Regina de Vivie-Riedle

List of Publications by Year
in descending order

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184	6,699	57758	74163
papers	citations	44 h-index	75 g-index

196	196	196	4235
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Whither the Future of Controlling Quantum Phenomena?. Science, 2000, 288, 824-828.	12.6	1,045
2	Quantum Computation with Vibrationally Excited Molecules. Physical Review Letters, 2002, 89, 157901.	7.8	277
3	Extensions to quantum optimal control algorithms and applications to special problems in state selective molecular dynamics. Journal of Chemical Physics, 1999, 110, 1896-1904.	3.0	163
4	Ultrafast Excited-State Proton Transfer of 2-(2â€˜-Hydroxyphenyl)benzothiazole: Theoretical Analysis of the Skeletal Deformations and the Active Vibrational Modesâ€. Journal of Physical Chemistry A, 2003, 107, 10591-10599.	2.5	154
5	Attosecond Control of Electron Dynamics in Carbon Monoxide. Physical Review Letters, 2009, 103, 103002.	7.8	151
6	Applying optimal control theory for elements of quantum computation in molecular systems. Chemical Physics Letters, 2001, 343, 633-641.	2.6	118
7	Theoretical spectroscopy of the NO radical. I. Potential curves and lifetimes of excited states. Journal of Chemical Physics, 1988, 89, 3028-3043.	3.0	116
8	Singlet Oxygen Reactivity with Carbonate Solvents Used for Li-Ion Battery Electrolytes. Journal of Physical Chemistry A, 2018, 122, 8828-8839.	2.5	114
9	Controlling molecular ground-state dissociation by optimizing vibrational ladder climbing. Journal of Chemical Physics, 2003, 118, 2021-2024.	3.0	107
10	Subcycle Controlled Charge-Directed Reactivity with Few-Cycle Midinfrared Pulses. Physical Review Letters, 2012, 108, 063002.	7.8	99
11	Vibrational molecular quantum computing: Basis set independence and theoretical realization of the Deutschâ€“Jozsa algorithm. Journal of Chemical Physics, 2004, 121, 12158.	3.0	98
12	The interplay of skeletal deformations and ultrafast excited-state intramolecular proton transfer: Experimental and theoretical investigation of 10-hydroxybenzo[h]quinoline. Chemical Physics, 2008, 347, 446-461.	1.9	91
13	Femtosecond Lasers for Quantum Information Technology. Chemical Reviews, 2007, 107, 5082-5100.	47.7	88
14	(Sub-)femtosecond control of molecular reactions via tailoring the electric field of light. Physical Chemistry Chemical Physics, 2013, 15, 9448.	2.8	86
15	Quantum dynamics of photoexcited cyclohexadiene introducing reactive coordinates. Journal of Chemical Physics, 2000, 112, 5054-5059.	3.0	82
16	Electroâ€mediated PhotoRedox Catalysis for Selective C(sp³)â€“O Cleavages of Phosphinated Alcohols to Carbanions. Angewandte Chemie - International Edition, 2021, 60, 20817-20825.	13.8	81
17	Making Fast Photoswitches Fasterâ€”Using Hammett Analysis to Understand the Limit of Donorâ€“Acceptor Approaches for Faster Hemithioindigo Photoswitches. Chemistry - A European Journal, 2014, 20, 13984-13992.	3.3	78
18	Subfemtosecond steering of hydrocarbon deprotonation through superposition of vibrational modes. Nature Communications, 2014, 5, 3800.	12.8	78

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19	Adiabatic approach for ultrafast quantum dynamics mediated by simultaneously active conical intersections. Chemical Physics Letters, 2001, 346, 299-304.	2.6	75
20	Complete Mechanism of Hemithioindigo Motor Rotation. Journal of the American Chemical Society, 2018, 140, 5311-5318.	13.7	75
