

# Roland Mitric

## List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Density functional study of structural and electronic properties of bimetallic silver-gold clusters: Comparison with pure gold and silver clusters. <i>Journal of Chemical Physics</i> , <b>2002</b> , 117, 3120-3131	3.9	289
180	Reactivity of atomic gold anions toward oxygen and the oxidation of CO: experiment and theory. <i>Journal of the American Chemical Society</i> , <b>2004</b> , 126, 2526-35	16.4	188
179	Ab initio study of the absorption spectra of Ag <sub>n</sub> (n=58) clusters. <i>Journal of Chemical Physics</i> , <b>2001</b> , 115, 10450	3.9	187
178	Theoretical and experimental consideration of the reactions between V <sub>x</sub> O <sub>y</sub> <sup>+</sup> and ethylene. <i>Journal of the American Chemical Society</i> , <b>2003</b> , 125, 6289-99	16.4	180
177	Clusters as model systems for investigating nanoscale oxidation catalysis. <i>Chemical Physics Letters</i> , <b>2009</b> , 475, 1-9	2.5	151
176	Influence of charge state on the mechanism of CO oxidation on gold clusters. <i>Journal of the American Chemical Society</i> , <b>2008</b> , 130, 1694-8	16.4	138
175	Influence of charge state on catalytic oxidation reactions at metal oxide clusters containing radical oxygen centers. <i>Journal of the American Chemical Society</i> , <b>2009</b> , 131, 5460-70	16.4	129
174	Nonadiabatic dynamics within the time dependent density functional theory: Ultrafast photodynamics in pyrazine. <i>Chemical Physics</i> , <b>2008</b> , 349, 319-324	2.3	127
173	Stoichiometric zirconium oxide cations as potential building blocks for cluster assembled catalysts. <i>Journal of the American Chemical Society</i> , <b>2008</b> , 130, 13912-20	16.4	118
172	Non-adiabatic dynamics of pyrrole: Dependence of deactivation mechanisms on the excitation energy. <i>Chemical Physics</i> , <b>2010</b> , 375, 26-34	2.3	115
171	Oxygen adsorption on hydrated gold cluster anions: experiment and theory. <i>Journal of the American Chemical Society</i> , <b>2003</b> , 125, 8408-14	16.4	94
170	Theoretical exploration of ultrafast dynamics in atomic clusters: analysis and control. <i>Chemical Reviews</i> , <b>2005</b> , 105, 11-66	68.1	93
169	Nonadiabatic dynamics and simulation of time resolved photoelectron spectra within time-dependent density functional theory: Ultrafast photoswitching in benzyldeneaniline. <i>Journal of Chemical Physics</i> , <b>2008</b> , 129, 164118	3.9	92
168	Cooperative effects in the activation of molecular oxygen by anionic silver clusters. <i>Journal of the American Chemical Society</i> , <b>2004</b> , 126, 3442-3	16.4	92
167	Laser-field-induced surface-hopping method for the simulation and control of ultrafast photodynamics. <i>Physical Review A</i> , <b>2009</b> , 79,	2.6	90
166	Nonadiabatic dynamics within time-dependent density functional tight binding method. <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 12700-5	2.8	79
165	Synthesis, characterization and optical properties of low nuclearity liganded silver clusters: Ag <sub>31</sub> (SG) <sub>19</sub> and Ag <sub>15</sub> (SG) <sub>11</sub> . <i>Nanoscale</i> , <b>2013</b> , 5, 5637-43	7.7	77

164	The mechanism of excimer formation: an experimental and theoretical study on the pyrene dimer. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 25002-25015	3.6	76
163	Isomer-specific spectroscopy of metal clusters trapped in a matrix: Ag <sub>9</sub> . <i>Physical Review A</i> , <b>2004</b> , 70,	2.6	74
162	Generation of oxygen radical centers in binary neutral metal oxide clusters for catalytic oxidation reactions. <i>Angewandte Chemie - International Edition</i> , <b>2010</b> , 49, 407-10	16.4	65
161	Ultrafast photodynamics of furan. <i>Journal of Chemical Physics</i> , <b>2010</b> , 133, 234303	3.9	60
160	The structures of vanadium oxide cluster-ethene complexes. A combined IR multiple photon dissociation spectroscopy and DFT calculation study. <i>Journal of the American Chemical Society</i> , <b>2003</b> , 125, 15716-7	16.4	57
