Roland Mitric

List of Publications by Year in Descending Order

181 papers	5,131 citations	41 h-index	64 g-index
191 ext. papers	5,495 ext. citations	5.6 avg, IF	5.59 L-index

#	Paper	IF	Citations
181	The Role of Molecular Arrangement on the Strongly Coupled Exciton-Plasmon Polariton Dispersion in Metal-Organic Hybrid Structures. *Journal of Physical Chemistry C*, **2022**, 126, 4163-4171	3.8	1
180	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	16.4	6
179	On the quantum and classical control of laser-driven isomerization in the Wigner representation. *Journal of Chemical Physics*, **2021**, 154, 174103	3.9	0
178	Ultrafast Resonance Energy Transfer in Ethylene-Bridged BODIPY Heterooligomers: From Frenkel to Förster Coupling Limit. *Journal of the American Chemical Society*, **2021**, 143, 7414-7425	16.4	12
177	Solvent Induced Helix Folding of Defined Indolenine Squaraine Oligomers. *Chemistry - A European Journal*, **2021**, 27, 8380-8389	4.8	2
176	Isolated 2-hydroxypyrene and its dimer: a frequency- and time-resolved spectroscopic study. *New Journal of Chemistry*, **2021**, 45, 14949-14956	3.6	1
175	Electronic relaxation of aqueous aminoazobenzenes studied by time-resolved photoelectron spectroscopy and surface hopping TDDFT dynamics calculations. *Faraday Discussions*, **2021**, 228, 226-241	3.6	3
174	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	3.9	5
173	Ultrafast Energy Transfer Dynamics in a Squaraine Heterotriad. *Journal of Physical Chemistry A*, **2021**, 125, 2504-2511	2.8	2
172	Excimer formation dynamics in the isolated tetracene dimer. *Chemical Science*, **2021**, 12, 11965-11975	9.4	4
171	Innentitelbild: The Optical Spectrum of Au2+ (Angew. Chem. 48/2020). *Angewandte Chemie*, **2020**, 132, 21434-21434	3.6	
170	Do Xylylenes Isomerize in Pyrolysis?. *ChemPhysChem*, **2020**, 21, 1515-1518	3.2	3
169	Excitation energy transport in DNA modelled by multi-chromophoric field-induced surface hopping. *Physical Chemistry Chemical Physics*, **2020**, 22, 16536-16551	3.6	5
168	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	3.9	18
167	Impact of substituents on molecular properties and catalytic activities of trinuclear Ru macrocycles in water oxidation. *Chemical Science*, **2020**, 11, 7654-7664	9.4	9
166	Direct observation of -benzyne formation in photochemical hexadehydro-Diels-Alder (-HDDA) reactions. *Chemical Science*, **2020**, 11, 9198-9208	9.4	6
165	Dibortetraiodid (B2I4) ist im Festkörper ein Polymer aus sp3-hybridisiertem Bor. *Angewandte Chemie*, **2020**, 132, 5574-5579	3.6	

164	Tetraiododiborane(4) (B I) is a Polymer Based on sp Boron in the Solid State. *Angewandte Chemie - International Edition*, **2020**, 59, 5531-5535	16.4	1
163	Size Dependence of Non-Radiative Decay Rates in J-Aggregates. *Journal of Physical Chemistry A*, **2020**, 124, 10143-10151	2.8	8
162	Correlating Nanoscale Optical Coherence Length and Microscale Topography in Organic Materials by Coherent Two-Dimensional Microspectroscopy. *Nano Letters*, **2020**, 20, 6452-6458	11.5	4
161	The Optical Spectrum of Au. *Angewandte Chemie - International Edition*, **2020**, 59, 21403-21408	16.4	6
160	The Optical Spectrum of Au2+. *Angewandte Chemie*, **2020**, 132, 21587-21592	3.6	2
159	Comparison of moving and fixed basis sets for nonadiabatic quantum dynamics at conical intersections. *Chemical Physics*, **2020**, 528, 110526	2.3	1
158	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	2.8	7
157	metaFALCON: A Program Package for Automatic Sampling of Conical Intersection Seams Using Multistate Metadynamics. *Journal of Chemical Theory and Computation*, **2019**, 15, 3450-3460	6.4	14
