Roland Mitric

List of Publications by Year
in descending order

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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	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
2	Transforming Dyes into Fluorophores: Excitonâ€Induced Emission with Chainâ€like Oligoâ€BODIPY Superstructures. Angewandte Chemie, 2022, 134, .	1.6	4
3	Transforming Dyes into Fluorophores: Excitonâ€Induced Emission with Chainâ€like Oligoâ€BODIPY Superstructures. Angewandte Chemie - International Edition, 2022, 61, .	7.2	15
4	(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
5	Isolated 2-hydroxypyrene and its dimer: a frequency- and time-resolved spectroscopic study. New Journal of Chemistry, 2021, 45, 14949-14956.	1.4	3
6	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
7	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
8	Ultrafast Energy Transfer Dynamics in a Squaraine Heterotriad. Journal of Physical Chemistry A, 2021, 125, 2504-2511.	1.1	4
9	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
10	On the quantum and classical control of laser-driven isomerization in the Wigner representation. Journal of Chemical Physics, 2021, 154, 174103.	1.2	1
11	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
12	Solvent Induced Helix Folding of Defined Indolenine Squaraine Oligomers. Chemistry - A European Journal, 2021, 27, 8380-8389.	1.7	6
13	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
14	Excimer formation dynamics in the isolated tetracene dimer. Chemical Science, 2021, 12, 11965-11975.	3.7	12
15	Comparison of moving and fixed basis sets for nonadiabatic quantum dynamics at conical intersections. Chemical Physics, 2020, 528, 110526.	0.9	1
16	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
17	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
18	Size Dependence of Non-Radiative Decay Rates in J-Aggregates. Journal of Physical Chemistry A, 2020, 124, 10143-10151.	1.1	14

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19	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
20	The Optical Spectrum of Au 2 +. Angewandte Chemie - International Edition, 2020, 59, 21403-21408.	7.2	9
21	The Optical Spectrum of Au 2 +. Angewandte Chemie, 2020, 132, 21587-21592.	1.6	4
22	Innentitelbild: The Optical Spectrum of Au₂⁺ (Angew. Chem. 48/2020). Angewandte Chemie, 2020, 132, 21434-21434.	1.6	0
23	Do Xylylenes Isomerize in Pyrolysis?. ChemPhysChem, 2020, 21, 1515-1518.	1.0	5
24	Excitation energy transport in DNA modelled by multi-chromophoric field-induced surface hopping. Physical Chemistry Chemical Physics, 2020, 22, 16536-16551.	1.3	9
25	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
26	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
27	Direct observation of o-benzyne formation in photochemical hexadehydro-Dielsâ€“Alder (hÎ½-HDDA) reactions. Chemical Science, 2020, 11, 9198-9208.	3.7	11
28	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
29	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
30	Dynamic exciton localisation in a pyreneâ€“BODIPYâ€“pyrene dye conjugate. Physical Chemistry Chemical Physics, 2019, 21, 9013-9025.	1.3	13
31	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
32	Collective Response in DNA-Stabilized Silver Cluster Assemblies from First-Principles Simulations. Journal of Physical Chemistry Letters, 2019, 10, 7884-7889.	2.1	5
33	The origin of the solvent dependence of fluorescence quantum yields in dipolar merocyanine dyes. Chemical Science, 2019, 10, 11013-11022.	3.7	67
34	Probing ultrafast dynamics during and after passing through conical intersections. Physical Chemistry Chemical Physics, 2019, 21, 13902-13905.	1.3	28
35	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
36	Isolation of diborenes and their 90Â°-twisted diradical congeners. Nature Communications, 2018, 9, 1197.	5.8	62