21	Steering Proton Migration in Hydrocarbons Using Intense Few-Cycle Laser Fields. Physical Review Letters, 2016, 116, 193001.	7.8	74
22	Femtosecond Study of Multiphoton Ionization Processes in K2:Â From Pumpâ˜Probe to Control#. The Journal of Physical Chemistry, 1996, 100, 7789-7796.	2.9	72
23	Manganese pentacarbonyl bromide as candidate for a molecular qubit system operated in the infrared regime. Journal of Chemical Physics, 2005, 123, 244509.	3.0	67
24	Cavity Cooling of Internal Molecular Motion. Physical Review Letters, 2007, 99, 073001.	7.8	67
25	Monotonic Convergent Optimal Control Theory with Strict Limitations on the Spectrum of Optimized Laser Fields. Physical Review Letters, 2008, 101, 073002.	7.8	67
26	Mechanism of UVâ€Induced Formation of Dewar Lesions in DNA. Angewandte Chemie - International Edition, 2012, 51, 408-411.	13.8	67
27	Proximity-Induced H-Aggregation of Cyanine Dyes on DNA-Duplexes. Journal of Physical Chemistry A, 2016, 120, 9941-9947.	2.5	66
28	Electron dynamics in molecules: a new combination of nuclear quantum dynamics and electronic structure theory. Journal of Physics B: Atomic, Molecular and Optical Physics, 2008, 41, 074006.	1.5	64
29	Laser control schemes for molecular switches. Applied Physics B: Lasers and Optics, 2004, 79, 987-992.	2.2	63
30	Optimal control theory â€“ closing the gap between theory and experiment. Physical Chemistry Chemical Physics, 2012, 14, 14460.	2.8	63
31	Adapting optimal control theory and using learning loops to provide experimentally feasible shaping mask patterns. Journal of Chemical Physics, 2001, 115, 3105-3111.	3.0	62
32	Norbornenes in Inverse Electronâ€Demand Dielsâ€“Alder Reactions. Chemistry - A European Journal, 2013, 19, 13309-13312.	3.3	61
33	Molecular Driving Forces for Z/E Isomerization Mediated by Heteroatoms: The Example Hemithioindigo. Journal of Physical Chemistry A, 2010, 114, 13016-13030.	2.5	58
34	Preparation and addressability of molecular vibrational qubit states in the presence of anharmonic resonance. Chemical Physics Letters, 2003, 378, 273-280.	2.6	57
35	Quantum optimal control strategies for photoisomerization via electronically excited states. Chemical Physics Letters, 1998, 290, 415-422.	2.6	55
36	The role of anharmonicity and coupling in quantum computing based on vibrational qubits. New Journal of Physics, 2006, 8, 48-48.	2.9	54

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37	Beyond the van der Lugt/Oosterhoff Model: When the Conical Intersection Seam and the S₁Minimum Energy Path Do Not Cross. Journal of Organic Chemistry, 2010, 75, 123-129.	3.2	52
38	Adaptive strong-field control of chemical dynamics guided by three-dimensional momentum imaging. Nature Communications, 2013, 4, 2895.	12.8	51
39	Mechanisms of local and global molecular quantum gates and their implementation prospects. Journal of Chemical Physics, 2005, 122, 154105.	3.0	50
40	Femtosecond wave-packet propagation in spin-orbit-coupled electronic states ofK239,39andK239,41. Physical Review A, 1996, 54, 306-313.	2.5	49
41	Attosecond control of the dissociative ionization via electron localization: A comparison between and CO. Chemical Physics, 2009, 366, 139-147.	1.9	48
42	Photoprotecting Uracil by Coupling with Lossy Nanocavities. Journal of Physical Chemistry Letters, 2020, 11, 8810-8818.	4.6	47
43	Teaching optimal control theory to distill robust pulses even under experimental constraints. Physical Review A, 2002, 65, .	2.5	46