156	Dynamic exciton localisation in a pyrene-BODIPY-pyrene dye conjugate. *Physical Chemistry Chemical Physics*, **2019**, 21, 9013-9025	3.6	7
155	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	3.6	6
154	Collective Response in DNA-Stabilized Silver Cluster Assemblies from First-Principles Simulations. *Journal of Physical Chemistry Letters*, **2019**, 10, 7884-7889	6.4	3
153	The origin of the solvent dependence of fluorescence quantum yields in dipolar merocyanine dyes. *Chemical Science*, **2019**, 10, 11013-11022	9.4	34
152	Probing ultrafast dynamics during and after passing through conical intersections. *Physical Chemistry Chemical Physics*, **2019**, 21, 13902-13905	3.6	19
151	Exciton Dynamics from Strong to Weak Coupling Limit Illustrated on a Series of Squaraine Dimers. *Journal of Physical Chemistry C*, **2018**, 122, 8082-8093	3.8	33
150	Isolation of diborenes and their 90°-twisted diradical congeners. *Nature Communications*, **2018**, 9, 1197	17.4	41
149	Excited state dynamics and time-resolved photoelectron spectroscopy of para-xylylene. *Faraday Discussions*, **2018**, 212, 83-100	3.6	6
148	A block Jacobi method for complex skew-symmetric matrices with applications in the time-dependent variational principle. *Computer Physics Communications*, **2018**, 231, 187-197	4.2	1
147	Multistate metadynamics for automatic exploration of conical intersections. *Physical Review A*, **2018**, 97,	2.6	6

146	Ultrafast Photodynamics of Glucose. *Journal of Physical Chemistry B*, **2018**, 122, 19-27	3.4	2
145	Diborene: Generation and Photoelectron Spectroscopy of an Inorganic Biradical. *Journal of Physical Chemistry Letters*, **2018**, 9, 5921-5925	6.4	12
144	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	3.9	11
143	Exciton localization in excited-state dynamics of a tetracene trimer: a surface hopping LC-TDDFTB study. *Physical Chemistry Chemical Physics*, **2018**, 20, 25995-26007	3.6	15
142	Disentangling the photochemistry of benzocyclobutenedione. *Physical Chemistry Chemical Physics*, **2018**, 20, 15434-15444	3.6	3
141	Femtosecond dynamics of the 2-methylallyl radical: A computational and experimental study. *Journal of Chemical Physics*, **2017**, 147, 013902	3.9	9
140	Femtosecond time-resolved photoelectron spectroscopy of the benzyl radical. *Physical Chemistry Chemical Physics*, **2017**, 19, 12365-12374	3.6	7
139	The mechanism of excimer formation: an experimental and theoretical study on the pyrene dimer. *Physical Chemistry Chemical Physics*, **2017**, 19, 25002-25015	3.6	76
138	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	4.2	41
137	Deciphering environment effects in peptide bond solvation dynamics by experiment and theory. *Physical Chemistry Chemical Physics*, **2017**, 19, 22564-22572	3.6	8
136	Cooperative water oxidation catalysis in a series of trinuclear metallosupramolecular ruthenium macrocycles. *Energy and Environmental Science*, **2017**, 10, 2137-2153	35.4	27
135	Excited state nonadiabatic dynamics of bare and hydrated anionic gold clusters Au3(-)[H2O]n (n = 0-2). *Physical Chemistry Chemical Physics*, **2016**, 18, 6411-9	3.6	7
134	Photochemical Chiral Symmetry Breaking in Alanine. *Journal of Physical Chemistry A*, **2016**, 120, 8976-8982	2.8	4
133	First-principles simulation of light propagation and exciton dynamics in metal cluster nanostructures. *Applied Physics B: Lasers and Optics*, **2016**, 122, 1	1.9	2
132	Excitonic Properties of Ordered Metal Nanocluster Arrays: 2D Silver Clusters at Multiporphyrin Templates. *Journal of Physical Chemistry A*, **2016**, 120, 4465-72	2.8	5
131	Dynamics of Isolated 1,8-Naphthalimide and N-Methyl-1,8-naphthalimide: An Experimental and Computational Study. *Journal of Physical Chemistry A*, **2016**, 120, 2089-95	2.8	17