159	How shaped light discriminates nearly identical biochromophores. <i>Physical Review Letters</i> , <b>2010</b> , 105, 073003	7.4	54
158	Kinetic analysis of the reaction between (V <sub>2</sub> O <sub>5</sub> ) <sub>n=1,2+</sub> and ethylene. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 3015-22	3.4	54
157	Time-resolved photoelectron imaging spectra from non-adiabatic molecular dynamics simulations. <i>Journal of Chemical Physics</i> , <b>2013</b> , 139, 134104	3.9	51
156	Time-resolved femtosecond photoelectron spectroscopy by field-induced surface hopping. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 3755-65	2.8	51
155	Joint experimental and theoretical investigations of the reactivity of Au <sub>2</sub> O-(n) and Au <sub>3</sub> O-(n) (n=1-5) with carbon monoxide. <i>Journal of Chemical Physics</i> , <b>2006</b> , 125, 204311	3.9	50
154	Time-dependent density functional theory excited state nonadiabatic dynamics combined with quantum mechanical/molecular mechanical approach: photodynamics of indole in water. <i>Journal of Chemical Physics</i> , <b>2011</b> , 135, 054105	3.9	49
153	Silver cluster-biomolecule hybrids: from basics towards sensors. <i>Physical Chemistry Chemical Physics</i> , <b>2012</b> , 14, 9282-90	3.6	48
152	Simulation of laser-induced coupled electron-nuclear dynamics and time-resolved harmonic spectra in complex systems. <i>Physical Review A</i> , <b>2011</b> , 83,	2.6	48
151	Absorption enhancement and conformational control of peptides by small silver clusters. <i>Physical Review Letters</i> , <b>2008</b> , 101, 213001	7.4	48
150	Ab Initio Adiabatic Dynamics Combined with Wigner Distribution Approach to Femtosecond Pump-Probe Negative Ion to Neutral to Positive Ion (NeNePo) Spectroscopy of Ag <sub>2</sub> Au, Ag <sub>4</sub> , and Au <sub>4</sub> Clusters. <i>Journal of Physical Chemistry A</i> , <b>2001</b> , 105, 8892-8905	2.8	48
149	Time- and angle-resolved photoemission spectroscopy of hydrated electrons near a liquid water surface. <i>Physical Review Letters</i> , <b>2014</b> , 112, 187603	7.4	44
148	2p core-level binding energies of size-selected free silicon clusters: Chemical shifts and cluster structure. <i>Physical Review B</i> , <b>2012</b> , 85,	3.3	44
147	Simulation of time resolved photoelectron spectra with Stieltjes imaging illustrated on ultrafast internal conversion in pyrazine. <i>Journal of Chemical Physics</i> , <b>2010</b> , 132, 174301	3.9	44

146	Optimal Control of Ionization Processes in NaK: Comparison between Theory and Experiment. <i>Journal of Physical Chemistry A</i> , <b>2004</b> , 108, 4175-4179	2.8	44
145	Long-range correction for tight-binding TD-DFT. <i>Journal of Chemical Physics</i> , <b>2015</b> , 143, 134120	3.9	43
144	Structural properties and reactivity of bimetallic silver-gold clusters. <i>European Physical Journal D</i> , <b>2003</b> , 24, 41-44	1.3	42
143	Isolation of diborenes and their 90°-twisted diradical congeners. <i>Nature Communications</i> , <b>2018</b> , 9, 1197	17.4	41
142	DFTBaby: A software package for non-adiabatic molecular dynamics simulations based on long-range corrected tight-binding TD-DFT(B). <i>Computer Physics Communications</i> , <b>2017</b> , 221, 174-202	4.2	41
141	Energy Transfer Between Squaraine Polymer Sections: From Helix to Zigzag and All the Way Back. <i>Journal of the American Chemical Society</i> , <b>2015</b> , 137, 7851-61	16.4	41
140	Reactivity of stoichiometric titanium oxide cations. <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 4243-93.6	3.6	38
139	Ab initio nonadiabatic dynamics study of ultrafast radiationless decay over conical intersections illustrated on the Na3F cluster. <i>Journal of Chemical Physics</i> , <b>2006</b> , 125, 24303	3.9	38
138	Tuning cluster reactivity by charge state and composition: experimental and theoretical investigation of CO binding energies to Ag(n)Au(m)(+/-) (n + m = 3). <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 951-9	2.8	37
