Wolfgang Domcke

List of Publications by Year
in descending order

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396 papers	24,044 citations	6254 80 h-index	11939 134 g-index
400 all docs	400 docs citations	400 times ranked	7948 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.	2.6	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.	2.5	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.	2.8	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.	2.8	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.	2.8	28
6	Simulation of UV absorption spectra and relaxation dynamics of uracil and uracilâ€“water clusters. Physical Chemistry Chemical Physics, 2021, 23, 2594-2604.	2.8	17
7	Strong static and dynamic Jahnâ€“Teller and pseudo-Jahnâ€“Teller effects in niobium tetrafluoride. Journal of Chemical Physics, 2021, 154, 124305.	3.0	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.	5.3	16
9	Can Hydrated Electrons be Produced from Water with Visible Light?. ChemPhotoChem, 2021, 5, 680-690.	3.0	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.	4.6	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.	5.3	11
12	Quantum dynamics with ab initio potentials. Journal of Chemical Physics, 2021, 155, 080401.	3.0	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.	2.5	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.	4.6	9
15	Multi-faceted spectroscopic mapping of ultrafast nonadiabatic dynamics near conical intersections: A computational study. Journal of Chemical Physics, 2020, 153, 174111.	3.0	29
16	Photooxidation of water with heptazine-based molecular photocatalysts: Insights from spectroscopy and computational chemistry. Journal of Chemical Physics, 2020, 153, 100902.	3.0	17
17	Photoinduced water oxidation in pyrimidineâ€“water clusters: a combined experimental and theoretical study. Physical Chemistry Chemical Physics, 2020, 22, 12502-12514.	2.8	16
18	Tracking both ultrafast electrons and nuclei. Science, 2020, 368, 820-821.	12.6	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.	3.0	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.	3.1	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.	2.5	20
22	Effects of high pulse intensity and chirp in two-dimensional electronic spectroscopy of an atomic vapor. Optics Express, 2020, 28, 25806.	3.4	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.	3.0	5
24	Spin-orbit vibronic coupling in Î4 states of linear triatomic molecules. Journal of Chemical Physics, 2019, 151, 134103.	3.0	1
25	Singletâ€“Triplet Inversion in Heptazine and in Polymeric Carbon Nitrides. Journal of Physical Chemistry A, 2019, 123, 8099-8108.	2.5	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.	4.6	21
27	Mechanisms of photoreactivity in hydrogen-bonded adenineâ€“H‹sub›2‹/sub›O complexes. Physical Chemistry Chemical Physics, 2019, 21, 14238-14249.	2.8	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.	2.8	28
29	Beyond artificial photosynthesis: general discussion. Faraday Discussions, 2019, 215, 422-438.	3.2	0
30	Synthetic approaches to artificial photosynthesis: general discussion. Faraday Discussions, 2019, 215, 242-281.	3.2	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.	3.0	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.	4.6	19
33	Assessing the performance of trajectory surface hopping methods: Ultrafast internal conversion in pyrazine. Journal of Chemical Physics, 2019, 150, 154119.	3.0	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.	2.5	4
35	Monitoring of Nonadiabatic Effects in Individual Chromophores by Femtosecond Double-Pump Single-Molecule Spectroscopy: A Model Study. Molecules, 2019, 24, 231.	3.8	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.	2.8	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.	3.1	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.	3.0	32
39	Solar Energy Harvesting with Carbon Nitrides and Nâ€Heterocyclic Frameworks: Do We Understand the Mechanism?. ChemPhotoChem, 2019, 3, 10-23.	3.0	31
40	Proton-Coupled Electron Transfer from Water to a Model Heptazine-Based Molecular Photocatalyst. Journal of Physical Chemistry Letters, 2018, 9, 6257-6261.	4.6	51
41	Photoinduced hydrogen-transfer reactions in pyridine-water clusters: Insights from excited-state electronic-structure calculations. Chemical Physics, 2018, 515, 550-556.	1.9	10
42	Enhanced S₂ Fluorescence from a Free-Base Tetraphenylporphyrin Surface-Mounted Metal Organic Framework. Journal of Physical Chemistry C, 2018, 122, 23321-23328.	3.1	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.	4.6	8
44	Mechanism of Photocatalytic Water Oxidation by Graphitic Carbon Nitride. Journal of Physical Chemistry Letters, 2018, 9, 4695-4699.	4.6	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.	2.8	35
46	Resonant femtosecond stimulated Raman spectroscopy with an intense actinic pump pulse: Application to conical intersections. Journal of Chemical Physics, 2017, 146, 084105.	3.0	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.	2.5	85
48	Photodissociation dynamics of the pyridinyl radical: Time-dependent quantum wave-packet calculations. Journal of Chemical Physics, 2017, 146, 124304.	3.0	18