44	Effects of multi orbital contributions in the angular-dependent ionization of molecules in intense few-cycle laser pulses. Applied Physics B: Lasers and Optics, 2010, 98, 659-666.	2.2	46
45	Photochemical formation of intricarene. Nature Communications, 2014, 5, 5597.	12.8	44
46	Visualizing conical intersection passages via vibronic coherence maps generated by stimulated ultrafast X-ray Raman signals. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 24069-24075.	7.1	44
47	Coherent control of the molecular four-wave-mixing response by phase and amplitude shaped pulses. Chemical Physics, 2001, 267, 261-276.	1.9	43
48	Accelerated and Efficient Photochemistry from Higher Excited Electronic States in Fulgide Molecules. Journal of Physical Chemistry A, 2008, 112, 13364-13371.	2.5	41
49	Ground state normal mode analysis: Linking excited state dynamics and experimental observables. Journal of Chemical Physics, 2001, 114, 6151-6159.	3.0	38
50	The role of phases and their interplay in molecular vibrational quantum computing with multiple qubits. New Journal of Physics, 2006, 8, 100-100.	2.9	38
51	A molecular conveyor belt by controlled delivery of single molecules into ultrashort laser pulses. Nature Physics, 2012, 8, 238-242.	16.7	38
52	Photostability of 4,4â€²â€Dihydroxythioindigo, a Mimetic of Indigo. Angewandte Chemie - International Edition, 2014, 53, 591-594.	13.8	38
53	Monitoring conical intersections in the ring opening of furan by attosecond stimulated X-ray Raman spectroscopy. Structural Dynamics, 2016, 3, 023601.	2.3	38
54	Deactivation pathways of thiophene and oligothiophenes: internal conversion versus intersystem crossing. Physical Chemistry Chemical Physics, 2016, 18, 7903-7915.	2.8	38

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55	Waveform control of orientation-dependent ionization of DCl in few-cycle laser fields. Physical Chemistry Chemical Physics, 2011, 13, 8653.	2.8	37
56	The detailed balance limit of photochemical energy conversion. Physical Chemistry Chemical Physics, 2010, 12, 422-432.	2.8	36
57	Ab initio molecular dynamics of thiophene: the interplay of internal conversion and intersystem crossing. Physical Chemistry Chemical Physics, 2017, 19, 25662-25670.	2.8	36
58	Ultrafast molecular dynamics controlled by pulse duration: The Na3 molecule. Journal of Chemical Physics, 1996, 104, 8857-8864.	3.0	35
59	Optimal conversion of an atomic to a molecular Bose-Einstein condensate. Physical Review A, 2002, 66, .	2.5	35
60	Controlling Photorelaxation in Uracil with Shaped Laser Pulses: AÂTheoretical Assessment. Journal of the American Chemical Society, 2017, 139, 5061-5066.	13.7	35
61	Spin-forbidden transitions in the presence of an intersystem crossing: application to the b1Î£+ state in OH+. Chemical Physics, 1987, 112, 349-361.	1.9	34
62	Photoinduced Heterocyclic Ring Opening of Furfural: Distinct Open-Chain Product Identification by Ultrafast X-ray Transient Absorption Spectroscopy. Journal of the American Chemical Society, 2018, 140, 12538-12544.	13.7	34
63	Laser control strategies for energy transfer reactions in atom molecule collisions. Faraday Discussions, 1999, 113, 303-317.	3.2	33
64	Charge Oscillation Controlled Molecular Excitation. Physical Review Letters, 2013, 110, 123003.	7.8	33
65	Theoretical spectroscopy of the NO radical. III. Î› doubling and predissociation in the Câ€‰2Î state. Journal of Chemical Physics, 1990, 92, 3613-3618.	3.0	32