130	Vibrationally resolved optical spectra and ultrafast electronic relaxation dynamics of diamantane. *Physical Chemistry Chemical Physics*, **2016**, 18, 8701-9	3.6	5
129	Non-adiabatic dynamics around a conical intersection with surface-hopping coupled coherent states. *Journal of Chemical Physics*, **2016**, 144, 234108	3.9	5

128	Laser-induced fluorescence of free diamondoid molecules. *Physical Chemistry Chemical Physics*, **2015**, 17, 4739-49	3.6	15
127	Single water solvation dynamics in the 4-aminobenzonitrile-water cluster cation revealed by picosecond time-resolved infrared spectroscopy. *Physical Chemistry Chemical Physics*, **2015**, 17, 29969-77	3.6	16
126	Optimal control of light propagation and exciton transfer in arrays of molecular-like noble-metal clusters. *Physical Review B*, **2015**, 91,	3.3	3
125	Long-range correction for tight-binding TD-DFT. *Journal of Chemical Physics*, **2015**, 143, 134120	3.9	43
124	Energy Transfer Between Squaraine Polymer Sections: From Helix to Zigzag and All the Way Back. *Journal of the American Chemical Society*, **2015**, 137, 7851-61	16.4	41
123	Time-Resolved Study of 1,8-Naphthalic Anhydride and 1,4,5,8-Naphthalene-tetracarboxylic Dianhydride. *Journal of Physical Chemistry A*, **2015**, 119, 6006-16	2.8	8
122	Site-dependence of van der Waals interaction explains exciton spectra of double-walled tubular J-aggregates. *Physical Chemistry Chemical Physics*, **2015**, 17, 6741-7	3.6	36
121	Femtosecond Time and Angle Resolved Photoemission Spectroscopy of Liquids. *Springer Proceedings in Physics*, **2015**, 305-308	0.2	1
120	Photodissociation dynamics of propargylene, HCCCH. *Physical Chemistry Chemical Physics*, **2014**, 16, 6294-302	3.6	11
119	The nature of electronic excitations at the metal-bioorganic interface illustrated on histidine-silver hybrids. *Physical Chemistry Chemical Physics*, **2014**, 16, 1257-61	3.6	15
118	Exploring ultrafast dynamics of pyrazine by time-resolved photoelectron imaging. *Journal of Physical Chemistry A*, **2014**, 118, 8437-45	2.8	16
117	Photo-oxidation by laser pulse induced desorption of phthalocyanines. *International Journal of Mass Spectrometry*, **2014**, 365-366, 89-92	1.9	
116	Size and shape dependent photoluminescence and excited state decay rates of diamondoids. *Physical Chemistry Chemical Physics*, **2014**, 16, 3070-6	3.6	27
115	Excited states from quantum Monte Carlo in the basis of Slater determinants. *Journal of Chemical Physics*, **2014**, 141, 194104	3.9	13
114	Solvation dynamics of a single water molecule probed by infrared spectra--theory meets experiment. *Angewandte Chemie - International Edition*, **2014**, 53, 14601-4	16.4	27
113	Aufklärung der Solvatationsdynamik eines einzelnen Wassermoleküls durch Infrarotspektroskopie: Theorie und Experiment. *Angewandte Chemie*, **2014**, 126, 14830-14834	3.6	
112	Time- and angle-resolved photoemission spectroscopy of hydrated electrons near a liquid water surface. *Physical Review Letters*, **2014**, 112, 187603	7.4	44
111	Ab initio simulations of light propagation in silver cluster nanostructures. *Physical Review B*, **2014**, 89,	3.3	7

110	Cation induced electrochromism in 2,4-dinitrophenylhydrazine (DNPH): Tuning optical properties of aromatic rings. *Chemical Physics Letters*, **2013**, 570, 22-25	2.5	4
109	Formation and characterization of thioglycolic acid-silver cluster complexes. *Dalton Transactions*, **2013**, 42, 8328-33	4.3	13
108	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	3.8	32
107	Synthesis, characterization and optical properties of low nuclearity liganded silver clusters: Ag31(SG)19 and Ag15(SG)11. *Nanoscale*, **2013**, 5, 5637-43	7.7	77
