Wolfgang Domcke

List of Publications by Year
in descending order

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396 papers	24,044 citations	7251 80 h-index	13635 134 g-index
400 all docs	400 docs citations	400 times ranked	8874 citing authors

#	Article	IF	Citations
1	Water Oxidation and Hydrogen Evolution with Organic Photooxidants: A Theoretical Perspective. Journal of Physical Chemistry B, 2022, 126, 2777-2788.	1.2	2
2	Ab Initio Electronic Structure Study of the Photoinduced Reduction of Carbon Dioxide with the Heptazinyl Radical. Journal of Physical Chemistry A, 2022, 126, 2778-2787.	1.1	2
3	On the propensity of formation of cyclobutane dimers in face-to-face and face-to-back uracil stacks in solution. Physical Chemistry Chemical Physics, 2022, 24, 14836-14845.	1.3	1
4	Ab initio trajectory surface-hopping dynamics studies of excited-state proton-coupled electron transfer reactions in trianisoleheptazineâ€“phenol complexes. Physical Chemistry Chemical Physics, 2022, 24, 15925-15936.	1.3	3
5	Triangular boron carbon nitrides: an unexplored family of chromophores with unique properties for photocatalysis and optoelectronics. Physical Chemistry Chemical Physics, 2021, 23, 12968-12975.	1.3	28
6	Simulation of UV absorption spectra and relaxation dynamics of uracil and uracilâ€“water clusters. Physical Chemistry Chemical Physics, 2021, 23, 2594-2604.	1.3	17
7	Strong static and dynamic Jahnâ€“Teller and pseudo-Jahnâ€“Teller effects in niobium tetrafluoride. Journal of Chemical Physics, 2021, 154, 124305.	1.2	3
8	Ab Initio Surface-Hopping Simulation of Femtosecond Transient-Absorption Pumpâ€“Probe Signals of Nonadiabatic Excited-State Dynamics Using the Doorwayâ€“Window Representation. Journal of Chemical Theory and Computation, 2021, 17, 2394-2408.	2.3	16
9	Can Hydrated Electrons be Produced from Water with Visible Light?. ChemPhotoChem, 2021, 5, 680-690.	1.5	4
10	Are Heptazine-Based Organic Light-Emitting Diode Chromophores Thermally Activated Delayed Fluorescence or Inverted Singletâ€“Triplet Systems?. Journal of Physical Chemistry Letters, 2021, 12, 6852-6860.	2.1	45
11	Combined Surface-Hopping, Dyson Orbital, and B-Spline Approach for the Computation of Time-Resolved Photoelectron Spectroscopy Signals: The Internal Conversion in Pyrazine. Journal of Chemical Theory and Computation, 2021, 17, 5098-5109.	2.3	11
12	Quantum dynamics with ab initio potentials. Journal of Chemical Physics, 2021, 155, 080401.	1.2	2
13	Ab Initio Nonadiabatic Surface-Hopping Trajectory Simulations of Photocatalytic Water Oxidation and Hydrogen Evolution with the Heptazine Chromophore. Journal of Physical Chemistry A, 2021, 125, 9917-9931.	1.1	10
14	Ab Initio Quasiclassical Simulation of Femtosecond Time-Resolved Two-Dimensional Electronic Spectra of Pyrazine. Journal of Physical Chemistry Letters, 2021, 12, 11736-11744.	2.1	9
15	Multi-faceted spectroscopic mapping of ultrafast nonadiabatic dynamics near conical intersections: A computational study. Journal of Chemical Physics, 2020, 153, 174111.	1.2	29
16	Photooxidation of water with heptazine-based molecular photocatalysts: Insights from spectroscopy and computational chemistry. Journal of Chemical Physics, 2020, 153, 100902.	1.2	17
17	Photoinduced water oxidation in pyrimidineâ€“water clusters: a combined experimental and theoretical study. Physical Chemistry Chemical Physics, 2020, 22, 12502-12514.	1.3	16
18	Tracking both ultrafast electrons and nuclei. Science, 2020, 368, 820-821.	6.0	3

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19	First-principles study of large-amplitude dynamic Jahnâ€“Teller effects in vanadium tetrafluoride. Journal of Chemical Physics, 2020, 152, 094304.	1.2	4
20	Control of Excited-State Proton-Coupled Electron Transfer by Ultrafast Pump-Push-Probe Spectroscopy in Heptazine-Phenol Complexes: Implications for Photochemical Water Oxidation. Journal of Physical Chemistry C, 2020, 124, 9151-9160.	1.5	18