66	Theoretical optimization and prediction in the experimental search space for vibrational quantum processes. Physical Review A, 2008, 78, .	2.5	30
67	Theoretical spectroscopy of the NO radical. II. Î› doubling in the ground Xâ€‰2Î state and spinâ€“orbit effects in the excited Î states. Journal of Chemical Physics, 1989, 90, 3660-3670.	3.0	28
68	Control of a collision complex via a conical intersection. Journal of Chemical Physics, 2003, 119, 5901-5906.	3.0	28
69	Buildup and Decay of the Optical Absorption in the Ultrafast Photo-Generation and Reaction of Benzhydryl Cations in Solution. Journal of Physical Chemistry A, 2012, 116, 11064-11074.	2.5	27
70	Reaction velocity control by manipulating the momentum of a nuclear wavepacket with phase-sensitive optimal control theory. Chemical Physics Letters, 2005, 404, 289-295.	2.6	26
71	Nucleophilic Substitution Dynamics: Comparing Wave Packet Calculations with Experiment. Journal of Physical Chemistry A, 2014, 118, 4661-4669.	2.5	26
72	Visualization of bond rearrangements in acetylene using near single-cycle laser pulses. Faraday Discussions, 2016, 194, 495-508.	3.2	26

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73	Pathways to New Applications for Quantum Control. Accounts of Chemical Research, 2018, 51, 2279-2286.	15.6	26
74	ONIOM approach for non-adiabatic on-the-fly molecular dynamics demonstrated for the backbone controlled Dewar valence isomerization. Journal of Chemical Physics, 2012, 136, 204307.	3.0	25
75	Dynamics of ultraviolet-induced DNA lesions: Dewar formation guided by pre-tension induced by the backbone. New Journal of Physics, 2012, 14, 065006.	2.9	24
76	Modified ant-colony-optimization algorithm as an alternative to genetic algorithms. Physical Review A, 2009, 79, .	2.5	23
77	Chemoselective quantum control of carbonyl bonds in Grignard reactions using shaped laser pulses. Physical Chemistry Chemical Physics, 2010, 12, 15780.	2.8	22
78	Ionâ€Pairing of Phosphonium Salts in Solution: Cï£¿Hâ‹…â‹…â‹…Halogen and Cï£¿Hâ‹…â‹…â‹…Ï€ Hydrogen Bonds. Chemistry - A European Journal, 2013, 19, 14612-14630.	3.3	22
79	A Comprehensive Microscopic Picture of the Benzhydryl Radical and Cation Photogeneration and Interconversion through Electron Transfer. ChemPhysChem, 2013, 14, 1423-1437.	2.1	22
80	Compensating for spatial laser profile effects on the control of quantum systems. Physical Review A, 2000, 62, .	2.5	21
81	Design of optimal infrared femtosecond laser pulses for the overtone excitation in acetylene. Chemical Physics, 2001, 267, 173-185.	1.9	21
82	Control strategies for reactive processes involving vibrationally hot product states. Journal of Photochemistry and Photobiology A: Chemistry, 2006, 180, 282-288.	3.9	21
83	Electron Dynamics and Its Control in Molecules: From Diatomics to Larger Molecular Systems. IEEE Journal of Selected Topics in Quantum Electronics, 2012, 18, 119-129.	2.9	21
84	Design of specially adapted reactive coordinates to economically compute potential and kinetic energy operators including geometry relaxation. Journal of Chemical Physics, 2016, 144, 234104.	3.0	21
85	RNA Environment Is Responsible for Decreased Photostability of Uracil. Journal of the American Chemical Society, 2018, 140, 8714-8720.	13.7	21
86	From laser control of vibrationally mediated photodissociation to photodesorption: Model simulations of breaking metal-ligand bonds in organometallic molecules, clusters, and adsorbates at surfaces. International Journal of Quantum Chemistry, 1996, 57, 595-609.	2.0	20
