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	Insights into the Impact of Gold Nanoclusters Au₁₀SG₁₀ on Human Microglia. ACS Chemical Neuroscience, 2022, 13, 464-476.	3.5	7
2	Open questions on proteins interacting with nanoclusters. Communications Chemistry, 2022, 5, .	4.5	10
3	Size and ligand effects of gold nanoclusters in alteration of organellar state and translocation of transcription factors in human primary astrocytes. Nanoscale, 2021, 13, 3173-3183.	5.6	11
4	Insights into Interactions between Interleukin-6 and Dendritic Polyglycerols. International Journal of Molecular Sciences, 2021, 22, 2415.	4.1	6
5	Functionalized Au15 nanoclusters as luminescent probes for protein carbonylation detection. Communications Chemistry, 2021, 4, .	4.5	16
6	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
7	Phenyl argentate aggregates [AgnPhn+1]â^' (n = 2â€“8): Models for the self-assembly of atom-precise polynuclear organometallics. Journal of Chemical Physics, 2021, 154, 224301.	3.0	3
8	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
9	Size Dependence of Non-Radiative Decay Rates in J-Aggregates. Journal of Physical Chemistry A, 2020, 124, 10143-10151.	2.5	14
10	Rationale Strategy to Tune the Optical Properties of Gold Catenane Nanoclusters by Doping with Silver Atoms. Journal of Physical Chemistry C, 2020, 124, 19368-19374.	3.1	7
11	Intrazeolite CO Methanation by Small Ruthenium Carbonyl Complexes: Translation from Free Clusters into the Cage. ChemCatChem, 2020, 12, 3857-3862.	3.7	0
12	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
13	Structure of the ligated Ag60 nanoparticle [{Cl@Ag12}@Ag48(dppm)12] (where) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 262 Td	1.3	7
14	Enhanced two-photon absorption of ligated silver and gold nanoclusters: theoretical and experimental assessments. Nanoscale, 2019, 11, 12436-12448.	5.6	54
15	Models Facilitating the Design of a New Metalâ€Organic Framework Catalyst for the Selective Decomposition of Formic Acid into Hydrogen and Carbon Dioxide. ChemCatChem, 2019, 11, 2372-2372.	3.7	0
16	Models Facilitating the Design of a New Metalâ€Organic Framework Catalyst for the Selective Decomposition of Formic Acid into Hydrogen and Carbon Dioxide. ChemCatChem, 2019, 11, 2443-2448.	3.7	11
17	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
18	Catenane Structures of Homoleptic Thioglycolic Acid-Protected Gold Nanoclusters Evidenced by Ion Mobility-Mass Spectrometry and DFT Calculations. Nanomaterials, 2019, 9, 457.	4.1	12

#	ARTICLE	IF	CITATIONS
19	Structural characterization and gas-phase studies of the [Ag₁₀H₈(L)₆]²⁺ nanocluster dication. Nanoscale, 2019, 11, 22880-22889.	5.6	16
20	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
21	pH-Induced transformation of ligated Au₂₅ to brighter Au₂₃ nanoclusters. Nanoscale, 2018, 10, 11335-11341.	5.6	39
22	Why Do Silver Trimers Intercalated in DNA Exhibit Unique Nonlinear Properties That Are Promising for Applications?. Journal of Physical Chemistry Letters, 2018, 9, 2584-2589.	4.6	8
23	A Brief Survey of Nonlinear Optics: Second Harmonic Generation and Two-Photon Absorption. SpringerBriefs in Materials, 2018, , 21-27.	0.3	1
24	Liganded Silver and Gold Quantum Clusters: Background of Their Structural, Electronic, and Optical Properties. SpringerBriefs in Materials, 2018, , 5-20.	0.3	4
25	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
26	Computational Evaluation of Optical Nonlinearities: Quantum Chemical Approaches. SpringerBriefs in Materials, 2018, , 29-38.	0.3	0
27	Selected Studied Cases. SpringerBriefs in Materials, 2018, , 63-75.	0.3	0
28	Concluding Remarks and Outlook. SpringerBriefs in Materials, 2018, , 77-82.	0.3	0
29	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
30	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
31	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
32	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
33	Theoretical design of new class of optical materials based on small noble metal nanocluster-biomolecule hybrids and its potential for medical applications. Advances in Physics: X, 2017, 2, 695-716.	4.1	6
34	ESI/MS investigation of routes to the formation of silver hydride nanocluster dications [Ag x H xâ^'2 L y] 2+ and gas-phase unimolecular chemistry of [Ag 10 H 8 L 6] 2+. International Journal of Mass Spectrometry, 2017, 413, 97-105.	1.5	13
35	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
36	Tuning Ag₂₉ nanocluster light emission from red to blue with one and two-photon excitation. Nanoscale, 2016, 8, 2892-2898.	5.6	75