21	Molecular Design of Heptazine-Based Photocatalysts: Effect of Substituents on Photocatalytic Efficiency and Photostability. Journal of Physical Chemistry A, 2020, 124, 3698-3710.	1.1	20
22	Effects of high pulse intensity and chirp in two-dimensional electronic spectroscopy of an atomic vapor. Optics Express, 2020, 28, 25806.	1.7	13
23	Orientational relaxation of a quantum linear rotor in a dissipative environment: Simulations with the hierarchical equations-of-motion method. Journal of Chemical Physics, 2019, 151, 034101.	1.2	5
24	Spin-orbit vibronic coupling in Î4 states of linear triatomic molecules. Journal of Chemical Physics, 2019, 151, 134103.	1.2	1
25	Singletâ€“Triplet Inversion in Heptazine and in Polymeric Carbon Nitrides. Journal of Physical Chemistry A, 2019, 123, 8099-8108.	1.1	87
26	Mapping of Wave Packet Dynamics at Conical Intersections by Time- and Frequency-Resolved Fluorescence Spectroscopy: A Computational Study. Journal of Physical Chemistry Letters, 2019, 10, 5873-5880.	2.1	21
27	Mechanisms of photoreactivity in hydrogen-bonded adenineâ€“H‹sub›2‹/sub›O complexes. Physical Chemistry Chemical Physics, 2019, 21, 14238-14249.	1.3	9
28	Photoinduced electron-driven proton transfer from water to an N-heterocyclic chromophore: nonadiabatic dynamics studies for pyridineâ€“water clusters. Physical Chemistry Chemical Physics, 2019, 21, 14073-14079.	1.3	28
29	Beyond artificial photosynthesis: general discussion. Faraday Discussions, 2019, 215, 422-438.	1.6	0
30	Synthetic approaches to artificial photosynthesis: general discussion. Faraday Discussions, 2019, 215, 242-281.	1.6	5
31	Analysis of transient-absorption pump-probe signals of nonadiabatic dissipative systems: â€œidealâ€•and â€œrealâ€•spectra. Journal of Chemical Physics, 2019, 150, 204102.	1.2	19
32	Origin of Unexpectedly Simple Oscillatory Responses in the Excited-State Dynamics of Disordered Molecular Aggregates. Journal of Physical Chemistry Letters, 2019, 10, 2806-2810.	2.1	19
33	Assessing the performance of trajectory surface hopping methods: Ultrafast internal conversion in pyrazine. Journal of Chemical Physics, 2019, 150, 154119.	1.2	44
34	Role of the Pyridinyl Radical in the Light-Driven Reduction of Carbon Dioxide: A First-Principles Study. Journal of Physical Chemistry A, 2019, 123, 3678-3684.	1.1	4
35	Monitoring of Nonadiabatic Effects in Individual Chromophores by Femtosecond Double-Pump Single-Molecule Spectroscopy: A Model Study. Molecules, 2019, 24, 231.	1.7	4
36	UV absorption spectra of DNA bases in the 350â€“190 nm range: assignment and state specific analysis of solvation effects. Physical Chemistry Chemical Physics, 2019, 21, 22782-22793.	1.3	14

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37	Barrierless Heptazine-Driven Excited State Proton-Coupled Electron Transfer: Implications for Controlling Photochemistry of Carbon Nitrides and Aza-Arenes. Journal of Physical Chemistry C, 2019, 123, 29580-29588.	1.5	21
38	Multimode quantum dynamics with multiple Davydov D2 trial states: Application to a 24-dimensional conical intersection model. Journal of Chemical Physics, 2019, 150, 024101.	1.2	32
39	Solar Energy Harvesting with Carbon Nitrides and Nâ€Heterocyclic Frameworks: Do We Understand the Mechanism?. ChemPhotoChem, 2019, 3, 10-23.	1.5	31
40	Proton-Coupled Electron Transfer from Water to a Model Heptazine-Based Molecular Photocatalyst. Journal of Physical Chemistry Letters, 2018, 9, 6257-6261.	2.1	51
41	Photoinduced hydrogen-transfer reactions in pyridine-water clusters: Insights from excited-state electronic-structure calculations. Chemical Physics, 2018, 515, 550-556.	0.9	10
42	Enhanced S₂ Fluorescence from a Free-Base Tetraphenylporphyrin Surface-Mounted Metal Organic Framework. Journal of Physical Chemistry C, 2018, 122, 23321-23328.	1.5	12