87	Pulse trains in molecular dynamics and coherent spectroscopy: a theoretical study. New Journal of Physics, 2009, 11, 105036.	2.9	19
88	Molecular Model of the Ring-Opening and Ring-Closure Reaction of a Fluorinated Indolylfulgide. Journal of Physical Chemistry A, 2012, 116, 10518-10528.	2.5	19
89	Quantum Dynamics in an Explicit Solvent Environment: A Photochemical Bond Cleavage Treated with a Combined QD/MD Approach. Journal of Chemical Theory and Computation, 2015, 11, 1987-1995.	5.3	19
90	Substituent effects on the relaxation dynamics of furan, furfural and Î²-furfural: a combined theoretical and experimental approach. Physical Chemistry Chemical Physics, 2017, 19, 2025-2035.	2.8	19

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91	CARS spectroscopy of the NaH2 collision complex: the nature of the Na(32 P)H2 exciplex ? ab initio calculations and experimental results. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1990, 17, 299-308.	1.0	18
92	Interaction of electronic structure and nuclear dynamics on the S1 reaction surface for the ring opening of cyclohexadiene. Applied Physics B: Lasers and Optics, 2000, 71, 391-396.	2.2	18
93	Geometrical and substituent effects in conical intersections: Linking chemical structure and photoreactivity in polyenes. Journal of Chemical Physics, 2011, 135, 034304.	3.0	18
94	Quantum Dynamics of a Photochemical Bond Cleavage Influenced by the Solvent Environment: A Dynamic Continuum Approach. Journal of Physical Chemistry Letters, 2014, 5, 3480-3485.	4.6	18
95	Unravelling Photochemical Relationships Among Natural Products from Aplysia dactylomela. ACS Central Science, 2017, 3, 39-46.	11.3	18
96	Electroâ€mediated PhotoRedox Catalysis for Selective C(sp 3)â€“O Cleavages of Phosphinated Alcohols to Carbanions. Angewandte Chemie, 2021, 133, 20985-20993.	2.0	18
97	Ultrafast dissociation pathways of diphenylmethyl chloride to generate reactive carbo cations. Chemical Physics, 2008, 343, 329-339.	1.9	17
98	Ultrafast relaxation from <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si2.gif" overflow="scroll"><mml:mrow><mml:msup><mml:mrow /><mml:mrow><mml:mn>1</mml:mn></mml:mrow></mml:msup><mml:msub><mml:mrow><mml:mi>L</mml:mi></mml:mrow><mml:r to <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:msup><mml:mrow /><mml:mrow><mml:mn>1</mml:mn></mml:mrow></mml:msup><mml:msub><mml:mm. Chemical Physics, 201	1.9	17
99	Intersystem Crossing as a Key Component of the Nonadiabatic Relaxation Dynamics of Bithiophene and Terthiophene. Journal of Chemical Theory and Computation, 2018, 14, 4530-4540.	5.3	17
100	Stereoselective Csp 3 â^'Csp 2 Crossâ€Couplings of Chiral Secondary Alkylzinc Reagents with Alkenyl and Aryl Halides. Angewandte Chemie - International Edition, 2020, 59, 320-324.	13.8	17
101	Coherent control for ultrafast photochemical reactions. Pure and Applied Chemistry, 2001, 73, 525-528.	1.9	15
102	Chirp-driven vibrational distribution in transition metal carbonyl complexes. Physical Chemistry Chemical Physics, 2007, 9, 369-376.	2.8	15
103	Oxidative Ring Contraction of Cyclobutenes: General Approach to Cyclopropylketones including Mechanistic Insights. Journal of Organic Chemistry, 2018, 83, 4905-4921.	3.2	15
104	Activation of 2â€Cyclohexenone by BF 3 Coordination: Mechanistic Insights from Theory and Experiment. Angewandte Chemie - International Edition, 2021, 60, 10155-10163.	13.8	15
105	Coupled electron-nuclear wavepacket dynamics in potassium dimers. Journal of Physics B: Atomic, Molecular and Optical Physics, 2014, 47, 124015.	1.5	15