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37	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
38	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
39	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
40	Water activation by small free ruthenium oxide clusters. Physical Chemistry Chemical Physics, 2014, 16, 26578-26583.	2.8	11
41	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
42	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
43	Gas-Phase Synthesis and Structure of Wade-Type Ruthenium Carbonyl and Hydrido Carbonyl Clusters. Journal of Physical Chemistry A, 2014, 118, 8356-8359.	2.5	4
44	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
45	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
46	Cation induced electrochromism in 2,4-dinitrophenylhydrazine (DNPH): Tuning optical properties of aromatic rings. Chemical Physics Letters, 2013, 570, 22-25.	2.6	5
47	Formation and characterization of thioglycolic acidâ€“silver cluster complexes. Dalton Transactions, 2013, 42, 8328.	3.3	13
48	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
49	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
50	Nonlinear Absorption Dynamics Using Fieldâ€Induced Surface Hopping: Zinc Porphyrin in Water. ChemPhysChem, 2013, 14, 1377-1386.	2.1	16
51	Structure and reactivity of small particles: from clusters to aerosols. Physical Chemistry Chemical Physics, 2012, 14, 9252.	2.8	6
52	Theoretical study of structural and optical properties of noble metal clusterâ€“dipeptide hybrids at defect centers of MgO. Physical Chemistry Chemical Physics, 2012, 14, 9330.	2.8	5
53	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
54	Silver clusterâ€“biomolecule hybrids: from basics towards sensors. Physical Chemistry Chemical Physics, 2012, 14, 9282.	2.8	51