137	Site-dependence of van der Waals interaction explains exciton spectra of double-walled tubular J-aggregates. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 6741-7	3.6	36
136	Spectroscopy of isolated, mass-selected tryptophan-Ag3 complexes: a model for photoabsorption enhancement in nanoparticle-biomolecule hybrid systems. <i>Journal of Chemical Physics</i> , <b>2006</b> , 125, 164326-9	3.9	34
135	The origin of the solvent dependence of fluorescence quantum yields in dipolar merocyanine dyes. <i>Chemical Science</i> , <b>2019</b> , 10, 11013-11022	9.4	34
134	Exciton Dynamics from Strong to Weak Coupling Limit Illustrated on a Series of Squaraine Dimers. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 8082-8093	3.8	33
133	Doubly charged silver clusters stabilized by tryptophan: Ag4(2+) as an optical marker for monitoring particle growth. <i>Angewandte Chemie - International Edition</i> , <b>2011</b> , 50, 878-81	16.4	33
132	New Strategy for Optimal Control of Femtosecond Pump-Dump Processes. <i>Journal of Physical Chemistry A</i> , <b>2002</b> , 106, 10477-10481	2.8	33
131	Tuning Structural and Optical Properties of Thiolate-Protected Silver Clusters by Formation of a Silver Core with Confined Electrons. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 14824-14831	3.8	32
130	Structural and Optical Properties of Isolated Noble Metal-Glutathione Complexes: Insight into the Chemistry of Liganded Nanoclusters. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 24549-24554	3.8	30
129	Photoabsorption and photofragmentation of isolated cationic silver cluster-tryptophan hybrid systems. <i>Journal of Chemical Physics</i> , <b>2007</b> , 127, 134301	3.9	30

128	Experimental and theoretical study of the absorption properties of thiolated diamondoids. <i>Journal of Chemical Physics</i> , <b>2010</b> , 132, 144305	3.9	29
127	Optical properties of gas-phase tryptophan-silver cations: charge transfer from the indole ring to the silver atom. <i>ChemPhysChem</i> , <b>2006</b> , 7, 524-8	3.2	29
126	Femtosecond time-resolved geometry relaxation and ultrafast intramolecular energy redistribution in Ag <sub>2</sub> Au. <i>ChemPhysChem</i> , <b>2005</b> , 6, 243-53	3.2	29
125	Optical and structural properties of copper-oxytocin dications in the gas phase. <i>Journal of Physical Chemistry B</i> , <b>2009</b> , 113, 11293-300	3.4	28
124	Size and shape dependent photoluminescence and excited state decay rates of diamondoids. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 3070-6	3.6	27
123	Solvation dynamics of a single water molecule probed by infrared spectra--theory meets experiment. <i>Angewandte Chemie - International Edition</i> , <b>2014</b> , 53, 14601-4	16.4	27
122	Binding motifs of silver in prion octarepeat model peptides: a joint ion mobility, IR and UV spectroscopies, and theoretical approach. <i>Physical Chemistry Chemical Physics</i> , <b>2012</b> , 14, 11433-40	3.6	27
121	Composition dependent adsorption of multiple CO molecules on binary silver-gold clusters Ag(n)Au(m)+ (n + m = 5): theory and experiment. <i>Physical Chemistry Chemical Physics</i> , <b>2010</b> , 12, 7865-73	3.6	27
120	Field-induced surface hopping method for probing transition state nonadiabatic dynamics of Ag <sub>3</sub> . <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 8690-6	3.6	27
119	Cooperative water oxidation catalysis in a series of trinuclear metallosupramolecular ruthenium macrocycles. <i>Energy and Environmental Science</i> , <b>2017</b> , 10, 2137-2153	35.4	27
118	Electronic coherence within the semiclassical field-induced surface hopping method: strong field quantum control in K <sub>2</sub> . <i>Physical Chemistry Chemical Physics</i> , <b>2012</b> , 14, 8299-306	3.6	26
117	Generation of Oxygen Radical Centers in Binary Neutral Metal Oxide Clusters for Catalytic Oxidation Reactions. <i>Angewandte Chemie</i> , <b>2010</b> , 122, 417-420	3.6	25
116	Size-dependent dynamics in excited states of gold clusters: from oscillatory motion to photoinduced melting. <i>Journal of Chemical Physics</i> , <b>2007</b> , 127, 164312	3.9	25