106	Searching for pathways involving dressed states in optimal control theory. Faraday Discussions, 2011, 153, 159.	3.2	14
107	Two New Methods To Generate Internal Coordinates for Molecular Wave Packet Dynamics in Reduced Dimensions. Journal of Chemical Theory and Computation, 2016, 12, 5698-5708.	5.3	14
108	Sub-cycle directional control of the dissociative ionization of H₂in tailored femtosecond laser fields. Journal of Physics B: Atomic, Molecular and Optical Physics, 2017, 50, 172001.	1.5	14

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109	Constructing Grids for Molecular Quantum Dynamics Using an Autoencoder. Journal of Chemical Theory and Computation, 2018, 14, 55-62.	5.3	14
110	Resonance CARS overtones of NaH in a Na (3p) + H2 gas mixture. Chemical Physics Letters, 1991, 186, 531-538.	2.6	13
111	Influence of static and dynamical structural changes on ultrafast processes mediated by conical intersections. Journal of Photochemistry and Photobiology A: Chemistry, 2007, 190, 352-358.	3.9	13
112	Robustness of quantum gates operating on the high frequency modes of MnBr(CO)5. Chemical Physics, 2007, 338, 291-298.	1.9	13
113	Multi-objective genetic algorithm optimization of 2D- and 3D-Pareto fronts for vibrational quantum processes. New Journal of Physics, 2009, 11, 013019.	2.9	13
114	A multi target approach to control chemical reactions in their inhomogeneous solvent environment. Journal of Physics B: Atomic, Molecular and Optical Physics, 2015, 48, 234003.	1.5	13
115	Photoisomerization of hemithioindigo compounds: Combining solvent- and substituent- effects into an advanced reaction model. Chemical Physics, 2018, 515, 614-621.	1.9	13
116	Design criteria for optimal photosynthetic energy conversion. Chemical Physics Letters, 2008, 466, 209-213.	2.6	12
117	Simulating the control of molecular reactions via modulated light fields: from gas phase to solution. Journal of Physics B: Atomic, Molecular and Optical Physics, 2017, 50, 082001.	1.5	12
118	Waveform control of molecular dynamics close to a conical intersection. Journal of Chemical Physics, 2020, 153, 224307.	3.0	12
119	Coupled nuclear and electron dynamics in the vicinity of a conical intersection. Journal of Chemical Physics, 2021, 154, 134306.	3.0	12
120	Design and interpretation of laser pulses for the control of quantum systems. Applied Physics B: Lasers and Optics, 2000, 71, 285-292.	2.2	11
121	Conical intersection seams in polyenes derived from their chemical composition. Journal of Chemical Physics, 2012, 137, 074101.	3.0	11
122	Theoretical study of the absorption spectrum of the pseudorotating Na3(B). Chemical Physics, 1997, 223, 1-14.	1.9	10
123	Molecular population control including rotation. Europhysics Letters, 2003, 64, 703-708.	2.0	10
124	Cavity cooling of translational and ro-vibrational motion of molecules: ab initio-based simulations for OH and NO. Applied Physics B: Lasers and Optics, 2007, 89, 459-467.	2.2	10
125	Cavity sideband cooling of trapped molecules. Physical Review A, 2011, 84, .	2.5	10
126	Sub-cycle steering of the deprotonation of acetylene by intense few-cycle mid-infrared laser fields. Optics Express, 2017, 25, 14192.	3.4	10

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127	Optimal use of time-dependent probability density data to extract potential-energy surfaces. Physical Review A, 2002, 65, .	2.5	9