43	Simulation of Femtosecond Phase-Locked Double-Pump Signals of Individual Light-Harvesting Complexes LH2. Journal of Physical Chemistry Letters, 2018, 9, 4488-4494.	2.1	8
44	Mechanism of Photocatalytic Water Oxidation by Graphitic Carbon Nitride. Journal of Physical Chemistry Letters, 2018, 9, 4695-4699.	2.1	22
45	Mechanism of photocatalytic water splitting with triazine-based carbon nitrides: insights from ab initio calculations for the triazineâ€“water complex. Physical Chemistry Chemical Physics, 2018, 20, 14420-14430.	1.3	35
46	Resonant femtosecond stimulated Raman spectroscopy with an intense actinic pump pulse: Application to conical intersections. Journal of Chemical Physics, 2017, 146, 084105.	1.2	7
47	Mechanism of Photocatalytic Water Splitting with Graphitic Carbon Nitride: Photochemistry of the Heptazineâ€“Water Complex. Journal of Physical Chemistry A, 2017, 121, 4754-4764.	1.1	85
48	Photodissociation dynamics of the pyridinyl radical: Time-dependent quantum wave-packet calculations. Journal of Chemical Physics, 2017, 146, 124304.	1.2	18
49	Efficient orientational averaging of nonlinear optical signals in multi-chromophore systems. Journal of Chemical Physics, 2017, 147, 044114.	1.2	13
50	Accuracy of trajectory surface-hopping methods: Test for a two-dimensional model of the photodissociation of phenol. Journal of Chemical Physics, 2017, 147, 184114.	1.2	43
51	Theoretical aspects of femtosecond double-pump single-molecule spectroscopy. II. Strong-field regime. Physical Chemistry Chemical Physics, 2017, 19, 32307-32319.	1.3	12
52	Theoretical aspects of femtosecond double-pump single-molecule spectroscopy. I. Weak-field regime. Physical Chemistry Chemical Physics, 2017, 19, 32296-32306.	1.3	13
53	Nonperturbative response functions: A tool for the interpretation of four-wave-mixing signals beyond third order. Journal of Chemical Physics, 2017, 147, 234104.	1.2	11
54	Role of Electron-Driven Proton-Transfer Processes in the Ultrafast Deactivation of Photoexcited Anionic 8-oxoGuanine-Adenine and 8-oxoGuanine-Cytosine Base Pairs. Molecules, 2017, 22, 135.	1.7	11

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55	Structural dynamics: general discussion. Faraday Discussions, 2016, 194, 583-620.	1.6	0
56	Vibrational and condensed phase dynamics: general discussion. Faraday Discussions, 2016, 194, 747-775.	1.6	1
57	Attosecond processes and X-ray spectroscopy: general discussion. Faraday Discussions, 2016, 194, 427-462.	1.6	0
58	Electronic and non-adiabatic dynamics: general discussion. Faraday Discussions, 2016, 194, 209-257.	1.6	3
59	State-specific tunneling lifetimes from classical trajectories: H-atom dissociation in electronically excited pyrrole. Journal of Chemical Physics, 2016, 144, 104105.	1.2	11
60	Relativistic theory of the Jahn-Teller effect: p-orbitals in tetrahedral and trigonal systems. Journal of Chemical Physics, 2016, 144, 124101.	1.2	18
61	Femtosecond stimulated Raman spectroscopy as a tool to detect molecular vibrations in ground and excited electronic states. Journal of Chemical Physics, 2016, 144, 184307.	1.2	4
62	Alternative view of two-dimensional spectroscopy. Journal of Chemical Physics, 2016, 144, 194104.	1.2	11
63	Onset of the Electronic Absorption Spectra of Isolated and Ï€-Stacked Oligomers of 5,6-Dihydroxyindole: An Ab Initio Study of the Building Blocks of Eumelanin. Journal of Physical Chemistry B, 2016, 120, 3493-3502.	1.2	37
64	Dissipative dynamics at conical intersections: simulations with the hierarchy equations of motion method. Faraday Discussions, 2016, 194, 61-80.	1.6	39
65	Conical-Intersection Topographies Suggest That Ribose Exhibits Enhanced UV Photostability. Journal of Physical Chemistry B, 2016, 120, 10729-10735.	1.2	12