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55	Exploring similarities in reactivity of superatom species: a combined theoretical and experimental investigation. Physical Chemistry Chemical Physics, 2012, 14, 1846.	2.8	4
56	Laser pulse trains for controlling excited state dynamics of adenine in water. Physical Chemistry Chemical Physics, 2012, 14, 4687.	2.8	23
57	Synthesis and Spectroscopic Characterization of Diphenylargentate, [(C₆H₅)₂Ag]^{â^'}. Journal of Physical Chemistry Letters, 2012, 3, 1197-1201.	4.6	16
58	Speciation of Copperâ€"Peptide Complexes in Water Solution Using DFTB and DFT Approaches: Case of the [Cu(HGGG)(Py)] Complex. Journal of Physical Chemistry B, 2012, 116, 6250-6260.	2.6	9
59	Binary Neutral Metal Oxide Clusters with Oxygen Radical Centers for Catalytic Oxidation Reactions: From Cluster Models Toward Surfaces. Journal of Physical Chemistry C, 2012, 116, 11570-11574.	3.1	8
60	BLUF Hydrogen network dynamics and UV/Vis spectra: A combined molecular dynamics and quantum chemical study. Journal of Computational Chemistry, 2012, 33, 2233-2242.	3.3	12
61	Theoretical Methods for Nonadiabatic Dynamics â€œon the flyâ€•in Complex Systems and its Control by Laser Fields. Progress in Theoretical Chemistry and Physics, 2012, , 299-325.	0.2	1
62	Analysis and control of ultrafast photon-induced processes. Physical Chemistry Chemical Physics, 2011, 13, 8619.	2.8	0
63	Reactivity of stoichiometric titanium oxide cations. Physical Chemistry Chemical Physics, 2011, 13, 4243.	2.8	39
64	Field-induced surface hopping method for probing transition state nonadiabatic dynamics of Ag3. Physical Chemistry Chemical Physics, 2011, 13, 8690.	2.8	28
65	Investigating Reactive Superoxide Units Bound to Zirconium Oxide Cations. Journal of Physical Chemistry C, 2011, 115, 21559-21566.	3.1	5
66	Structural and Photochemical Properties of Organosilver Reactive Intermediates MeAg₂⁺and PhAg₂⁺. Journal of Physical Chemistry A, 2011, 115, 9120-9127.	2.5	24
67	Electronic Structure Similarities in Pb_xSb_y^{â€"}and Sn_xBi_y^{â€"}Clusters. Journal of Physical Chemistry A, 2011, 115, 10276-10280.	2.5	12
68	Time-Resolved Femtosecond Photoelectron Spectroscopy by Field-Induced Surface Hopping. Journal of Physical Chemistry A, 2011, 115, 3755-3765.	2.5	52
69	Gas-Phase Synthesis and Vibronic Action Spectroscopy of Ag2H+. Journal of Physical Chemistry Letters, 2011, 2, 548-552.	4.6	19
70	Tuning Cluster Reactivity by Charge State and Composition: Experimental and Theoretical Investigation of CO Binding Energies to Ag_nAu_m^{+/â^'} (n +) Tj ETQq0 0 0 rgBT /Overlock 1	2.5	68
71	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
72	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

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73	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
74	Unique optical properties of silver cluster-biochromophore hybrids: Comparison with copper and gold. Chemical Physics Letters, 2011, 501, 211-214.	2.6	8
75	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
76	Non-adiabatic dynamics of pyrrole: Dependence of deactivation mechanisms on the excitation energy. Chemical Physics, 2010, 375, 26-34.	1.9	124
77	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
78	Generation of Oxygen Radical Centers in Binary Neutral Metal Oxide Clusters for Catalytic Oxidation Reactions. Angewandte Chemie - International Edition, 2010, 49, 2272-2272.	13.8	3
79	A harmonic approximation of intramolecular vibrations in a mixed quantumâ€“classical methodology: Linear absorbance of a dissolved Pheophorbid-a molecule as an example. Chemical Physics, 2010, 377, 10-14.	1.9	15
80	Theoretical study of structural and optical properties of small silver and gold clusters at defect centers of MgO. Physica Status Solidi (B): Basic Research, 2010, 247, 1099-1108.	1.5	6
81	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
82	How Shaped Light Discriminates Nearly Identical Biochromophores. Physical Review Letters, 2010, 105, 073003.	7.8	57
83	Ultrafast photodynamics of furan. Journal of Chemical Physics, 2010, 133, 234303.	3.0	69
84	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
85	Experimental and theoretical study of the absorption properties of thiolated diamondoids. Journal of Chemical Physics, 2010, 132, 144305.	3.0	31
86	Tailoring Functionality of Clusters and Their Complexes with Biomolecules by Size, Structures, and Lasers. Science and Technology of Atomic, Molecular, Condensed Matter and Biological Systems, 2010, 1, 485-516.	0.6	0
87	Silver Cluster Chromophores for Absorption Enhancement of Peptides. Journal of Physical Chemistry A, 2009, 113, 3783-3788.	2.5	11
88	Gasâ€Phase Synthesis and Intense Visible Absorption of Tryptophanâ€“Gold Cations. Angewandte Chemie - International Edition, 2009, 48, 7829-7832.	13.8	20
89	Clusters as model systems for investigating nanoscale oxidation catalysis. Chemical Physics Letters, 2009, 475, 1-9.	2.6	160
90	Silver cluster induced absorption enhancement and conformation control of peptides. European Physical Journal D, 2009, 52, 203-206.	1.3	6