49	Efficient orientational averaging of nonlinear optical signals in multi-chromophore systems. Journal of Chemical Physics, 2017, 147, 044114.	3.0	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.	3.0	43
51	Theoretical aspects of femtosecond double-pump single-molecule spectroscopy. II. Strong-field regime. Physical Chemistry Chemical Physics, 2017, 19, 32307-32319.	2.8	12
52	Theoretical aspects of femtosecond double-pump single-molecule spectroscopy. I. Weak-field regime. Physical Chemistry Chemical Physics, 2017, 19, 32296-32306.	2.8	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.	3.0	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.	3.8	11

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55	Structural dynamics: general discussion. Faraday Discussions, 2016, 194, 583-620.	3.2	0
56	Vibrational and condensed phase dynamics: general discussion. Faraday Discussions, 2016, 194, 747-775.	3.2	1
57	Attosecond processes and X-ray spectroscopy: general discussion. Faraday Discussions, 2016, 194, 427-462.	3.2	0
58	Electronic and non-adiabatic dynamics: general discussion. Faraday Discussions, 2016, 194, 209-257.	3.2	3
59	State-specific tunneling lifetimes from classical trajectories: H-atom dissociation in electronically excited pyrrole. Journal of Chemical Physics, 2016, 144, 104105.	3.0	11
60	Relativistic theory of the Jahn-Teller effect: p-orbitals in tetrahedral and trigonal systems. Journal of Chemical Physics, 2016, 144, 124101.	3.0	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.	3.0	4
62	Alternative view of two-dimensional spectroscopy. Journal of Chemical Physics, 2016, 144, 194104.	3.0	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.	2.6	37
64	Dissipative dynamics at conical intersections: simulations with the hierarchy equations of motion method. Faraday Discussions, 2016, 194, 61-80.	3.2	39
65	Conical-Intersection Topographies Suggest That Ribose Exhibits Enhanced UV Photostability. Journal of Physical Chemistry B, 2016, 120, 10729-10735.	2.6	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.	2.1	19
67	Resonant Femtosecond Stimulated Raman Spectra: Theory and Simulations. Journal of Physical Chemistry A, 2016, 120, 3286-3295.	2.5	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.	2.8	78
69	Photocatalytic water splitting with acridine dyes: Guidelines from computational chemistry. Chemical Physics, 2016, 464, 78-85.	1.9	10
70	Excited-state deactivation in 8-oxo-deoxyguanosine: comparison between anionic and neutral forms. Physical Chemistry Chemical Physics, 2016, 18, 947-955.	2.8	15
71	Microscopic derivation of the Keilsonâ€“Storer master equation. Chemical Physics, 2015, 462, 35-40.	1.9	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.	3.0	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> cation and its signatures in the. Chemical Physics, 2015, 460, 51-55.	1.9	4
74	Theory of femtosecond coherent double-pump single-molecule spectroscopy: Application to light harvesting complexes. Journal of Chemical Physics, 2015, 142, 164106.	3.0	24
75	Nonadiabatic nuclear dynamics of the ammonia cation studied by surface hopping classical trajectory calculations. Journal of Chemical Physics, 2015, 142, 104307.	3.0	46
76	Simulation of femtosecond two-dimensional electronic spectra of conical intersections. Journal of Chemical Physics, 2015, 143, 074308.	3.0	29
77	Photocatalytic Water Splitting with the Acridine Chromophore: A Computational Study. Journal of Physical Chemistry B, 2015, 119, 10664-10672.	2.6	41
78	Photoinduced water splitting via benzoquinone and semiquinone sensitisation. Physical Chemistry Chemical Physics, 2015, 17, 32183-32193.	2.8	30
79	Quasi-classical nonadiabatic transition probability for G3/2Ã—(t2+e) Jahnâ€“Teller systems. Chemical Physics, 2015, 463, 1-4.	1.9	2
80	Mechanisms of Photostability in Kynurenines: A Joint Electronic-Structure and Dynamics Study. Journal of Physical Chemistry B, 2015, 119, 2112-2124.	2.6	33
81	Signatures of conical intersections in two-dimensional electronic spectra. Journal of Physics B: Atomic, Molecular and Optical Physics, 2014, 47, 124019.	1.5	32
82	Electronically excited states and photochemical reaction mechanisms of Î²-glucose. Physical Chemistry Chemical Physics, 2014, 16, 38-47.	2.8	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.	2.5	7
84	Mechanisms of Ultrafast Excited-State Deactivation in Adenosine. Journal of Physical Chemistry A, 2014, 118, 122-127.	2.5	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.	2.5	23
86	Photochemical Mechanisms of Radiationless Deactivation Processes in Urocanic Acid. Journal of Physical Chemistry B, 2014, 118, 976-985.	2.6	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.	2.5	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.	2.5	90
89	Photochemistry of 2-Aminooxazole, a Hypothetical Prebiotic Precursor of RNA Nucleotides. Journal of Physical Chemistry Letters, 2013, 4, 2785-2788.	4.6	29
90	Interpolation of multi-sheeted multi-dimensional potential-energy surfaces via a linear optimization procedure. Journal of Chemical Physics, 2013, 138, 224103.	3.0	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.	3.9	4