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37	Ultrafast Photodynamics of Glucose. Journal of Physical Chemistry B, 2018, 122, 19-27.	1.2	4
38	Diborene: Generation and Photoelectron Spectroscopy of an Inorganic Biradical. Journal of Physical Chemistry Letters, 2018, 9, 5921-5925.	2.1	19
39	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
40	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
41	Disentangling the photochemistry of benzocyclobutenedione. Physical Chemistry Chemical Physics, 2018, 20, 15434-15444.	1.3	3
42	Excited state dynamics and time-resolved photoelectron spectroscopy of para-xylylene. Faraday Discussions, 2018, 212, 83-100.	1.6	6
43	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
44	Multistate metadynamics for automatic exploration of conical intersections. Physical Review A, 2018, 97, .	1.0	9
45	Femtosecond dynamics of the 2-methylallyl radical: A computational and experimental study. Journal of Chemical Physics, 2017, 147, 013902.	1.2	12
46	Femtosecond time-resolved photoelectron spectroscopy of the benzyl radical. Physical Chemistry Chemical Physics, 2017, 19, 12365-12374.	1.3	10
47	Supramolecular Approaches to Improve the Performance of Ruthenium‐Based Water Oxidation Catalysts. Advanced Energy Materials, 2017, 7, 1602939.	10.2	26
48	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
49	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
50	Deciphering environment effects in peptide bond solvation dynamics by experiment and theory. Physical Chemistry Chemical Physics, 2017, 19, 22564-22572.	1.3	11
51	Cooperative water oxidation catalysis in a series of trinuclear metallosupramolecular ruthenium macrocycles. Energy and Environmental Science, 2017, 10, 2137-2153.	15.6	40
52	Non-adiabatic dynamics around a conical intersection with surface-hopping coupled coherent states. Journal of Chemical Physics, 2016, 144, 234108.	1.2	7
53	Photochemical Chiral Symmetry Breaking in Alanine. Journal of Physical Chemistry A, 2016, 120, 8976-8982.	1.1	8
54	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

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55	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
56	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
57	Vibrationally resolved optical spectra and ultrafast electronic relaxation dynamics of diamantane. Physical Chemistry Chemical Physics, 2016, 18, 8701-8709.	1.3	7
58	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
59	Optimal control of light propagation and exciton transfer in arrays of molecular-like noble-metal clusters. Physical Review B, 2015, 91, .	1.1	4
60	Long-range correction for tight-binding TD-DFT. Journal of Chemical Physics, 2015, 143, 134120.	1.2	51
61	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
62	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
63	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
64	Laser-induced fluorescence of free diamondoid molecules. Physical Chemistry Chemical Physics, 2015, 17, 4739-4749.	1.3	20
65	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
66	Femtosecond Time and Angle Resolved Photoemission Spectroscopy of Liquids. Springer Proceedings in Physics, 2015, , 305-308.	0.1	1
67	Time- and Angle-Resolved Photoemission Spectroscopy of Hydrated Electrons Near a Liquid Water Surface. Physical Review Letters, 2014, 112, 187603.	2.9	49
68	Ab initiosimulations of light propagation in silver cluster nanostructures. Physical Review B, 2014, 89, .	1.1	8
69	Photodissociation dynamics of propargylene, HCCCH. Physical Chemistry Chemical Physics, 2014, 16, 6294-6302.	1.3	12
70	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
71	Exploring Ultrafast Dynamics of Pyrazine by Time-Resolved Photoelectron Imaging. Journal of Physical Chemistry A, 2014, 118, 8437-8445.	1.1	18
72	Photo-oxidation by laser pulse induced desorption of phthalocyanines. International Journal of Mass Spectrometry, 2014, 365-366, 89-92.	0.7	0