128	Mechanism of UV-induced Dewar lesion repair catalysed by DNA (6-4) photolyase. Chemical Science, 2012, 3, 1794.	7.4	9
129	Hole-transfer induced energy transfer in perylene diimide dyads with a donorâ€“spacerâ€“acceptor motif. Physical Chemistry Chemical Physics, 2015, 17, 25061-25072.	2.8	9
130	Ultrafast photochemistry with two product channels: Wavepacket motion through two distinct conical intersections. Chemical Physics Letters, 2017, 683, 128-134.	2.6	9
131	Electronic and Geometric Characterization of TICT Formation in Hemithioindigo Photoswitches by Picosecond Infrared Spectroscopy. Journal of Physical Chemistry A, 2021, 125, 4390-4400.	2.5	9
132	Dielsâ€“Alder Reaction of Photochemically Generated (E)-Cyclohept-2-enones: Diene Scope, Reaction Pathway, and Synthetic Application. Journal of Organic Chemistry, 2022, 87, 4838-4851.	3.2	9
133	Ultrafast excitation process in NaNH3: a combined theoretical and experimental analysis. Chemical Physics, 1997, 225, 299-308.	1.9	8
134	Phase- and intensity-dependence of ultrafast dynamics in hydrocarbon molecules in few-cycle laser fields. Molecular Physics, 2017, 115, 1835-1845.	1.7	8
135	The importance of Rydberg orbitals in dissociative ionization of small hydrocarbon molecules in intense laser fields. Scientific Reports, 2017, 7, 4441.	3.3	8
136	Time-resolved nuclear dynamics in bound and dissociating acetylene. Structural Dynamics, 2018, 5, 044302.	2.3	8
137	Regio- and diastereoselective reactions of chiral secondary alkylcopper reagents with propargylic phosphates: preparation of chiral allenes. Chemical Science, 2020, 11, 5328-5332.	7.4	8
138	Ultrafast strong-field dissociation of vinyl bromide: An attosecond transient absorption spectroscopy and non-adiabatic molecular dynamics study. Structural Dynamics, 2021, 8, 034104.	2.3	8
139	Field-dressed orbitals in strong-field molecular ionization. Physical Review A, 2015, 92, .	2.5	7
140	Molecular features in complex environment: Cooperative team players during excited state bond cleavage. Structural Dynamics, 2016, 3, 043205.	2.3	7
141	Ultrafast Reactive Quantum Dynamics Coupled to Classical Solvent Dynamics Using an Ehrenfest Approach. Journal of Physical Chemistry A, 2018, 122, 2849-2857.	2.5	7
142	H₂ Evolution from Electrocatalysts with Redox-Active Ligands: Mechanistic Insights from Theory and Experiment vis-Ã-vis Co-Mabiq. Inorganic Chemistry, 2021, 60, 13888-13902.	4.0	7
143	Comment on â€œAnharmonic properties of the vibrational quantum computerâ€•[J. Chem. Phys. 126, 204102 (2007)]. Journal of Chemical Physics, 2008, 128, 167101.	3.0	6
144	Ground and Excited State Surfaces for the Photochemical Bond Cleavage in Phenylmethylphenylphosphonium Ions. Journal of Physical Chemistry A, 2013, 117, 10626-10633.	2.5	6

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145	Wavepacket Splitting in the First 100 fs Determines the Products from the Bond Cleavage of Diphenylmethylchloride. EPJ Web of Conferences, 2013, 41, 05042.	0.3	6
146	Multiscale Conformational Sampling Reveals Excited-State Locality in DNA Self-Repair Mechanism. Journal of Physical Chemistry A, 2020, 124, 9133-9140.	2.5	6
147	NONADIABATIC QUANTUM DYNAMICS AND CONTROL STRATEGIES. Advanced Series in Physical Chemistry, 2004, , 803-827.	1.5	5
148	Activation of 2â€Cyclohexenone by BF 3 Coordination: Mechanistic Insights from Theory and Experiment. Angewandte Chemie, 2021, 133, 10243-10251.	2.0	5
149	Photo-Induced Coupled Nuclear and Electron Dynamics in the Nucleobase Uracil. Frontiers in Physics, 2021, 9, .	2.1	5