106	Time-resolved photoelectron imaging spectra from non-adiabatic molecular dynamics simulations. *Journal of Chemical Physics*, **2013**, 139, 134104	3.9	51
105	Nonlinear absorption dynamics using field-induced surface hopping: zinc porphyrin in water. *ChemPhysChem*, **2013**, 14, 1377-86	3.2	14
104	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	2.5	9
103	Theoretical study of structural and optical properties of noble metal cluster-dipeptide hybrids at defect centers of MgO. *Physical Chemistry Chemical Physics*, **2012**, 14, 9330-5	3.6	5
102	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, 11433-40	3.6	27
101	Silver cluster-biomolecule hybrids: from basics towards sensors. *Physical Chemistry Chemical Physics* , **2012**, 14, 9282-90	3.6	48
100	Exploring similarities in reactivity of superatom species: a combined theoretical and experimental investigation. *Physical Chemistry Chemical Physics*, **2012**, 14, 1846-9	3.6	4
99	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, 9301-5	3.6	
98	Electronic coherence within the semiclassical field-induced surface hopping method: strong field quantum control in K2. *Physical Chemistry Chemical Physics*, **2012**, 14, 8299-306	3.6	26
97	Laser pulse trains for controlling excited state dynamics of adenine in water. *Physical Chemistry Chemical Physics*, **2012**, 14, 4687-94	3.6	22
96	Synthesis and Spectroscopic Characterization of Diphenylargentate, [(C6H5)2Ag](.). *Journal of Physical Chemistry Letters*, **2012**, 3, 1197-201	6.4	15
95	Speciation of copper-peptide complexes in water solution using DFTB and DFT approaches: case of the [Cu(HGGG)(Py)] complex. *Journal of Physical Chemistry B*, **2012**, 116, 6250-60	3.4	9
94	Photodynamics of free and solvated tyrosine. *Journal of Physical Chemistry B*, **2012**, 116, 8762-70	3.4	17
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	3.8	8

92	BLUF hydrogen network dynamics and UV/Vis spectra: a combined molecular dynamics and quantum chemical study. *Journal of Computational Chemistry*, **2012**, 33, 2233-42	3.5	11
91	2p core-level binding energies of size-selected free silicon clusters: Chemical shifts and cluster structure. *Physical Review B*, **2012**, 85,	3.3	44
90	Switching from molecular to bulklike dynamics in electronic relaxation of a small gold cluster. *Physical Review A*, **2012**, 85,	2.6	17
89	Theoretical Methods for Nonadiabatic Dynamics on the fly in Complex Systems and its Control by Laser Fields. *Progress in Theoretical Chemistry and Physics*, **2012**, 299-325	0.6	
88	Multistate Nonadiabatic Dynamics on the Fly in Complex Systems and Its Control by Laser Fieldes. *Advanced Series in Physical Chemistry*, **2011**, 497-568		7
87	Gas-Phase Synthesis and Vibronic Action Spectroscopy of Ag2H+. *Journal of Physical Chemistry Letters*, **2011**, 2, 548-552	6.4	19
86	Tuning cluster reactivity by charge state and composition: experimental and theoretical investigation of CO binding energies to Ag(n)Au(m)(+/-) (n + m = 3). *Journal of Physical Chemistry A*, **2011**, 115, 951-9	2.8	37
85	Structural and Optical Properties of Isolated Noble Metal Glutathione Complexes: Insight into the Chemistry of Liganded Nanoclusters. *Journal of Physical Chemistry C*, **2011**, 115, 24549-24554	3.8	30
84	Doubly charged silver clusters stabilized by tryptophan: Ag4(2+) as an optical marker for monitoring particle growth. *Angewandte Chemie - International Edition*, **2011**, 50, 878-81	16.4	33
83	Doubly Charged Silver Clusters Stabilized by Tryptophan: Ag42+ as an Optical Marker for Monitoring Particle Growth. *Angewandte Chemie*, **2011**, 123, 908-911	3.6	2
82	Reactivity of stoichiometric titanium oxide cations. *Physical Chemistry Chemical Physics*, **2011**, 13, 4243-9	3.6	38