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73	Size and shape dependent photoluminescence and excited state decay rates of diamondoids. Physical Chemistry Chemical Physics, 2014, 16, 3070-3076.	1.3	35
74	Excited states from quantum Monte Carlo in the basis of Slater determinants. Journal of Chemical Physics, 2014, 141, 194104.	1.2	14
75	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
76	Cation induced electrochromism in 2,4-dinitrophenylhydrazine (DNPH): Tuning optical properties of aromatic rings. Chemical Physics Letters, 2013, 570, 22-25.	1.2	5
77	Formation and characterization of thioglycolic acidâ€"silver cluster complexes. Dalton Transactions, 2013, 42, 8328.	1.6	13
78	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
79	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
80	Time-resolved photoelectron imaging spectra from non-adiabatic molecular dynamics simulations. Journal of Chemical Physics, 2013, 139, 134104.	1.2	59
81	Nonlinear Absorption Dynamics Using Fieldâ€Induced Surface Hopping: Zinc Porphyrin in Water. ChemPhysChem, 2013, 14, 1377-1386.	1.0	16
82	Switching from molecular to bulklike dynamics in electronic relaxation of a small gold cluster. Physical Review A, 2012, 85, .	1.0	17
83	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
84	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
85	Silver clusterâ€"biomolecule hybrids: from basics towards sensors. Physical Chemistry Chemical Physics, 2012, 14, 9282.	1.3	51
86	Exploring similarities in reactivity of superatom species: a combined theoretical and experimental investigation. Physical Chemistry Chemical Physics, 2012, 14, 1846.	1.3	4
87	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
88	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
89	Laser pulse trains for controlling excited state dynamics of adenine in water. Physical Chemistry Chemical Physics, 2012, 14, 4687.	1.3	23
90	Synthesis and Spectroscopic Characterization of Diphenylargentate, [(C₆H₅)₂Ag]^{â^'}. Journal of Physical Chemistry Letters, 2012, 3, 1197-1201.	2.1	16

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91	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
92	Photodynamics of Free and Solvated Tyrosine. Journal of Physical Chemistry B, 2012, 116, 8762-8770.	1.2	18
93	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
94	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
95	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
96	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
97	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
98	Reactivity of stoichiometric titanium oxide cations. Physical Chemistry Chemical Physics, 2011, 13, 4243.	1.3	39
99	Field-induced surface hopping method for probing transition state nonadiabatic dynamics of Ag3. Physical Chemistry Chemical Physics, 2011, 13, 8690.	1.3	28
100	Investigating Reactive Superoxide Units Bound to Zirconium Oxide Cations. Journal of Physical Chemistry C, 2011, 115, 21559-21566.	1.5	5
101	Structural and Photochemical Properties of Organosilver Reactive Intermediates MeAg₂⁺and PhAg₂⁺. Journal of Physical Chemistry A, 2011, 115, 9120-9127.	1.1	24
102	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
103	Time-Resolved Femtosecond Photoelectron Spectroscopy by Field-Induced Surface Hopping. Journal of Physical Chemistry A, 2011, 115, 3755-3765.	1.1	52
104	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
105	Gas-Phase Synthesis and Vibronic Action Spectroscopy of Ag2H+. Journal of Physical Chemistry Letters, 2011, 2, 548-552.	2.1	19
106	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	8
107	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
108	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

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109	Unique optical properties of silver cluster-biochromophore hybrids: Comparison with copper and gold. Chemical Physics Letters, 2011, 501, 211-214.	1.2	8
110	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
111	Simulation of laser-induced coupled electron-nuclear dynamics and time-resolved harmonic spectra in complex systems. Physical Review A, 2011, 83, .	1.0	54
112	Non-adiabatic dynamics of pyrrole: Dependence of deactivation mechanisms on the excitation energy. Chemical Physics, 2010, 375, 26-34.	0.9	124
113	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
114	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
115	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
116	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
117	How Shaped Light Discriminates Nearly Identical Biochromophores. Physical Review Letters, 2010, 105, 073003.	2.9	57
118	Ultrafast photodynamics of furan. Journal of Chemical Physics, 2010, 133, 234303.	1.2	69
119	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
120	Experimental and theoretical study of the absorption properties of thiolated diamondoids. Journal of Chemical Physics, 2010, 132, 144305.	1.2	31
121	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
122	Silver Cluster Chromophores for Absorption Enhancement of Peptides. Journal of Physical Chemistry A, 2009, 113, 3783-3788.	1.1	11
123	Gasâ€Phase Synthesis and Intense Visible Absorption of Tryptophanâ€“Gold Cations. Angewandte Chemie - International Edition, 2009, 48, 7829-7832.	7.2	20
124	Clusters as model systems for investigating nanoscale oxidation catalysis. Chemical Physics Letters, 2009, 475, 1-9.	1.2	160
125	Silver cluster induced absorption enhancement and conformation control of peptides. European Physical Journal D, 2009, 52, 203-206.	0.6	6
126	Optical and Structural Properties of Copperâ^'Oxytocin Dications in the Gas Phase. Journal of Physical Chemistry B, 2009, 113, 11293-11300.	1.2	29