66	Excitedâ€State Deactivation of Adenine by Electronâ€Driven Protonâ€Transfer Reactions in Adenineâ€“Water Clusters: Aâ€…Computational Study. ChemPhysChem, 2016, 17, 1298-1304.	1.0	19
67	Resonant Femtosecond Stimulated Raman Spectra: Theory and Simulations. Journal of Physical Chemistry A, 2016, 120, 3286-3295.	1.1	15
68	A â€˜bottom upâ€™, ab initio computational approach to understanding fundamental photophysical processes in nitrogen containing heterocycles, DNA bases and base pairs. Physical Chemistry Chemical Physics, 2016, 18, 20007-20027.	1.3	78
69	Photocatalytic water splitting with acridine dyes: Guidelines from computational chemistry. Chemical Physics, 2016, 464, 78-85.	0.9	10
70	Excited-state deactivation in 8-oxo-deoxyguanosine: comparison between anionic and neutral forms. Physical Chemistry Chemical Physics, 2016, 18, 947-955.	1.3	15
71	Microscopic derivation of the Keilsonâ€“Storer master equation. Chemical Physics, 2015, 462, 35-40.	0.9	4
72	Quantum dynamics on a three-sheeted six-dimensional ab initio potential-energy surface of the phosphine cation: Simulation of the photoelectron spectrum and the ultrafast radiationless decay dynamics. Journal of Chemical Physics, 2015, 143, 194301.	1.2	7

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73	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si3.gif" overflow="scroll"><mml:mrow><mml:mi>E</mml:mi><mml:mo>Ã—</mml:mo><mml:mi>e</mml:mi></mml:mrow></mml:math> Jahnâ€“Teller effect in the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:msubsup><mml:mrow><mml:mtext>P</mml:mtext></mml:mrow><mml:mrow><mml:mn>4</mml:mn>	0.9	4
74	Theory of femtosecond coherent double-pump single-molecule spectroscopy: Application to light harvesting complexes. Journal of Chemical Physics, 2015, 142, 164106.	1.2	24
75	Nonadiabatic nuclear dynamics of the ammonia cation studied by surface hopping classical trajectory calculations. Journal of Chemical Physics, 2015, 142, 104307.	1.2	46
76	Simulation of femtosecond two-dimensional electronic spectra of conical intersections. Journal of Chemical Physics, 2015, 143, 074308.	1.2	29
77	Photocatalytic Water Splitting with the Acridine Chromophore: A Computational Study. Journal of Physical Chemistry B, 2015, 119, 10664-10672.	1.2	41
78	Photoinduced water splitting via benzoquinone and semiquinone sensitisation. Physical Chemistry Chemical Physics, 2015, 17, 32183-32193.	1.3	30
79	Quasi-classical nonadiabatic transition probability for G3/2Ã—(t2+e) Jahnâ€“Teller systems. Chemical Physics, 2015, 463, 1-4.	0.9	2
80	Mechanisms of Photostability in Kynurenines: A Joint Electronic-Structure and Dynamics Study. Journal of Physical Chemistry B, 2015, 119, 2112-2124.	1.2	33
81	Signatures of conical intersections in two-dimensional electronic spectra. Journal of Physics B: Atomic, Molecular and Optical Physics, 2014, 47, 124019.	0.6	32
82	Electronically excited states and photochemical reaction mechanisms of Î²-glucose. Physical Chemistry Chemical Physics, 2014, 16, 38-47.	1.3	20
83	Infrared Absorption Spectra of Jahnâ€“Teller Systems: Application to the Transition-Metal Trifluorides MnF₃ and NiF₃. Journal of Physical Chemistry A, 2014, 118, 3726-3734.	1.1	7
84	Mechanisms of Ultrafast Excited-State Deactivation in Adenosine. Journal of Physical Chemistry A, 2014, 118, 122-127.	1.1	76
85	The (E + A) Ã— (e + a) Jahnâ€“Teller and Pseudo-Jahnâ€“Teller Hamiltonian Including Spinâ€“Orbit Coupling for Trigonal Systems. Journal of Physical Chemistry A, 2014, 118, 11962-11970.	1.1	23
86	Photochemical Mechanisms of Radiationless Deactivation Processes in Urocanic Acid. Journal of Physical Chemistry B, 2014, 118, 976-985.	1.2	35
87	Photoinduced Oxidation of Water in the Pyridineâ€“Water Complex: Comparison of the Singlet and Triplet Photochemistries. Journal of Physical Chemistry A, 2014, 118, 7788-7795.	1.1	33