81	Field-induced surface hopping method for probing transition state nonadiabatic dynamics of Ag3. *Physical Chemistry Chemical Physics*, **2011**, 13, 8690-6	3.6	27
80	Investigating Reactive Superoxide Units Bound to Zirconium Oxide Cations. *Journal of Physical Chemistry C*, **2011**, 115, 21559-21566	3.8	5
79	Structural and photochemical properties of organosilver reactive intermediates MeAg2(+) and PhAg2(+). *Journal of Physical Chemistry A*, **2011**, 115, 9120-7	2.8	23
78	Electronic structure similarities in Pb(x)Sb(y)(-) and Sn(x)Bi(y)(-) clusters. *Journal of Physical Chemistry A*, **2011**, 115, 10276-80	2.8	11
77	Time-resolved femtosecond photoelectron spectroscopy by field-induced surface hopping. *Journal of Physical Chemistry A*, **2011**, 115, 3755-65	2.8	51
76	Unique optical properties of silver cluster-biochromophore hybrids: Comparison with copper and gold. *Chemical Physics Letters*, **2011**, 501, 211-214	2.5	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	3.9	49

74	Simulation of laser-induced coupled electron-nuclear dynamics and time-resolved harmonic spectra in complex systems. *Physical Review A*, **2011**, 83,	2.6	48
73	Simulation of time resolved photoelectron spectra with Stieltjes imaging illustrated on ultrafast internal conversion in pyrazine. *Journal of Chemical Physics*, **2010**, 132, 174301	3.9	44
72	How shaped light discriminates nearly identical biochromophores. *Physical Review Letters*, **2010**, 105, 073003	7.4	54
71	Ultrafast photodynamics of furan. *Journal of Chemical Physics*, **2010**, 133, 234303	3.9	60
70	Composition dependent adsorption of multiple CO molecules on binary silver-gold clusters Ag(n)Au(m)+ (n + m = 5): theory and experiment. *Physical Chemistry Chemical Physics*, **2010**, 12, 7865-73	3.6	27
69	Experimental and theoretical study of the absorption properties of thiolated diamondoids. *Journal of Chemical Physics*, **2010**, 132, 144305	3.9	29
68	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		
67	Non-adiabatic dynamics of pyrrole: Dependence of deactivation mechanisms on the excitation energy. *Chemical Physics*, **2010**, 375, 26-34	2.3	115
66	Generation of Oxygen Radical Centers in Binary Neutral Metal Oxide Clusters for Catalytic Oxidation Reactions. *Angewandte Chemie*, **2010**, 122, 417-420	3.6	25
65	Generation of oxygen radical centers in binary neutral metal oxide clusters for catalytic oxidation reactions. *Angewandte Chemie - International Edition*, **2010**, 49, 407-10	16.4	65
64	Generation of Oxygen Radical Centers in Binary Neutral Metal Oxide Clusters for Catalytic Oxidation Reactions. *Angewandte Chemie - International Edition*, **2010**, 49, 2272-2272	16.4	3
63	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, n/a-n/a	1.3	6
62	Silver cluster chromophores for absorption enhancement of peptides. *Journal of Physical Chemistry A*, **2009**, 113, 3783-8	2.8	11
61	Gas-Phase Synthesis and Intense Visible Absorption of Tryptophan□Gold Cations. *Angewandte Chemie*, **2009**, 121, 7969-7972	3.6	2
60	Gas-phase synthesis and intense visible absorption of tryptophan-gold cations. *Angewandte Chemie - International Edition*, **2009**, 48, 7829-32	16.4	19
59	Clusters as model systems for investigating nanoscale oxidation catalysis. *Chemical Physics Letters*, **2009**, 475, 1-9	2.5	151
58	Silver cluster induced absorption enhancement and conformation control of peptides. *European Physical Journal D*, **2009**, 52, 203-206	1.3	6
57	Optical and structural properties of copper-oxytocin dications in the gas phase. *Journal of Physical Chemistry B*, **2009**, 113, 11293-300	3.4	28

