Cluster Cations with Ethene in the Presence of Molecular Oxygen. Journal of Physical Chemistry A, 2000, 104, 6983-6992.	2.5	27
118	Size-dependent dynamics in excited states of gold clusters: From oscillatory motion to photoinduced melting. Journal of Chemical Physics, 2007, 127, 164312.	3.0	27
119	Nanotechnology in Tumor Biomarker Detection: The Potential of Liganded Nanoclusters as Nonlinear Optical Contrast Agents for Molecular Diagnostics of Cancer. Cancers, 2021, 13, 4206.	3.7	27
120	ECP-CI study of electronic structure and geometry of small neutral and charged Ag n clusters; Predictions and interpretation of measured properties. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1993, 26, 287-289.	1.0	26
121	A DFT study of EPR parameters in Cu(ii) complexes of the octarepeat region of the prion protein. Physical Chemistry Chemical Physics, 2008, 10, 4573.	2.8	26
122	Ab initio configuration interaction study of excited states of LiNa3 and Li2Na2 clusters: Interpretation of absorption spectra. Journal of Chemical Physics, 1992, 96, 4934-4944.	3.0	25
123	Electronic properties and geometric structures of Li4H and Li9H from optical absorption spectra. Journal of Chemical Physics, 1995, 102, 2727-2736.	3.0	25
124	Gas-phase VUV photoionisation and photofragmentation of the silver deuteride nanocluster [Ag₁₀D₈L₆]²⁺ (L = bis(diphenylphosphino)methane). A joint experimental and theoretical study. Physical Chemistry Chemical Physics, 2015, 17, 25772-25777.	2.8	25
125	Interactions of CO with AunOmâ‚ (nâ‰¥4). International Journal of Mass Spectrometry, 2006, 254, 163-167.	1.5	24
126	Structural and Photochemical Properties of Organosilver Reactive Intermediates MeAg₂⁺and PhAg₂⁺. Journal of Physical Chemistry A, 2011, 115, 9120-9127.	2.5	24

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127	How to Translate the [LCu₂(H)]⁺â€Catalysed Selective Decomposition of Formic Acid into H₂ and CO₂ from the Gas Phase into a Zeolite.. ChemCatChem, 2018, 10, 1173-1177.	3.7	24
128	Ligand shell size effects on one- and two-photon excitation fluorescence of zwitterion functionalized gold nanoclusters. Physical Chemistry Chemical Physics, 2019, 21, 23916-23921.	2.8	24
129	Ground and excited states properties of Na4F m=1â^'3, Li4H and Li4H2 clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1993, 26, 192-194.	1.0	23
130	Laser pulse trains for controlling excited state dynamics of adenine in water. Physical Chemistry Chemical Physics, 2012, 14, 4687.	2.8	23
131	Structural and optical properties of small oxygen-doped- and pure-silver clusters. European Physical Journal D, 1999, 9, 183-187.	1.3	22
132	Ab initio CI study of the hydrogen abstraction by imidogen (NH(a1.DELTA.)). Journal of the American Chemical Society, 1984, 106, 4061-4062.	13.7	20
133	Ab initio three-dimensional quantum dynamics of Ag3 clusters in the NeNePo process. Chemical Physics Letters, 2000, 318, 256-262.	2.6	20
134	Observation and Theoretical Description of Periodic Geometric Rearrangement in Electronically Excited Nonstoichiometric Sodium-Fluoride Clusters. Physical Review Letters, 2002, 89, 213404.	7.8	20
135	DFT investigation of copperâ€“peptide complexes related to the octarepeat domain of the prion protein. Inorganic Chemistry Communication, 2003, 6, 650-653.	3.9	20
136	Gasâ€Phase Synthesis and Intense Visible Absorption of Tryptophanâ€“Gold Cations. Angewandte Chemie - International Edition, 2009, 48, 7829-7832.	13.8	20
137	Formation and Characterisation of the Silver Hydride Nanocluster Cation [Ag₃H₂((Ph₂P)₂CH₂)]⁺ and Its Release of Hydrogen. Chemistry - A European Journal, 2014, 20, 16626-16633.	3.3	20