88	Ab Initio Study of Potential Ultrafast Internal Conversion Routes in Oxybenzone, Caffeic Acid, and Ferulic Acid: Implications for Sunscreens. Journal of Physical Chemistry A, 2014, 118, 11999-12010.	1.1	90
89	Photochemistry of 2-Aminooxazole, a Hypothetical Prebiotic Precursor of RNA Nucleotides. Journal of Physical Chemistry Letters, 2013, 4, 2785-2788.	2.1	29
90	Interpolation of multi-sheeted multi-dimensional potential-energy surfaces via a linear optimization procedure. Journal of Chemical Physics, 2013, 138, 224103.	1.2	22

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91	Ab initio study of the cyclodimerization of uracil through butane-like and oxetane-like conical intersections. Journal of Photochemistry and Photobiology A: Chemistry, 2013, 271, 1-7.	2.0	4
92	Strong-pump strong-probe spectroscopy: effects of higher excited electronic states. Physical Chemistry Chemical Physics, 2013, 15, 8119.	1.3	22
93	A multi-sheeted three-dimensional potential-energy surface for the H-atom photodissociation of phenol. Faraday Discussions, 2013, 163, 73.	1.6	33
94	Computational investigation of the photoinduced homolytic dissociation of water in the pyridineâ€“water complex. Physical Chemistry Chemical Physics, 2013, 15, 5957.	1.3	51
95	Calculation of third-order signals via driven SchrÃ¶dinger equations: General results and application to electronic 2D photon echo spectroscopy. Chemical Physics, 2013, 422, 53-62.	0.9	23
96	Pump-probe spectroscopy with strong pulses as a tool to enhance weak electronic transitions. Physical Review A, 2013, 87, .	1.0	10
97	Spectroscopy meets theory. Nature Chemistry, 2013, 5, 257-258.	6.6	28
98	Jahn-Teller theory beyond the standard model. Journal of Physics: Conference Series, 2013, 428, 012015.	0.3	13
99	Simple Recipes for Separating Excited-State Absorption and Cascading Signals by Polarization-Sensitive Measurements. Journal of Physical Chemistry A, 2013, 117, 11509-11513.	1.1	10
100	Simulation of femtosecond â€œdouble-slitâ€•experiments for a chromophore in a dissipative environment. Journal of Chemical Physics, 2013, 139, 214302.	1.2	19
101	Domain of validity of the perturbative approach to femtosecond optical spectroscopy. Journal of Chemical Physics, 2013, 139, 224107.	1.2	13
102	Ultrafast non-adiabatic dynamics of ethylene including Rydberg states. Molecular Physics, 2013, 111, 2439-2450.	0.8	41
103	Quantum dynamics of electron-transfer reactions: photoinduced intermolecular electron transfer in a porphyrinâ€“quinone complex. Molecular Physics, 2012, 110, 751-763.	0.8	25
104	Theoretical analysis of photoinduced H-atom elimination in thiophenol. Journal of Chemical Physics, 2012, 136, 174312.	1.2	45
105	Bath-induced correlations and relaxation of vibronic dimers. Journal of Chemical Physics, 2012, 136, 034507.	1.2	22
106	Nonadiabatic Nuclear Dynamics in the Ammonia Cation Studied by the Branching Classical Trajectory Method. Journal of Physics: Conference Series, 2012, 388, 102005.	0.3	0
107	On the nature and signatures of the solvated electron in water. Physical Chemistry Chemical Physics, 2012, 14, 22-34.	1.3	141
108	Relativistic Jahnâ€“Teller and pseudo-Jahnâ€“Teller couplings in systems. Chemical Physics, 2012, 407, 1-8.	0.9	18

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109	Jahn-Teller, pseudo-Jahn-Teller, and spin-orbit coupling Hamiltonian of a d electron in an octahedral environment. Journal of Chemical Physics, 2012, 137, 114101.	1.2	36
110	Photoinduced water splitting with oxotitanium porphyrin: a computational study. Physical Chemistry Chemical Physics, 2012, 14, 12807.	1.3	25
111	Ab initio study of dynamical E Ã— e Jahn-Teller and spin-orbit coupling effects in the transition-metal trifluorides TiF3, CrF3, and NiF3. Journal of Chemical Physics, 2012, 136, 084308.	1.2	33