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91	Optical and Structural Properties of Copperâ"Oxytocin Dications in the Gas Phase. Journal of Physical Chemistry B, 2009, 113, 11293-11300.	2.6	29
92	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
93	Nonadiabatic Dynamics within Time-Dependent Density Functional Tight Binding Method. Journal of Physical Chemistry A, 2009, 113, 12700-12705.	2.5	88
94	Laser-field-induced surface-hopping method for the simulation and control of ultrafast photodynamics. Physical Review A, 2009, 79, .	2.5	99
95	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
96	Ultrafast dynamics in noble metal clusters: The role of internal vibrational redistribution. Chemical Physics, 2008, 350, 111-117.	1.9	1
97	Nonadiabatic dynamics within the time dependent density functional theory: Ultrafast photodynamics in pyrazine. Chemical Physics, 2008, 349, 319-324.	1.9	137
98	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
99	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
100	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
101	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
102	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
103	Absorption Enhancement and Conformational Control of Peptides by Small Silver Clusters. Physical Review Letters, 2008, 101, 213001.	7.8	50
104	Optimal control of mode-selective femtochemistry in multidimensional systems. Physical Review A, 2007, 76, .	2.5	15
105	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
106	Photoabsorption and photofragmentation of isolated cationic silver clusterâ€"tryptophan hybrid systems. Journal of Chemical Physics, 2007, 127, 134301.	3.0	31
107	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
108	Photophysics of Internal Twisting. Advances in Chemical Physics, 2007, , 1-174.	0.3	203

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109	Analysis and control of small isolated molecular systems. , 2007, , 25-152.		4
110	Complex systems in the gas phase. , 2007, , 153-256.		1
111	Kinetic Analysis of the Reaction between (V2O5)n=1,2+ and Ethylene. Journal of Physical Chemistry B, 2006, 110, 3015-3022.	2.6	54
112	Cluster properties in the regime in which each atom counts. Computational Materials Science, 2006, 35, 151-157.	3.0	9
113	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
114	Emissive properties of silver particles at silver oxide surface defects. Applied Physics A: Materials Science and Processing, 2006, 82, 117-123.	2.3	13
115	Interactions of CO with AunOmâ^' (nâ‰¥4). International Journal of Mass Spectrometry, 2006, 254, 163-167.	1.5	24
116	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
117	The Gas-Phase Chemistry ofcis-Diammineplatinum(II) Complexes: A Joint Experimental and Theoretical Study. ChemPhysChem, 2006, 7, 1779-1785.	2.1	8
118	Photostabilization of the ultracold Rb2molecule by optimal control. Journal of Physics B: Atomic, Molecular and Optical Physics, 2006, 39, S1043-S1053.	1.5	5
119	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
120	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
121	Ultrafast dynamics in atomic clusters: Analysis and control. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 10594-10599.	7.1	13
122	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
123	Isotope selective photoionization of NaK by optimal control: Theory and experiment. Journal of Chemical Physics, 2006, 125, 214310.	3.0	16
124	Analysis and Control of Ultrafast Dynamics in Clusters. , 2006, , 466-478.		0
125	Femtosecond Time-Resolved Geometry Relaxation and Ultrafast Intramolecular Energy Redistribution in Ag2Au. ChemPhysChem, 2005, 6, 243-253.	2.1	33
126	Theoretical Exploration of Ultrafast Dynamics in Atomic Clusters: Analysis and Control. ChemInform, 2005, 36, no.	0.0	1