56	Influence of charge state on catalytic oxidation reactions at metal oxide clusters containing radical oxygen centers. *Journal of the American Chemical Society*, **2009**, 131, 5460-70	16.4	129
55	Nonadiabatic dynamics within time-dependent density functional tight binding method. *Journal of Physical Chemistry A*, **2009**, 113, 12700-5	2.8	79
54	Laser-field-induced surface-hopping method for the simulation and control of ultrafast photodynamics. *Physical Review A*, **2009**, 79,	2.6	90
53	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	3.9	92
52	A DFT study of EPR parameters in Cu(II) complexes of the octarepeat region of the prion protein. *Physical Chemistry Chemical Physics*, **2008**, 10, 4573-83	3.6	24
51	Influence of charge state on the mechanism of CO oxidation on gold clusters. *Journal of the American Chemical Society*, **2008**, 130, 1694-8	16.4	138
50	Stoichiometric zirconium oxide cations as potential building blocks for cluster assembled catalysts. *Journal of the American Chemical Society*, **2008**, 130, 13912-20	16.4	118
49	Absorption enhancement and conformational control of peptides by small silver clusters. *Physical Review Letters*, **2008**, 101, 213001	7.4	48
48	Absorption properties of cationic silver cluster–tryptophan complexes: A model for photoabsorption and photoemission enhancement in nanoparticle–biomolecule systems. *Chemical Physics*, **2008**, 343, 372-380	2.3	13
47	Ultrafast dynamics in noble metal clusters: The role of internal vibrational redistribution. *Chemical Physics*, **2008**, 350, 111-117	2.3	1
46	Nonadiabatic dynamics within the time dependent density functional theory: Ultrafast photodynamics in pyrazine. *Chemical Physics*, **2008**, 349, 319-324	2.3	127
45	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	1.3	1
44	Optical absorption of isolated silver cluster-tryptophan: A joint experimental and theoretical study. *European Physical Journal D*, **2007**, 43, 275-278	1.3	6
43	Reactivity of anionic gold oxide clusters towards CO: experiment and theory. *European Physical Journal D*, **2007**, 43, 205-208	1.3	19
42	Optical properties of small silver clusters supported at MgO. *European Physical Journal D*, **2007**, 45, 471-476	1.3	9
41	Mass-selected Ag3 clusters soft-landed onto MgO/Mo(100): femtosecond photoemission and first-principles simulations. *European Physical Journal D*, **2007**, 45, 477-483	1.3	13
40	Optimal control of mode-selective femtochemistry in multidimensional systems. *Physical Review A*, **2007**, 76,	2.6	14
39	Reactivity-promoting criterion based on internal vibrational energy redistribution. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 10314-7	11.5	19

38	Photoabsorption and photofragmentation of isolated cationic silver cluster-tryptophan hybrid systems. *Journal of Chemical Physics*, **2007**, 127, 134301	3.9	30
37	Size-dependent dynamics in excited states of gold clusters: from oscillatory motion to photoinduced melting. *Journal of Chemical Physics*, **2007**, 127, 164312	3.9	25
36	Complex systems in the gas phase **2007**, 153-256		1
35	Analysis and control of small isolated molecular systems **2007**, 25-152		3
34	Optical properties of gas-phase tryptophan-silver cations: charge transfer from the indole ring to the silver atom. *ChemPhysChem*, **2006**, 7, 524-8	3.2	29
33	The gas-phase chemistry of cis-diammineplatinum(II) complexes: a joint experimental and theoretical study. *ChemPhysChem*, **2006**, 7, 1779-85	3.2	8
32	Photostabilization of the ultracold Rb2molecule by optimal control. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2006**, 39, S1043-S1053	1.3	5
31	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	3.9	34