112	Role of Conical Intersections in Molecular Spectroscopy and Photoinduced Chemical Dynamics. Annual Review of Physical Chemistry, 2012, 63, 325-352.	4.8	401
113	Optical N-Wave-Mixing Spectroscopy with Strong and Temporally Well-Separated Pulses: The Doorwayâ^'Window Representation. Journal of Physical Chemistry B, 2011, 115, 5648-5658.	1.2	19
114	Strong and Long Makes Short: Strong-Pump Strong-Probe Spectroscopy. Journal of Physical Chemistry Letters, 2011, 2, 114-119.	2.1	22
115	Efficient Excited-State Deactivation in Organic Chromophores and Biologically Relevant Molecules: Role of Electron and Proton Transfer Processes. Advanced Series in Physical Chemistry, 2011, , 51-82.	1.5	5
116	Spin-Orbit Vibronic Coupling in Jahnâ€“Teller Systems. Advanced Series in Physical Chemistry, 2011, , 117-154.	1.5	9
117	Exact quantum master equation for a molecular aggregate coupled to a harmonic bath. Physical Review E, 2011, 84, 041139.	0.8	20
118	Relativistic Jahn-Teller effects in the photoelectron spectra of tetrahedral P4, As4, Sb4, and Bi4. Journal of Chemical Physics, 2011, 135, 104108.	1.2	19
119	Molecular mechanisms of the photostability of indigo. Physical Chemistry Chemical Physics, 2011, 13, 1618-1628.	1.3	86
120	Jahnâ€“Teller and spinâ€“orbit coupling effects in transition-metal trifluorides. Chemical Physics, 2011, 387, 56-65.	0.9	42
121	Effect of the Chirality of Residues and Î³â€Turns on the Electronic Excitation Spectra, Excitedâ€State Reaction Paths and Conical Intersections of Capped Phenylalanineâ€“Alanine Dipeptides. ChemPhysChem, 2011, 12, 1833-1840.	1.0	14
122	Conical Intersections. Advanced Series in Physical Chemistry, 2011, , .	1.5	300
123	First-principles study of photoinduced electron-transfer dynamics in a Mgâ€“porphyrinâ€“quinone complex. Chemical Physics Letters, 2010, 498, 230-234.	1.2	22
124	Relativistic TÃ—T and TÃ—E Jahnâ€“Teller coupling in tetrahedral systems. Chemical Physics, 2010, 374, 86-93.	0.9	28
125	High-order expansion of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si5.gif" display="inline" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mi>T</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> Jahnâ€“Teller potential-energy surfaces in tetrahedral systems. Chemical Physics Letters, 2010, 494, 134-138.	1.2	31
126	Photoinduced Proton Transfer as a Possible Mechanism for Highly Efficient Excited-State Deactivation in Proteins. Journal of Physical Chemistry Letters, 2010, 1, 425-428.	2.1	22

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127	High-order expansion of T2Ã—t2 Jahnâ€“Teller potential-energy surfaces in tetrahedral molecules. Journal of Chemical Physics, 2010, 132, 154108.	1.2	55
128	Relativistic Jahn-Teller effect in tetrahedral systems. Physical Review A, 2010, 81, .	1.0	33
129	Comparison of the non-radiative decay mechanisms of 4-pyrimidinone and uracil: an ab initio study. Physical Chemistry Chemical Physics, 2010, 12, 5007.	1.3	61
130	Role of excited-state hydrogen detachment and hydrogen-transfer processes for the excited-state deactivation of an aromatic dipeptide: N-acetyl tryptophan methyl amide. Physical Chemistry Chemical Physics, 2010, 12, 4899.	1.3	29
131	Efficient calculation of the polarization induced by N coherent laser pulses. Journal of Chemical Physics, 2009, 131, 194103.	1.2	22
132	Manipulating electronic couplings and nonadiabatic nuclear dynamics with strong laser pulses. Journal of Chemical Physics, 2009, 131, 124505.	1.2	27
133	Ab initio study of the energetics of photoinduced electron and proton transfer processes in a bio-inspired model of photochemical water splitting. Chemical Physics Letters, 2009, 479, 144-148.	1.2	12
134	Photophysics of the Trp-Gly dipeptide: Role of electron and proton transfer processes for efficient excited-state deactivation. Chemical Physics Letters, 2009, 482, 38-43.	1.2	27