115	A DFT study of EPR parameters in Cu(II) complexes of the octarepeat region of the prion protein. <i>Physical Chemistry Chemical Physics</i> , <b>2008</b> , 10, 4573-83	3.6	24
114	Structural and photochemical properties of organosilver reactive intermediates MeAg <sub>2</sub> (+) and PhAg <sub>2</sub> (+). <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 9120-7	2.8	23
113	Laser pulse trains for controlling excited state dynamics of adenine in water. <i>Physical Chemistry Chemical Physics</i> , <b>2012</b> , 14, 4687-94	3.6	22
112	Gas-Phase Synthesis and Vibronic Action Spectroscopy of Ag <sub>2</sub> H <sup>+</sup> . <i>Journal of Physical Chemistry Letters</i> , <b>2011</b> , 2, 548-552	6.4	19
111	Gas-phase synthesis and intense visible absorption of tryptophan-gold cations. <i>Angewandte Chemie - International Edition</i> , <b>2009</b> , 48, 7829-32	16.4	19

110	Reactivity of anionic gold oxide clusters towards CO: experiment and theory. <i>European Physical Journal D</i> , <b>2007</b> , 43, 205-208	1.3	19
109	Reactivity-promoting criterion based on internal vibrational energy redistribution. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2007</b> , 104, 10314-7	11.5	19
108	( $\{V\}_2\{O\}_5^+$ ) reaction with C <sub>2</sub> H <sub>4</sub> : theoretical considerations of experimental findings. <i>European Physical Journal D</i> , <b>2003</b> , 24, 331-334	1.3	19
107	Probing ultrafast dynamics during and after passing through conical intersections. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 13902-13905	3.6	19
106	Predicting fluorescence quantum yields for molecules in solution: A critical assessment of the harmonic approximation and the choice of the lineshape function. <i>Journal of Chemical Physics</i> , <b>2020</b> , 152, 054107	3.9	18
105	Dynamics of Isolated 1,8-Naphthalimide and N-Methyl-1,8-naphthalimide: An Experimental and Computational Study. <i>Journal of Physical Chemistry A</i> , <b>2016</b> , 120, 2089-95	2.8	17
104	Photodynamics of free and solvated tyrosine. <i>Journal of Physical Chemistry B</i> , <b>2012</b> , 116, 8762-70	3.4	17
103	Switching from molecular to bulklike dynamics in electronic relaxation of a small gold cluster. <i>Physical Review A</i> , <b>2012</b> , 85,	2.6	17
102	Single water solvation dynamics in the 4-aminobenzonitrile-water cluster cation revealed by picosecond time-resolved infrared spectroscopy. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 29969-77	3.6	16
101	Exploring ultrafast dynamics of pyrazine by time-resolved photoelectron imaging. <i>Journal of Physical Chemistry A</i> , <b>2014</b> , 118, 8437-45	2.8	16
100	Laser-induced fluorescence of free diamondoid molecules. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 4739-49	3.6	15
99	The nature of electronic excitations at the metal-bioorganic interface illustrated on histidine-silver hybrids. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 1257-61	3.6	15
98	Synthesis and Spectroscopic Characterization of Diphenylargentate, [(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> Ag](.). <i>Journal of Physical Chemistry Letters</i> , <b>2012</b> , 3, 1197-201	6.4	15
97	Exciton localization in excited-state dynamics of a tetracene trimer: a surface hopping LC-TDDFTB study. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 25995-26007	3.6	15
96	metaFALCON: A Program Package for Automatic Sampling of Conical Intersection Seams Using Multistate Metadynamics. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 3450-3460	6.4	14
95	Nonlinear absorption dynamics using field-induced surface hopping: zinc porphyrin in water. <i>ChemPhysChem</i> , <b>2013</b> , 14, 1377-86	3.2	14
94	Optimal control of mode-selective femtochemistry in multidimensional systems. <i>Physical Review A</i> , <b>2007</b> , 76,	2.6	14
93	Vibrational spectra and DFT calculations of PPV-oligomers. <i>Journal of Molecular Structure</i> , <b>2003</b> , 661-662, 33-40	3.4	14



92	Excited states from quantum Monte Carlo in the basis of Slater determinants. <i>Journal of Chemical Physics</i> , <b>2014</b> , 141, 194104	3.9	13