30	Joint experimental and theoretical investigations of the reactivity of Au2O-(n) and Au3O-(n) (n=1-5) with carbon monoxide. *Journal of Chemical Physics*, **2006**, 125, 204311	3.9	50
29	Ultrafast dynamics in atomic clusters: analysis and control. *Proceedings of the National Academy of Sciences of the United States of America*, **2006**, 103, 10594-9	11.5	11
28	Ab initio nonadiabatic dynamics study of ultrafast radiationless decay over conical intersections illustrated on the Na3F cluster. *Journal of Chemical Physics*, **2006**, 125, 24303	3.9	38
27	Kinetic analysis of the reaction between (V2O5)n=1,2+ and ethylene. *Journal of Physical Chemistry B* , **2006**, 110, 3015-22	3.4	54
26	Cluster properties in the regime in which each atom counts. *Computational Materials Science*, **2006**, 35, 151-157	3.2	8
25	Emissive properties of silver particles at silver oxide surface defects. *Applied Physics A: Materials Science and Processing*, **2006**, 82, 117-123	2.6	11
24	Analysis and Control of Ultrafast Dynamics in Clusters **2006**, 466-478		
23	Theoretical exploration of ultrafast dynamics in atomic clusters: analysis and control. *Chemical Reviews*, **2005**, 105, 11-66	68.1	93
22	Tailoring the chemical reactivity and optical properties of clusters by size, structures and lasers. *European Physical Journal D*, **2005**, 34, 113-118	1.3	4
21	Femtosecond time-resolved geometry relaxation and ultrafast intramolecular energy redistribution in Ag2Au. *ChemPhysChem*, **2005**, 6, 243-53	3.2	29

20	Analysis and Control of Ultrafast Dynamics in Clusters: Theory and Experiment. *Advances in Chemical Physics*, **2005**, 179-246		2
19	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, 9906-16	3.9	12
18	Different approaches for the calculation of electronic excited states of nonstoichiometric alkali halide clusters: the example of Na3F. *Journal of Chemical Physics*, **2004**, 121, 9898-905	3.9	11
17	Theoretical approach for simulation of femtosecond spectra: New strategies for optimal control of complex systems. *International Journal of Quantum Chemistry*, **2004**, 99, 408-420	2.1	3
16	Reactivity of atomic gold anions toward oxygen and the oxidation of CO: experiment and theory. *Journal of the American Chemical Society*, **2004**, 126, 2526-35	16.4	188
15	Optimal Control of Ionization Processes in NaK: Comparison between Theory and Experiment. *Journal of Physical Chemistry A*, **2004**, 108, 4175-4179	2.8	44
14	Isomer-specific spectroscopy of metal clusters trapped in a matrix: Ag9. *Physical Review A*, **2004**, 70,	2.6	74
13	Cooperative effects in the activation of molecular oxygen by anionic silver clusters. *Journal of the American Chemical Society*, **2004**, 126, 3442-3	16.4	92
12	The structures of vanadium oxide cluster-ethene complexes. A combined IR multiple photon dissociation spectroscopy and DFT calculation study. *Journal of the American Chemical Society*, **2003** , 125, 15716-7	16.4	57
11	New strategy for optimal control of femtosecond pump-dump processes applicable to systems of moderate complexity. *European Physical Journal D*, **2003**, 24, 177-180	1.3	1
10	({rm{V}}_2 {rm{O}}_5^ +) reaction with C2H4: theoretical considerations of experimental findings. *European Physical Journal D*, **2003**, 24, 331-334	1.3	19
9	Structural properties and reactivity of bimetallic silver-gold clusters. *European Physical Journal D*, **2003**, 24, 41-44	1.3	42
8	Kinetics and equilibrium of small metallic clusters: Ab initio confinement molecular dynamics study of 4. *European Physical Journal D*, **2003**, 24, 45-48	1.3	1
7	Vibrational spectra and DFT calculations of PPV-oligomers. *Journal of Molecular Structure*, **2003**, 661-662, 33-40	3.4	14
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