138	Reactivity-promoting criterion based on internal vibrational energy redistribution. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 10314-10317.	7.1	19
139	Gas-Phase Synthesis and Vibronic Action Spectroscopy of Ag2H+. Journal of Physical Chemistry Letters, 2011, 2, 548-552.	4.6	19
140	Gas-Phase Structural and Optical Properties of Homo- and Heterobimetallic Rhombic Dodecahedral Nanoclusters [Ag_{14â€“n}Cu_n(Câ‰¡CtBu)₁₂X]⁺ (X = Cl, I, ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 2017, 121, 10719-10727.	3.1	19
141	Ab initio predictions of optically allowed transitions in Na20. Nature of excitations and influence of geometry. Chemical Physics Letters, 1993, 213, 522-526.	2.6	18
142	General properties of the Hartree-Fock problem demonstrated on the frontier orbital model. Theoretica Chimica Acta, 1975, 36, 149-161.	0.8	17
143	An ab initio configuration interaction study of the reaction between small lithium clusters (Li4, Li6) and H2 molecule. Journal of Chemical Physics, 1991, 94, 5533-5543.	3.0	17
144	Composition dependent selectivity in the coadsorption of H2O and CO on pure and binary silverâ€“gold clusters. Chemical Physics Letters, 2013, 565, 74-79.	2.6	17

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145	Sub-100 nanometer silver doped goldâ€“cysteine supramolecular assemblies with enhanced nonlinear optical properties. Physical Chemistry Chemical Physics, 2019, 21, 12091-12099.	2.8	17
146	Core-valence correlation potentials based on density functional theory. Applications to valence-electron-only calculations on Na and K diatomics. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1989, 13, 355-361.	1.0	16
147	Ab-initio study of structural and optical properties of nonstoichiometric alkalimetal- oxides. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1997, 40, 445-447.	1.0	16
148	Ab-initio study of optical response properties of nonstoichiometric lithium-hydride and sodium-fluoride clusters. Chemical Physics, 1997, 225, 173-187.	1.9	16
149	Theoretical determination of the absolute electron impact ionization cross-section function for silver clusters Agn (n=2â€“7). Journal of Chemical Physics, 1999, 111, 1964-1971.	3.0	16
150	Isotope selective photoionization of NaK by optimal control: Theory and experiment. Journal of Chemical Physics, 2006, 125, 214310.	3.0	16
151	Synthesis and Spectroscopic Characterization of Diphenylargentate, [(C₆H₅)₂Ag]^{â^’}. Journal of Physical Chemistry Letters, 2012, 3, 1197-1201.	4.6	16
152	Nonlinear Absorption Dynamics Using Fieldâ€Induced Surface Hopping: Zinc Porphyrin in Water. ChemPhysChem, 2013, 14, 1377-1386.	2.1	16
153	The nature of electronic excitations at the metalâ€“bioorganic interface illustrated on histidineâ€“silver hybrids. Physical Chemistry Chemical Physics, 2014, 16, 1257-1261.	2.8	16
154	Structural characterization and gas-phase studies of the [Ag₁₀H₈(L)₆]²⁺ nanocluster dication. Nanoscale, 2019, 11, 22880-22889.	5.6	16
155	Functionalized Au15 nanoclusters as luminescent probes for protein carbonylation detection. Communications Chemistry, 2021, 4, .	4.5	16
156	Optimal control of mode-selective femtochemistry in multidimensional systems. Physical Review A, 2007, 76, .	2.5	15
157	Absorption properties of cationic silver clusterâ€“tryptophan complexes: A model for photoabsorption and photoemission enhancement in nanoparticleâ€“biomolecule systems. Chemical Physics, 2008, 343, 372-380.	1.9	15
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