91	Formation and characterization of thioglycolic acid-silver cluster complexes. <i>Dalton Transactions</i> , <b>2013</b> , 42, 8328-33	4.3	13
90	Mass-selected Ag <sub>3</sub> clusters soft-landed onto MgO/Mo(100): femtosecond photoemission and first-principles simulations. <i>European Physical Journal D</i> , <b>2007</b> , 45, 477-483	1.3	13
89	Absorption properties of cationic silver cluster-tryptophan complexes: A model for photoabsorption and photoemission enhancement in nanoparticle-biomolecule systems. <i>Chemical Physics</i> , <b>2008</b> , 343, 372-380	2.3	13
88	Ultrafast excited state dynamics of the Na <sub>3</sub> F cluster: quantum wave packet and classical trajectory calculations compared to experimental results. <i>Journal of Chemical Physics</i> , <b>2004</b> , 121, 9906-16	3.9	12
87	Ultrafast Resonance Energy Transfer in Ethylene-Bridged BODIPY Heterooligomers: From Frenkel to Förster Coupling Limit. <i>Journal of the American Chemical Society</i> , <b>2021</b> , 143, 7414-7425	16.4	12
86	Diborene: Generation and Photoelectron Spectroscopy of an Inorganic Biradical. <i>Journal of Physical Chemistry Letters</i> , <b>2018</b> , 9, 5921-5925	6.4	12
85	Photodissociation dynamics of propargylene, HCCCH. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 6294-302	5.302	11
84	BLUF hydrogen network dynamics and UV/Vis spectra: a combined molecular dynamics and quantum chemical study. <i>Journal of Computational Chemistry</i> , <b>2012</b> , 33, 2233-42	3.5	11
83	Electronic structure similarities in Pb(x)Sb(y)(-) and Sn(x)Bi(y)(-) clusters. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 10276-80	2.8	11
82	Silver cluster chromophores for absorption enhancement of peptides. <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 3783-8	2.8	11
81	Ultrafast dynamics in atomic clusters: analysis and control. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2006</b> , 103, 10594-9	11.5	11
80	Emissive properties of silver particles at silver oxide surface defects. <i>Applied Physics A: Materials Science and Processing</i> , <b>2006</b> , 82, 117-123	2.6	11
79	Different approaches for the calculation of electronic excited states of nonstoichiometric alkali halide clusters: the example of Na <sub>3</sub> F. <i>Journal of Chemical Physics</i> , <b>2004</b> , 121, 9898-905	3.9	11
78	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. <i>Journal of Chemical Physics</i> , <b>2018</b> , 149, 134111	3.9	11
77	Femtosecond dynamics of the 2-methylallyl radical: A computational and experimental study. <i>Journal of Chemical Physics</i> , <b>2017</b> , 147, 013902	3.9	9
76	Impact of substituents on molecular properties and catalytic activities of trinuclear Ru macrocycles in water oxidation. <i>Chemical Science</i> , <b>2020</b> , 11, 7654-7664	9.4	9
75	Transient absorption spectra of excitation energy transfer in supramolecular complexes: A mixed quantum-classical description of pheophorbide-a systems. <i>Chemical Physics Letters</i> , <b>2012</b> , 522, 103-107	2.5	9

74	Speciation of copper-peptide complexes in water solution using DFTB and DFT approaches: case of the [Cu(HGGG)(Py)] complex. <i>Journal of Physical Chemistry B</i> , <b>2012</b> , 116, 6250-60	3.4	9
73	Optical properties of small silver clusters supported at MgO. <i>European Physical Journal D</i> , <b>2007</b> , 45, 471-476	3.6	9
72	Deciphering environment effects in peptide bond solvation dynamics by experiment and theory. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 22564-22572	3.6	8
71	Time-Resolved Study of 1,8-Naphthalic Anhydride and 1,4,5,8-Naphthalene-tetracarboxylic Dianhydride. <i>Journal of Physical Chemistry A</i> , <b>2015</b> , 119, 6006-16	2.8	8
70	Binary Neutral Metal Oxide Clusters with Oxygen Radical Centers for Catalytic Oxidation Reactions: From Cluster Models Toward Surfaces. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 11570-11574	3.8	8