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127	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
128	Nonadiabatic Dynamics within Time-Dependent Density Functional Tight Binding Method. Journal of Physical Chemistry A, 2009, 113, 12700-12705.	1.1	88
129	Laser-field-induced surface-hopping method for the simulation and control of ultrafast photodynamics. Physical Review A, 2009, 79, .	1.0	99
130	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
131	Ultrafast dynamics in noble metal clusters: The role of internal vibrational redistribution. Chemical Physics, 2008, 350, 111-117.	0.9	1
132	Nonadiabatic dynamics within the time dependent density functional theory: Ultrafast photodynamics in pyrazine. Chemical Physics, 2008, 349, 319-324.	0.9	137
133	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
134	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
135	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
136	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
137	Absorption Enhancement and Conformational Control of Peptides by Small Silver Clusters. Physical Review Letters, 2008, 101, 213001.	2.9	50
138	Optimal control of mode-selective femtochemistry in multidimensional systems. Physical Review A, 2007, 76, .	1.0	15
139	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
140	Photoabsorption and photofragmentation of isolated cationic silver clusterâ€“tryptophan hybrid systems. Journal of Chemical Physics, 2007, 127, 134301.	1.2	31
141	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
142	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
143	Optical absorption of isolated silver cluster-tryptophan: A joint experimental and theoretical study. European Physical Journal D, 2007, 43, 275-278.	0.6	6
144	Reactivity of anionic gold oxide clusters towards CO: experiment and theory. European Physical Journal D, 2007, 43, 205-208.	0.6	20

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145	Optical properties of small silver clusters supported at MgO. European Physical Journal D, 2007, 45, 471-476.	0.6	10
146	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
147	Analysis and control of small isolated molecular systems. , 2007, , 25-152.		4
148	Complex systems in the gas phase. , 2007, , 153-256.		1
149	Kinetic Analysis of the Reaction between (V2O5)n=1,2+ and Ethylene. Journal of Physical Chemistry B, 2006, 110, 3015-3022.	1.2	54
150	Cluster properties in the regime in which each atom counts. Computational Materials Science, 2006, 35, 151-157.	1.4	9
151	Emissive properties of silver particles at silver oxide surface defects. Applied Physics A: Materials Science and Processing, 2006, 82, 117-123.	1.1	13
152	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
153	The Gas-Phase Chemistry ofcis-Diammineplatinum(II) Complexes: A Joint Experimental and Theoretical Study. ChemPhysChem, 2006, 7, 1779-1785.	1.0	8
154	Photostabilization of the ultracold Rb2molecule by optimal control. Journal of Physics B: Atomic, Molecular and Optical Physics, 2006, 39, S1043-S1053.	0.6	5
155	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
156	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
157	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
158	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
159	Analysis and Control of Ultrafast Dynamics in Clusters. , 2006, , 466-478.		0
160	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
161	Femtosecond Time-Resolved Geometry Relaxation and Ultrafast Intramolecular Energy Redistribution in Ag2Au. ChemPhysChem, 2005, 6, 243-253.	1.0	33
162	Theoretical Exploration of Ultrafast Dynamics in Atomic Clusters: Analysis and Control. ChemInform, 2005, 36, no.	0.1	1

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163	Analysis and Control of Ultrafast Dynamics in Clusters: Theory and Experiment. Advances in Chemical Physics, 2005, , 179-246.	0.3	3
164	Theoretical Exploration of Ultrafast Dynamics in Atomic Clusters:â€‰ Analysis and Control. Chemical Reviews, 2005, 105, 11-66.	23.0	110
165	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
166	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
167	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
168	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
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