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127	Analysis and Control of Ultrafast Dynamics in Clusters: Theory and Experiment. Advances in Chemical Physics, 2005, , 179-246.	0.3	3
128	Theoretical Exploration of Ultrafast Dynamics in Atomic Clusters:â€‰ Analysis and Control. Chemical Reviews, 2005, 105, 11-66.	47.7	110
129	Ultrafast excited state dynamics of the Na3F cluster: Quantum wave packet and classical trajectory calculations compared to experimental results. Journal of Chemical Physics, 2004, 121, 9906-9916.	3.0	12
130	Different approaches for the calculation of electronic excited states of nonstoichiometric alkali halide clusters: The example of Na3F. Journal of Chemical Physics, 2004, 121, 9898-9905.	3.0	11
131	Theoretical approach for simulation of femtosecond spectra: New strategies for optimal control of complex systems. International Journal of Quantum Chemistry, 2004, 99, 408-420.	2.0	3
132	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
133	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
134	Isomer-specific spectroscopy of metal clusters trapped in a matrix:Ag9. Physical Review A, 2004, 70, .	2.5	77
135	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
136	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
137	Oxygen Adsorption on Hydrated Gold Cluster Anions:â€‰ Experiment and Theory. Journal of the American Chemical Society, 2003, 125, 8408-8414.	13.7	100
138	Theoretical and Experimental Consideration of the Reactions between VxOy+ and Ethylene. Journal of the American Chemical Society, 2003, 125, 6289-6299.	13.7	182
139	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
140	Observation and Theoretical Description of Periodic Geometric Rearrangement in Electronically Excited Nonstoichiometric Sodium-Fluoride Clusters. Physical Review Letters, 2002, 89, 213404.	7.8	20
141	Vibrational structure in the optical response of small Li-cluster ions. Journal of Chemical Physics, 2002, 117, 3711-3714.	3.0	9
142	New Strategy for Optimal Control of Femtosecond Pumpâ^'Dump Processes. Journal of Physical Chemistry A, 2002, 106, 10477-10481.	2.5	34
143	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
144	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

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145	Theoretical exploration of ultrafast spectroscopy of small clusters. European Physical Journal D, 2001, 16, 133-138.	1.3	2
146	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
147	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
148	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
149	Ab initio three-dimensional quantum dynamics of Ag3 clusters in the NeNePo process. Chemical Physics Letters, 2000, 318, 256-262.	2.6	20
150	Theoretical exploration of stationary and of ultrafast spectroscopy of small clusters. Applied Physics B: Lasers and Optics, 2000, 71, 343-349.	2.2	1
151	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
152	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
153	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
154	Structural and optical properties of small oxygen-doped- and pure-silver clusters. European Physical Journal D, 1999, 9, 183-187.	1.3	22
155	Theoretical study of femtosecond pumpâ€“probe signals of nonstoichiometric alkali halide clusters. European Physical Journal D, 1999, 9, 393-397.	1.3	10
156	The electronic structure and magnetic properties of the nickel tetramer and its partially carbonylated forms. European Physical Journal D, 1999, 9, 467-473.	1.3	1
157	Title is missing!. European Physical Journal D, 1998, 48, 637-658.	0.4	4
158	Theoretical exploration of femtosecond multi-state nuclear dynamics of small clusters. Journal of Chemical Physics, 1998, 108, 3096-3113.	3.0	67
159	Ultrafast Dynamics of Small Clusters on the Time Scale of Nuclear Motion. Journal of Physical Chemistry A, 1998, 102, 4069-4074.	2.5	30
160	Ab initio Molecular Dynamics for Determination of Structures of Alkali Metal Clusters and Their Temperatures Behavior; An Example of Li9+. Collection of Czechoslovak Chemical Communications, 1998, 63, 1431-1446.	1.0	0
161	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
162	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

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163	AbÂ–initio molecular dynamics based on nonÂ–local density functional procedure with Gaussian basis; study of structural and temperature behaviour of metallic clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1997, 40, 486-489.	1.0	8
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