135	Efficient Excited-State Deactivation of the Gly-Phe-Ala Tripeptide via an Electron-Driven Proton-Transfer Process. Journal of the American Chemical Society, 2009, 131, 1374-1375.	6.6	65
136	Efficient Calculation of Time- and Frequency-Resolved Four-Wave-Mixing Signals. Accounts of Chemical Research, 2009, 42, 1290-1298.	7.6	87
137	Biradicalic excited states of zwitterionic phenol-ammonia clusters. Journal of Chemical Physics, 2009, 130, 024302.	1.2	31
138	Computational Studies of the Photophysics of Neutral and Zwitterionic Amino Acids in an Aqueous Environment: Tyrosineâ^'(H2O)2 and Tryptophanâ^'(H2O)2 Clusters. Journal of Physical Chemistry A, 2009, 113, 542-550.	1.1	57
139	Photophysics of xanthine: computational study of the radiationless decay mechanisms. Physical Chemistry Chemical Physics, 2009, 11, 10165.	1.3	34
140	Role of vibrational energy relaxation in the photoinduced nonadiabatic dynamics of pyrrole at the conical intersection. Chemical Physics, 2008, 350, 125-138.	0.9	27
141	Computational studies of the photophysics of neutral and zwitterionic glycine in an aqueous environment: The glycineâ€“(H2O)2 cluster. Chemical Physics Letters, 2008, 457, 404-407.	1.2	10
142	The 3EÃ—E, 4EÃ—E and 5EÃ—E Jahnâ€“Teller Hamiltonians of trigonal systems. Chemical Physics, 2008, 352, 125-134.	0.9	19
143	Renner-Teller and spin-orbit vibronic coupling effects in linear triatomic molecules with a half-filled Ï€ shell. Journal of Chemical Physics, 2008, 128, 124318.	1.2	10
144	Vibronic Effects in Single Molecule Conductance: First-Principles Description and Application to Benzenealkanethiolates between Gold Electrodes. Journal of Physical Chemistry C, 2008, 112, 9880-9890.	1.5	58

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145	Computational Model of Photocatalytic Water Splitting. Journal of Physical Chemistry A, 2008, 112, 7311-7313.	1.1	17
146	Ab Initio Studies on the Photophysics of Guanine Tautomers: Out-of-Plane Deformation and NH Dissociation Pathways to Conical Intersections. Journal of Physical Chemistry A, 2008, 112, 7090-7097.	1.1	51
147	Nonradiative Decay Mechanisms of the Biologically Relevant Tautomer of Guanine. Journal of Physical Chemistry A, 2008, 112, 11965-11968.	1.1	109
148	Photochemistry of hydrogen-bonded aromatic pairs: Quantum dynamical calculations for the pyrroleâ€“pyridine complex. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 12707-12712.	3.3	74
149	Ab initio characterization of the conical intersections involved in the photochemistry of phenol. Journal of Chemical Physics, 2008, 129, 224307.	1.2	105
150	Effects of intense femtosecond pumping on ultrafast electronic-vibrational dynamics in molecular systems with relaxation. Journal of Chemical Physics, 2008, 129, 214303.	1.2	45
151	Relativistic EÃ—T Jahnâ€“Teller effect in tetrahedral systems. Journal of Chemical Physics, 2008, 129, 224102.	1.2	32
152	Quasiclassical theory of the dynamicalEâ€‰Ã—â€‰EJahnâ€“Teller effect including spinâ€“orbit interaction. Molecular Physics, 2007, 105, 1471-1485.	0.8	8
153	Spin-orbit vibronic coupling in Î3 states of linear triatomic molecules. Journal of Chemical Physics, 2007, 126, 134312.	1.2	23
154	Computational Studies of the Photophysics of Hydrogen-Bonded Molecular Systems. Journal of Physical Chemistry A, 2007, 111, 11725-11735.	1.1	227
155	Conical intersections involving the dissociative1Ï€Ïƒ* state in 9H-adenine: a quantum chemical ab initio study. Physical Chemistry Chemical Physics, 2007, 9, 2075-2084.	1.3	57
156	Theory of Ultrafast Nonadiabatic Excited-State Processes and their Spectroscopic Detection in Real Time. Advances in Chemical Physics, 2007, , 1-169.	0.3	282
157	Computational studies of aqueous-phase photochemistry and the hydrated electron in finite-size clusters. Physical Chemistry Chemical Physics, 2007, 9, 3818.	1.3	48
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