150	A practical approach to multivariate interpolation. Computers in Physics, 1997, 11, 647.	0.5	4
151	Stereoselektive C(sp 3)â€C(sp 2)â€Kreuzkupplungen von chiralen sekundÃren Alkylzinkreagenzien mit Alkenylâ€•und Arylhalogeniden. Angewandte Chemie, 2020, 132, 328-332.	2.0	4
152	Photochemical Ring Contraction of 5,5-Dialkylcyclopent-2-enones and in situ Trapping by Primary Amines. Journal of Organic Chemistry, 2023, 88, 6294-6303.	3.2	4
153	Controlling near-field optical intensities in metal nanoparticle systems by polarization pulse shaping. Applied Physics B: Lasers and Optics, 2010, 100, 195-206.	2.2	3
154	Molecular wave packet dynamics decelerated by solvent environment: A theoretical approach. EPJ Web of Conferences, 2013, 41, 05043.	0.3	3
155	The Interplay of Nuclear and Electron Wavepacket Motion in the Control of Molecular Processes: A Theoretical Perspective. Physical Chemistry in Action, 2014, , 213-248.	0.6	3
156	Ultrafast spectroscopy of UV-induced DNA-lesions â€" on the search for strategies which keep DNA alive. EPJ Web of Conferences, 2013, 41, 07005.	0.3	2
157	Efficient attosecond control of electron dynamics in molecules. EPJ Web of Conferences, 2013, 41, 02026.	0.3	2
158	Molekulares Quantencomputing. Nachrichten Aus Der Chemie, 2004, 52, 555-559.	0.0	1
159	Kohlenstofftanz und Frequenzkamm. Nachrichten Aus Der Chemie, 2005, 53, 1112-1115.	0.0	1
160	Theoretical Quantum Control of Fluctuating Molecular Energy Levels in Complex Chemical Environments. Advanced Quantum Technologies, 2019, 2, 1800099.	3.9	1
161	Control strategies for molecular switches in donor-bridge-acceptor systems. Springer Series in Chemical Physics, 2007, , 258-260.	0.2	1
162	Does the proton move during ultrafast excited state intramolecular proton transfer?. Springer Series in Chemical Physics, 2001, , 645-647.	0.2	1

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163	Physikalische Chemie 2002. Nachrichten Aus Der Chemie, 2003, 51, 330-339.	0.0	0
164	Analysis of near-field control in a single-nanoparticle system. , 2009, , .		0
165	Keldysh-scaling in the waveform control of the dissociative ionization of D<inf>2</inf>. , 2011, , .		0
166	Femtosecond pump-probe spectroscopy for single trapped molecular ions. EPJ Web of Conferences, 2013, 41, 02028.	0.3	0
167	The importance of Rydberg orbitals in dissociative ionization of small hydrocarbon molecules in intense few-cycle laser pulses. Journal of Physics: Conference Series, 2015, 635, 112043.	0.4	0
168	Ultrafast non-adiabatic dynamics of excited diphenylmethyl bromide elucidated by quantum dynamics and semi-classical on-the-fly dynamics. Physical Chemistry Chemical Physics, 2018, 20, 22753-22761.	2.8	0
169	Ultrafast Photorelaxation of Uracil Embedded in an RNA Strand. EPJ Web of Conferences, 2019, 205, 10002.	0.3	0
170	Simulation of time-dependent ionization processes in acetylene. EPJ Web of Conferences, 2019, 205, 09023.	0.3	0
171	Observation of Ultrafast Dynamics in CO2 Highly Excited States. , 2019, , .		0
172	Molecular quantum computing: Implementation of global quantum gates applying optimal control theory. , 2002, , .		0
173	Laserfields obtained through optimal control theory throw light on Raman type control experiments. , 2002, , .		0
174	Molecular quantum computing: Implementation of global quantum gates applying optimal control theory. Springer Series in Chemical Physics, 2003, , 76-78.	0.2	0
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