92	Strong-pump strong-probe spectroscopy: effects of higher excited electronic states. Physical Chemistry Chemical Physics, 2013, 15, 8119.	2.8	22
93	A multi-sheeted three-dimensional potential-energy surface for the H-atom photodissociation of phenol. Faraday Discussions, 2013, 163, 73.	3.2	33
94	Computational investigation of the photoinduced homolytic dissociation of water in the pyridineâ€“water complex. Physical Chemistry Chemical Physics, 2013, 15, 5957.	2.8	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.	1.9	23
96	Pump-probe spectroscopy with strong pulses as a tool to enhance weak electronic transitions. Physical Review A, 2013, 87, .	2.5	10
97	Spectroscopy meets theory. Nature Chemistry, 2013, 5, 257-258.	13.6	28
98	Jahn-Teller theory beyond the standard model. Journal of Physics: Conference Series, 2013, 428, 012015.	0.4	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.	2.5	10
100	Simulation of femtosecond â€œdouble-slitâ€•experiments for a chromophore in a dissipative environment. Journal of Chemical Physics, 2013, 139, 214302.	3.0	19
101	Domain of validity of the perturbative approach to femtosecond optical spectroscopy. Journal of Chemical Physics, 2013, 139, 224107.	3.0	13
102	Ultrafast non-adiabatic dynamics of ethylene including Rydberg states. Molecular Physics, 2013, 111, 2439-2450.	1.7	41
103	Quantum dynamics of electron-transfer reactions: photoinduced intermolecular electron transfer in a porphyrinâ€“quinone complex. Molecular Physics, 2012, 110, 751-763.	1.7	25
104	Theoretical analysis of photoinduced H-atom elimination in thiophenol. Journal of Chemical Physics, 2012, 136, 174312.	3.0	45
105	Bath-induced correlations and relaxation of vibronic dimers. Journal of Chemical Physics, 2012, 136, 034507.	3.0	22
106	Nonadiabatic Nuclear Dynamics in the Ammonia Cation Studied by the Branching Classical Trajectory Method. Journal of Physics: Conference Series, 2012, 388, 102005.	0.4	0
107	On the nature and signatures of the solvated electron in water. Physical Chemistry Chemical Physics, 2012, 14, 22-34.	2.8	141
108	Relativistic Jahnâ€“Teller and pseudo-Jahnâ€“Teller couplings in systems. Chemical Physics, 2012, 407, 1-8.	1.9	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.	3.0	36
110	Photoinduced water splitting with oxotitanium porphyrin: a computational study. Physical Chemistry Chemical Physics, 2012, 14, 12807.	2.8	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.	3.0	33
112	Role of Conical Intersections in Molecular Spectroscopy and Photoinduced Chemical Dynamics. Annual Review of Physical Chemistry, 2012, 63, 325-352.	10.8	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.	2.6	19
114	Strong and Long Makes Short: Strong-Pump Strong-Probe Spectroscopy. Journal of Physical Chemistry Letters, 2011, 2, 114-119.	4.6	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.	2.1	20
118	Relativistic Jahn-Teller effects in the photoelectron spectra of tetrahedral P4, As4, Sb4, and Bi4. Journal of Chemical Physics, 2011, 135, 104108.	3.0	19
119	Molecular mechanisms of the photostability of indigo. Physical Chemistry Chemical Physics, 2011, 13, 1618-1628.	2.8	86
120	Jahnâ€“Teller and spinâ€“orbit coupling effects in transition-metal trifluorides. Chemical Physics, 2011, 387, 56-65.	1.9	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.	2.1	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.	2.6	22
124	Relativistic TÃ—T and TÃ—E Jahnâ€“Teller coupling in tetrahedral systems. Chemical Physics, 2010, 374, 86-93.	1.9	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.	2.6	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.	4.6	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.	3.0	55
128	Relativistic Jahn-Teller effect in tetrahedral systems. Physical Review A, 2010, 81, .	2.5	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.	2.8	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.	2.8	29
131	Efficient calculation of the polarization induced by N coherent laser pulses. Journal of Chemical Physics, 2009, 131, 194103.	3.0	22
132	Manipulating electronic couplings and nonadiabatic nuclear dynamics with strong laser pulses. Journal of Chemical Physics, 2009, 131, 124505.	3.0	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.	2.6	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.	2.6	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.	13.7	65
136	Efficient Calculation of Time- and Frequency-Resolved Four-Wave-Mixing Signals. Accounts of Chemical Research, 2009, 42, 1290-1298.	15.6	87
137	Biradicalic excited states of zwitterionic phenol-ammonia clusters. Journal of Chemical Physics, 2009, 130, 024302.	3.0	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.	2.5	57
139	Photophysics of xanthine: computational study of the radiationless decay mechanisms. Physical Chemistry Chemical Physics, 2009, 11, 10165.	2.8	34
140	Role of vibrational energy relaxation in the photoinduced nonadiabatic dynamics of pyrrole at the conical intersection. Chemical Physics, 2008, 350, 125-138.	1.9	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.	2.6	10
142	The 3EