Roland Mitric

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/4760926/publications.pdf

Version: 2024-02-01

183 papers	5,821 citations	61945 43 h-index	91828 69 g-index
191 all docs	191 docs citations	191 times ranked	4301 citing authors

#	Article	IF	Citations
1	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.	1.2	305
2	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.	6.6	198
3	Ab initio study of the absorption spectra of Ag[sub n] (n=5â€“8) clusters. Journal of Chemical Physics, 2001, 115, 10450.	1.2	196
4	Theoretical and Experimental Consideration of the Reactions between VxOy+ and Ethylene. Journal of the American Chemical Society, 2003, 125, 6289-6299.	6.6	182
5	Clusters as model systems for investigating nanoscale oxidation catalysis. Chemical Physics Letters, 2009, 475, 1-9.	1.2	160
6	Influence of Charge State on the Mechanism of CO Oxidation on Gold Clusters. Journal of the American Chemical Society, 2008, 130, 1694-1698.	6.6	147
7	Nonadiabatic dynamics within the time dependent density functional theory: Ultrafast photodynamics in pyrazine. Chemical Physics, 2008, 349, 319-324.	0.9	137
8	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.	6.6	135
9	Non-adiabatic dynamics of pyrrole: Dependence of deactivation mechanisms on the excitation energy. Chemical Physics, 2010, 375, 26-34.	0.9	124
10	Stoichiometric Zirconium Oxide Cations as Potential Building Blocks for Cluster Assembled Catalysts. Journal of the American Chemical Society, 2008, 130, 13912-13920.	6.6	120
11	The mechanism of excimer formation: an experimental and theoretical study on the pyrene dimer. Physical Chemistry Chemical Physics, 2017, 19, 25002-25015.	1.3	119
12	Theoretical Exploration of Ultrafast Dynamics in Atomic Clusters:â€‰ Analysis and Control. Chemical Reviews, 2005, 105, 11-66.	23.0	110
13	Cooperative Effects in the Activation of Molecular Oxygen by Anionic Silver Clusters. Journal of the American Chemical Society, 2004, 126, 3442-3443.	6.6	105
14	Oxygen Adsorption on Hydrated Gold Cluster Anions:â€‰ Experiment and Theory. Journal of the American Chemical Society, 2003, 125, 8408-8414.	6.6	100
15	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.	1.2	100
16	Laser-field-induced surface-hopping method for the simulation and control of ultrafast photodynamics. Physical Review A, 2009, 79, .	1.0	99
17	Nonadiabatic Dynamics within Time-Dependent Density Functional Tight Binding Method. Journal of Physical Chemistry A, 2009, 113, 12700-12705.	1.1	88
18	Synthesis, characterization and optical properties of low nuclearity liganded silver clusters: Ag31(SG)19 and Ag15(SG)11. Nanoscale, 2013, 5, 5637.	2.8	83

#	Article	IF	Citations
19	Isomer-specific spectroscopy of metal clusters trapped in a matrix:Ag9. Physical Review A, 2004, 70, .	1.0	77
20	Ultrafast photodynamics of furan. Journal of Chemical Physics, 2010, 133, 234303.	1.2	69
21	Generation of Oxygen Radical Centers in Binary Neutral Metal Oxide Clusters for Catalytic Oxidation Reactions. Angewandte Chemie - International Edition, 2010, 49, 407-410.	7.2	68
22	The origin of the solvent dependence of fluorescence quantum yields in dipolar merocyanine dyes. Chemical Science, 2019, 10, 11013-11022.	3.7	67
23	Isolation of diborenes and their 90Â°-twisted diradical congeners. Nature Communications, 2018, 9, 1197.	5.8	62
24	Time-resolved photoelectron imaging spectra from non-adiabatic molecular dynamics simulations. Journal of Chemical Physics, 2013, 139, 134104.	1.2	59
25	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.	6.6	57
26	How Shaped Light Discriminates Nearly Identical Biochromophores. Physical Review Letters, 2010, 105, 073003.	2.9	57
27	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.	1.2	55
28	Kinetic Analysis of the Reaction between (V2O5)n=1,2+ and Ethylene. Journal of Physical Chemistry B, 2006, 110, 3015-3022.	1.2	54
29	Simulation of laser-induced coupled electron-nuclear dynamics and time-resolved harmonic spectra in complex systems. Physical Review A, 2011, 83, .	1.0	54
30	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.	1.2	53
31	Time-Resolved Femtosecond Photoelectron Spectroscopy by Field-Induced Surface Hopping. Journal of Physical Chemistry A, 2011, 115, 3755-3765.	1.1	52
32	DFTBaby: A software package for non-adiabatic molecular dynamics simulations based on long-range corrected tight-binding TD-DFT(B). Computer Physics Communications, 2017, 221, 174-202.	3.0	52
33	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.	1.1	51
34	Silver clusterâ€“biomolecule hybrids: from basics towards sensors. Physical Chemistry Chemical Physics, 2012, 14, 9282.	1.3	51
35	Long-range correction for tight-binding TD-DFT. Journal of Chemical Physics, 2015, 143, 134120.	1.2	51
36	Absorption Enhancement and Conformational Control of Peptides by Small Silver Clusters. Physical Review Letters, 2008, 101, 213001.	2.9	50

#	Article	IF	Citations
37	Energy Transfer Between Squaraine Polymer Sections: From Helix to Zigzag and All the Way Back. Journal of the American Chemical Society, 2015, 137, 7851-7861.	6.6	50
38	Time- and Angle-Resolved Photoemission Spectroscopy of Hydrated Electrons Near a Liquid Water Surface. Physical Review Letters, 2014, 112, 187603.	2.9	49
39	Exciton Dynamics from Strong to Weak Coupling Limit Illustrated on a Series of Squaraine Dimers. Journal of Physical Chemistry C, 2018, 122, 8082-8093.	1.5	49
40	Optimal Control of Ionization Processes in NaK:â€‰ Comparison between Theory and Experiment. Journal of Physical Chemistry A, 2004, 108, 4175-4179.	1.1	48
41	Simulation of time resolved photoelectron spectra with Stieltjes imaging illustrated on ultrafast internal conversion in pyrazine. Journal of Chemical Physics, 2010, 132, 174301.	1.2	48
42	2<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>p</mml:mi></mml:math>core-level binding energies of size-selected free silicon clusters: Chemical shifts and cluster structure. Physical Review B, 2012, 85, .	1.1	46
43	Structural properties and reactivity of bimetallic silver-gold clusters. European Physical Journal D, 2003, 24, 41-44.	0.6	44
44	Site-dependence of van der Waals interaction explains exciton spectra of double-walled tubular J-aggregates. Physical Chemistry Chemical Physics, 2015, 17, 6741-6747.	1.3	41
45	Ab initio nonadiabatic dynamics study of ultrafast radiationless decay over conical intersections illustrated on the Na3F cluster. Journal of Chemical Physics, 2006, 125, 024303.	1.2	40
46	Cooperative water oxidation catalysis in a series of trinuclear metallosupramolecular ruthenium macrocycles. Energy and Environmental Science, 2017, 10, 2137-2153.	15.6	40
47	Reactivity of stoichiometric titanium oxide cations. Physical Chemistry Chemical Physics, 2011, 13, 4243.	1.3	39
48	Tuning Cluster Reactivity by Charge State and Composition: Experimental and Theoretical Investigation of CO Binding Energies to Ag_nAu_m^{+/â^’} (n +) Tj ETQq0 1 0 rgBT /Overlock 1	0.1	39
49	Doubly Charged Silver Clusters Stabilized by Tryptophan: Ag₄²⁺ as an Optical Marker for Monitoring Particle Growth. Angewandte Chemie - International Edition, 2011, 50, 878-881.	7.2	38
50	Size and shape dependent photoluminescence and excited state decay rates of diamondoids. Physical Chemistry Chemical Physics, 2014, 16, 3070-3076.	1.3	35
51	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.	1.2	35
52	New Strategy for Optimal Control of Femtosecond Pumpâ^’Dump Processes. Journal of Physical Chemistry A, 2002, 106, 10477-10481.	1.1	34
53	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.	1.2	34
54	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.	1.5	34

#	Article	IF	Citations
55	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.	1.5	34
56	Femtosecond Time-Resolved Geometry Relaxation and Ultrafast Intramolecular Energy Redistribution in Ag2Au. ChemPhysChem, 2005, 6, 243-253.	1.0	33
57	Photoabsorption and photofragmentation of isolated cationic silver clusterâ€“tryptophan hybrid systems. Journal of Chemical Physics, 2007, 127, 134301.	1.2	31
58	Experimental and theoretical study of the absorption properties of thiolated diamondoids. Journal of Chemical Physics, 2010, 132, 144305.	1.2	31
59	Solvation Dynamics of a Single Water Molecule Probed by Infrared Spectraâ€”Theory Meets Experiment. Angewandte Chemie - International Edition, 2014, 53, 14601-14604.	7.2	31
60	Optical Properties of Gas-Phase Tryptophan-Silver Cations: Charge Transfer from the Indole Ring to the Silver Atom. ChemPhysChem, 2006, 7, 524-528.	1.0	29
61	Optical and Structural Properties of Copperâ"Oxytocin Dications in the Gas Phase. Journal of Physical Chemistry B, 2009, 113, 11293-11300.	1.2	29
62	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.	1.3	28
63	Field-induced surface hopping method for probing transition state nonadiabatic dynamics of Ag3. Physical Chemistry Chemical Physics, 2011, 13, 8690.	1.3	28
64	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.	1.3	28
65	Probing ultrafast dynamics during and after passing through conical intersections. Physical Chemistry Chemical Physics, 2019, 21, 13902-13905.	1.3	28
66	Ultrafast Resonance Energy Transfer in Ethylene-Bridged BODIPY Heterooligomers: From Frenkel to FÃ¶rster Coupling Limit. Journal of the American Chemical Society, 2021, 143, 7414-7425.	6.6	28
67	Size-dependent dynamics in excited states of gold clusters: From oscillatory motion to photoinduced melting. Journal of Chemical Physics, 2007, 127, 164312.	1.2	27
68	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.	1.3	26
69	Electronic coherence within the semiclassical field-induced surface hopping method: strong field quantum control in K2. Physical Chemistry Chemical Physics, 2012, 14, 8299.	1.3	26
70	Supramolecular Approaches to Improve the Performance of Rutheniumâ€Based Water Oxidation Catalysts. Advanced Energy Materials, 2017, 7, 1602939.	10.2	26
71	Structural and Photochemical Properties of Organosilver Reactive Intermediates MeAg₂⁺and PhAg₂⁺. Journal of Physical Chemistry A, 2011, 115, 9120-9127.	1.1	24
72	Laser pulse trains for controlling excited state dynamics of adenine in water. Physical Chemistry Chemical Physics, 2012, 14, 4687.	1.3	23

#	Article	IF	Citations
73	Dynamics of Isolated 1,8-Naphthalimide and N-Methyl-1,8-naphthalimide: An Experimental and Computational Study. Journal of Physical Chemistry A, 2016, 120, 2089-2095.	1.1	23
74	Exciton localization in excited-state dynamics of a tetracene trimer: a surface hopping LC-TDDFTB study. Physical Chemistry Chemical Physics, 2018, 20, 25995-26007.	1.3	23
75	$$ {m{V}}_2 {m{O}}_5^ + $$ reaction with C 2 H 4 : theoretical considerations of experimental findings. European Physical Journal D, 2003, 24, 331-334.	0.6	20
76	Reactivity of anionic gold oxide clusters towards CO: experiment and theory. European Physical Journal D, 2007, 43, 205-208.	0.6	20
77	Gasâ€Phase Synthesis and Intense Visible Absorption of Tryptophanâ€“Gold Cations. Angewandte Chemie - International Edition, 2009, 48, 7829-7832.	7.2	20
78	Laser-induced fluorescence of free diamondoid molecules. Physical Chemistry Chemical Physics, 2015, 17, 4739-4749.	1.3	20
79	Single water solvation dynamics in the 4-aminobenzonitrileâ€“water cluster cation revealed by picosecond time-resolved infrared spectroscopy. Physical Chemistry Chemical Physics, 2015, 17, 29969-29977.	1.3	20
80	Ultrafast Ring-Opening Reaction of 1,3-Cyclohexadiene: Identification of Nonadiabatic Pathway via Doubly Excited State. Journal of the American Chemical Society, 2021, 143, 8034-8045.	6.6	20
81	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.	3.3	19
82	Gas-Phase Synthesis and Vibronic Action Spectroscopy of Ag2H+. Journal of Physical Chemistry Letters, 2011, 2, 548-552.	2.1	19
83	Diborene: Generation and Photoelectron Spectroscopy of an Inorganic Biradical. Journal of Physical Chemistry Letters, 2018, 9, 5921-5925.	2.1	19
84	metaFALCON: A Program Package for Automatic Sampling of Conical Intersection Seams Using Multistate Metadynamics. Journal of Chemical Theory and Computation, 2019, 15, 3450-3460.	2.3	19
85	Photodynamics of Free and Solvated Tyrosine. Journal of Physical Chemistry B, 2012, 116, 8762-8770.	1.2	18
86	Exploring Ultrafast Dynamics of Pyrazine by Time-Resolved Photoelectron Imaging. Journal of Physical Chemistry A, 2014, 118, 8437-8445.	1.1	18
87	Switching from molecular to bulklike dynamics in electronic relaxation of a small gold cluster. Physical Review A, 2012, 85, .	1.0	17
88	Davydov-type excitonic effects on the absorption spectra of parallel-stacked and herringbone aggregates of pentacene: Time-dependent density-functional theory and time-dependent density-functional tight binding. Journal of Chemical Physics, 2018, 149, 134111.	1.2	17
89	Synthesis and Spectroscopic Characterization of Diphenylargentate, [(C₆H₅)₂Ag]^{â^'}. Journal of Physical Chemistry Letters, 2012, 3, 1197-1201.	2.1	16
90	Nonlinear Absorption Dynamics Using Fieldâ€Induced Surface Hopping: Zinc Porphyrin in Water. ChemPhysChem, 2013, 14, 1377-1386.	1.0	16

#	Article	IF	Citations
91	The nature of electronic excitations at the metalâ€“bioorganic interface illustrated on histidineâ€“silver hybrids. Physical Chemistry Chemical Physics, 2014, 16, 1257-1261.	1.3	16
92	Vibrational spectra and DFT calculations of PPV-oligomers. Journal of Molecular Structure, 2003, 661-662, 33-40.	1.8	15
93	Optimal control of mode-selective femtochemistry in multidimensional systems. Physical Review A, 2007, 76, .	1.0	15
94	Mass-selected Ag3 clusters soft-landed onto MgO/Mo(100): femtosecond photoemission and first-principles simulations. European Physical Journal D, 2007, 45, 477-483.	0.6	15
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.	0.9	15
96	Impact of substituents on molecular properties and catalytic activities of trinuclear Ru macrocycles in water oxidation. Chemical Science, 2020, 11, 7654-7664.	3.7	15
97	Transforming Dyes into Fluorophores: Excitonâ€Induced Emission with Chainâ€like Oligoâ€BODIPY Superstructures. Angewandte Chemie - International Edition, 2022, 61, .	7.2	15
98	Excited states from quantum Monte Carlo in the basis of Slater determinants. Journal of Chemical Physics, 2014, 141, 194104.	1.2	14
99	Size Dependence of Non-Radiative Decay Rates in J-Aggregates. Journal of Physical Chemistry A, 2020, 124, 10143-10151.	1.1	14
100	Emissive properties of silver particles at silver oxide surface defects. Applied Physics A: Materials Science and Processing, 2006, 82, 117-123.	1.1	13
101	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.	3.3	13
102	Formation and characterization of thioglycolic acidâ€“silver cluster complexes. Dalton Transactions, 2013, 42, 8328.	1.6	13
103	Dynamic exciton localisation in a pyreneâ€“BODIPYâ€“pyrene dye conjugate. Physical Chemistry Chemical Physics, 2019, 21, 9013-9025.	1.3	13
104	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.	1.2	12
105	Electronic Structure Similarities in Pb_xSb_y^{â€“}and Sn_xBi_y^{â€“}Clusters. Journal of Physical Chemistry A, 2011, 115, 10276-10280.	1.1	12
106	BLUF Hydrogen network dynamics and UV/Vis spectra: A combined molecular dynamics and quantum chemical study. Journal of Computational Chemistry, 2012, 33, 2233-2242.	1.5	12
107	Photodissociation dynamics of propargylene, HCCCH. Physical Chemistry Chemical Physics, 2014, 16, 6294-6302.	1.3	12
108	Femtosecond dynamics of the 2-methylallyl radical: A computational and experimental study. Journal of Chemical Physics, 2017, 147, 013902.	1.2	12

#	Article	IF	Citations
109	Experimental and theoretical 2p core-level spectra of size-selected gas-phase aluminum and silicon cluster cations: chemical shifts, geometric structure, and coordination-dependent screening. Physical Chemistry Chemical Physics, 2019, 21, 6651-6661.	1.3	12
110	Excimer formation dynamics in the isolated tetracene dimer. Chemical Science, 2021, 12, 11965-11975.	3.7	12
111	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.	1.2	11
112	Silver Cluster Chromophores for Absorption Enhancement of Peptides. Journal of Physical Chemistry A, 2009, 113, 3783-3788.	1.1	11
113	Deciphering environment effects in peptide bond solvation dynamics by experiment and theory. Physical Chemistry Chemical Physics, 2017, 19, 22564-22572.	1.3	11
114	Exploring the Excited-State Dynamics of Hydrocarbon Radicals, Biradicals, and Carbenes Using Time-Resolved Photoelectron Spectroscopy and Field-Induced Surface Hopping Simulations. Journal of Physical Chemistry A, 2019, 123, 10643-10662.	1.1	11
115	Direct observation of o-benzyne formation in photochemical hexadehydro-Dielsâ€“Alder (hÎ½-HDDA) reactions. Chemical Science, 2020, 11, 9198-9208.	3.7	11
116	Optical properties of small silver clusters supported at MgO. European Physical Journal D, 2007, 45, 471-476.	0.6	10
117	Femtosecond time-resolved photoelectron spectroscopy of the benzyl radical. Physical Chemistry Chemical Physics, 2017, 19, 12365-12374.	1.3	10
118	Cluster properties in the regime in which each atom counts. Computational Materials Science, 2006, 35, 151-157.	1.4	9
119	Multistate Nonadiabatic Dynamics â€œon the Flyâ€•in Complex Systems and Its Control by Laser Fieldes. Advanced Series in Physical Chemistry, 2011, , 497-568.	1.5	9
120	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.	1.2	9
121	Transient absorption spectra of excitation energy transfer in supramolecular complexes: A mixed quantum-classical description of pheophorbide-a systems. Chemical Physics Letters, 2012, 522, 103-107.	1.2	9
122	Time-Resolved Study of 1,8-Naphthalic Anhydride and 1,4,5,8-Naphthalene-tetracarboxylic Dianhydride. Journal of Physical Chemistry A, 2015, 119, 6006-6016.	1.1	9
123	Multistate metadynamics for automatic exploration of conical intersections. Physical Review A, 2018, 97, .	1.0	9
124	The Optical Spectrum of Au 2 +. Angewandte Chemie - International Edition, 2020, 59, 21403-21408.	7.2	9
125	Excitation energy transport in DNA modelled by multi-chromophoric field-induced surface hopping. Physical Chemistry Chemical Physics, 2020, 22, 16536-16551.	1.3	9
126	Effect of varying the TD-lc-DFTB range-separation parameter on charge and energy transfer in a model pentacene/buckminsterfullerene heterojunction. Journal of Chemical Physics, 2021, 154, 054102.	1.2	9