69	Unique optical properties of silver cluster-biochromophore hybrids: Comparison with copper and gold. <i>Chemical Physics Letters</i> , <b>2011</b> , 501, 211-214	2.5	8
68	The gas-phase chemistry of cis-diammineplatinum(II) complexes: a joint experimental and theoretical study. <i>ChemPhysChem</i> , <b>2006</b> , 7, 1779-85	3.2	8
67	Cluster properties in the regime in which each atom counts. <i>Computational Materials Science</i> , <b>2006</b> , 35, 151-157	3.2	8
66	Size Dependence of Non-Radiative Decay Rates in J-Aggregates. <i>Journal of Physical Chemistry A</i> , <b>2020</b> , 124, 10143-10151	2.8	8
65	Excited state nonadiabatic dynamics of bare and hydrated anionic gold clusters Au <sub>3</sub> (-)[H <sub>2</sub> O] <sub>n</sub> (n = 0-2). <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 6411-9	3.6	7
64	Femtosecond time-resolved photoelectron spectroscopy of the benzyl radical. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 12365-12374	3.6	7
63	Exploring the Excited-State Dynamics of Hydrocarbon Radicals, Biradicals, and Carbenes Using Time-Resolved Photoelectron Spectroscopy and Field-Induced Surface Hopping Simulations. <i>Journal of Physical Chemistry A</i> , <b>2019</b> , 123, 10643-10662	2.8	7
62	Dynamic exciton localisation in a pyrene-BODIPY-pyrene dye conjugate. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 9013-9025	3.6	7
61	Ab initio simulations of light propagation in silver cluster nanostructures. <i>Physical Review B</i> , <b>2014</b> , 89,	3.3	7
60	Multistate Nonadiabatic Dynamics on the Fly in Complex Systems and Its Control by Laser Fields. <i>Advanced Series in Physical Chemistry</i> , <b>2011</b> , 497-568		7
59	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. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 6651-6661	3.6	6
58	Excited state dynamics and time-resolved photoelectron spectroscopy of para-xylylene. <i>Faraday Discussions</i> , <b>2018</b> , 212, 83-100	3.6	6
57	Multistate metadynamics for automatic exploration of conical intersections. <i>Physical Review A</i> , <b>2018</b> , 97,	2.6	6



56	Silver cluster induced absorption enhancement and conformation control of peptides. <i>European Physical Journal D</i> , <b>2009</b> , 52, 203-206	1.3	6
55	Theoretical study of structural and optical properties of small silver and gold clusters at defect centers of MgO. <i>Physica Status Solidi (B): Basic Research</i> , <b>2010</b> , 247, n/a-n/a	1.3	6
54	Optical absorption of isolated silver cluster-tryptophan: A joint experimental and theoretical study. <i>European Physical Journal D</i> , <b>2007</b> , 43, 275-278	1.3	6
53	Direct observation of -benzyne formation in photochemical hexadehydro-Diels-Alder (-HDDA) reactions. <i>Chemical Science</i> , <b>2020</b> , 11, 9198-9208	9.4	6
52	The Optical Spectrum of Au. <i>Angewandte Chemie - International Edition</i> , <b>2020</b> , 59, 21403-21408	16.4	6
51	Ultrafast Ring-Opening Reaction of 1,3-Cyclohexadiene: Identification of Nonadiabatic Pathway via Doubly Excited State. <i>Journal of the American Chemical Society</i> , <b>2021</b> , 143, 8034-8045	16.4	6
50	Excitation energy transport in DNA modelled by multi-chromophoric field-induced surface hopping. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 16536-16551	3.6	5
49	Excitonic Properties of Ordered Metal Nanocluster Arrays: 2D Silver Clusters at Multiporphyrin Templates. <i>Journal of Physical Chemistry A</i> , <b>2016</b> , 120, 4465-72	2.8	5
48	Vibrationally resolved optical spectra and ultrafast electronic relaxation dynamics of diamantane. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 8701-9	3.6	5
47	Theoretical study of structural and optical properties of noble metal cluster-dipeptide hybrids at defect centers of MgO. <i>Physical Chemistry Chemical Physics</i> , <b>2012</b> , 14, 9330-5	3.6	5
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45	Photostabilization of the ultracold Rb <sub>2</sub> molecule by optimal control. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , <b>2006</b> , 39, S1043-S1053	1.3	5
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