#	Article	IF	Citations
127	The Gas-Phase Chemistry ofcis-Diammineplatinum(II) Complexes: A Joint Experimental and Theoretical Study. ChemPhysChem, 2006, 7, 1779-1785.	1.0	8
128	Unique optical properties of silver cluster-biochromophore hybrids: Comparison with copper and gold. Chemical Physics Letters, 2011, 501, 211-214.	1.2	8
129	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.	1.5	8
130	Ab initiosimulations of light propagation in silver cluster nanostructures. Physical Review B, 2014, 89, .	1.1	8
131	Photochemical Chiral Symmetry Breaking in Alanine. Journal of Physical Chemistry A, 2016, 120, 8976-8982.	1.1	8
132	Correlating Nanoscale Optical Coherence Length and Microscale Topography in Organic Materials by Coherent Two-Dimensional Microspectroscopy. Nano Letters, 2020, 20, 6452-6458.	4.5	8
133	Real-time observation of photoionization-induced water migration dynamics in 4-methylformanilideâ€“water by picosecond time-resolved infrared spectroscopy and ab initio molecular dynamics simulations. Physical Chemistry Chemical Physics, 2021, 24, 73-85.	1.3	8
134	Non-adiabatic dynamics around a conical intersection with surface-hopping coupled coherent states. Journal of Chemical Physics, 2016, 144, 234108.	1.2	7
135	Excitonic Properties of Ordered Metal Nanocluster Arrays: 2D Silver Clusters at Multiporphyrin Templates. Journal of Physical Chemistry A, 2016, 120, 4465-4472.	1.1	7
136	Vibrationally resolved optical spectra and ultrafast electronic relaxation dynamics of diamantane. Physical Chemistry Chemical Physics, 2016, 18, 8701-8709.	1.3	7
137	Excited state nonadiabatic dynamics of bare and hydrated anionic gold clusters Au₃^{â^’}[H₂O]_n (n = 0â€“2). Physical Chemistry Chemical Physics, 2016, 18, 6411-6419.	1.3	7
138	Optical absorption of isolated silver cluster-tryptophan: A joint experimental and theoretical study. European Physical Journal D, 2007, 43, 275-278.	0.6	6
139	Silver cluster induced absorption enhancement and conformation control of peptides. European Physical Journal D, 2009, 52, 203-206.	0.6	6
140	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.	0.7	6
141	Excited state dynamics and time-resolved photoelectron spectroscopy of para-xylylene. Faraday Discussions, 2018, 212, 83-100.	1.6	6
142	Electronic relaxation of aqueous aminoazobenzenes studied by time-resolved photoelectron spectroscopy and surface hopping TDDFT dynamics calculations. Faraday Discussions, 2021, 228, 226-241.	1.6	6
143	Solvent Induced Helix Folding of Defined Indolenine Squaraine Oligomers. Chemistry - A European Journal, 2021, 27, 8380-8389.	1.7	6
144	Photostabilization of the ultracold Rb2molecule by optimal control. Journal of Physics B: Atomic, Molecular and Optical Physics, 2006, 39, S1043-S1053.	0.6	5

#	Article	IF	Citations
145	Investigating Reactive Superoxide Units Bound to Zirconium Oxide Cations. Journal of Physical Chemistry C, 2011, 115, 21559-21566.	1.5	5
146	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.	1.3	5
147	Cation induced electrochromism in 2,4-dinitrophenylhydrazine (DNPH): Tuning optical properties of aromatic rings. Chemical Physics Letters, 2013, 570, 22-25.	1.2	5
148	Collective Response in DNA-Stabilized Silver Cluster Assemblies from First-Principles Simulations. Journal of Physical Chemistry Letters, 2019, 10, 7884-7889.	2.1	5
149	Do Xylylenes Isomerize in Pyrolysis?. ChemPhysChem, 2020, 21, 1515-1518.	1.0	5
150	(De)localization dynamics of molecular excitons: comparison of mixed quantum-classical and fully quantum treatments. Physical Chemistry Chemical Physics, 2022, 24, 12136-12148.	1.3	5
151	Tailoring the chemical reactivity and optical properties of clusters by size, structures and lasers. European Physical Journal D, 2005, 34, 113-118.	0.6	4
152	Exploring similarities in reactivity of superatom species: a combined theoretical and experimental investigation. Physical Chemistry Chemical Physics, 2012, 14, 1846.	1.3	4
153	Optimal control of light propagation and exciton transfer in arrays of molecular-like noble-metal clusters. Physical Review B, 2015, 91, .	1.1	4
154	Ultrafast Photodynamics of Glucose. Journal of Physical Chemistry B, 2018, 122, 19-27.	1.2	4
155	The Optical Spectrum of Au 2 +. Angewandte Chemie, 2020, 132, 21587-21592.	1.6	4
156	Ultrafast Energy Transfer Dynamics in a Squaraine Heterotriad. Journal of Physical Chemistry A, 2021, 125, 2504-2511.	1.1	4
157	Analysis and control of small isolated molecular systems. , 2007, , 25-152.		4
158	The Role of Molecular Arrangement on the Strongly Coupled Excitonâ€“Plasmon Polariton Dispersion in Metalâ€“Organic Hybrid Structures. Journal of Physical Chemistry C, 2022, 126, 4163-4171.	1.5	4
159	Transforming Dyes into Fluorophores: Excitonâ€Induced Emission with Chainâ€like Oligoâ€BODIPY Superstructures. Angewandte Chemie, 2022, 134, .	1.6	4
160	Theoretical approach for simulation of femtosecond spectra: New strategies for optimal control of complex systems. International Journal of Quantum Chemistry, 2004, 99, 408-420.	1.0	3
161	Analysis and Control of Ultrafast Dynamics in Clusters: Theory and Experiment. Advances in Chemical Physics, 2005, , 179-246.	0.3	3
162	Generation of Oxygen Radical Centers in Binary Neutral Metal Oxide Clusters for Catalytic Oxidation Reactions. Angewandte Chemie - International Edition, 2010, 49, 2272-2272.	7.2	3

#	Article	IF	Citations
163	Disentangling the photochemistry of benzocyclobutenedione. Physical Chemistry Chemical Physics, 2018, 20, 15434-15444.	1.3	3
164	Tetraiododiborane(4) (B₂I₄) is a Polymer Based on sp³ Boron in the Solid State. Angewandte Chemie - International Edition, 2020, 59, 5531-5535.	7.2	3
165	Isolated 2-hydroxypyrene and its dimer: a frequency- and time-resolved spectroscopic study. New Journal of Chemistry, 2021, 45, 14949-14956.	1.4	3
166	First-principles simulation of light propagation and exciton dynamics in metal cluster nanostructures. Applied Physics B: Lasers and Optics, 2016, 122, 1.	1.1	2
167	New strategy for optimal control of femtosecond pump-dump processes applicable to systems of moderate complexity. European Physical Journal D, 2003, 24, 177-180.	0.6	1
168	Kinetics and equilibrium of small metallic clusters: Ab initio confinement molecular dynamics study of 4. European Physical Journal D, 2003, 24, 45-48.	0.6	1
169	Theoretical Exploration of Ultrafast Dynamics in Atomic Clusters: Analysis and Control. ChemInform, 2005, 36, no.	0.1	1
170	Dynamical aspects and the role of IVR for the reactivity of noble metal clusters towards molecular oxygen. European Physical Journal D, 2007, 43, 201-204.	0.6	1
171	Ultrafast dynamics in noble metal clusters: The role of internal vibrational redistribution. Chemical Physics, 2008, 350, 111-117.	0.9	1
172	A block Jacobi method for complex skew-symmetric matrices with applications in the time-dependent variational principle. Computer Physics Communications, 2018, 231, 187-197.	3.0	1
173	Comparison of moving and fixed basis sets for nonadiabatic quantum dynamics at conical intersections. Chemical Physics, 2020, 528, 110526.	0.9	1
174	On the quantum and classical control of laser-driven isomerization in the Wigner representation. Journal of Chemical Physics, 2021, 154, 174103.	1.2	1
175	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
176	Femtosecond Time and Angle Resolved Photoemission Spectroscopy of Liquids. Springer Proceedings in Physics, 2015, , 305-308.	0.1	1
177	Complex systems in the gas phase. , 2007, , 153-256.		1
178	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
179	Modification of the secondary structure of angiotensin II by substitution of hydrogen with Cs cations: an experimental and theoretical study. Physical Chemistry Chemical Physics, 2012, 14, 9301.	1.3	0
180	Photo-oxidation by laser pulse induced desorption of phthalocyanines. International Journal of Mass Spectrometry, 2014, 365-366, 89-92.	0.7	0

#	Article	IF	Citations
181	Dibortetraiodid (B 2 I 4) ist im FestkÃ¶rper ein Polymer aus sp 3 â€hybridisiertem Bor. Angewandte Chemie, 2020, 132, 5574-5579.	1.6	0
182	Innentitelbild: The Optical Spectrum of Au₂⁺ (Angew. Chem. 48/2020). Angewandte Chemie, 2020, 132, 21434-21434.	1.6	0
183	Analysis and Control of Ultrafast Dynamics in Clusters. , 2006, , 466-478.		0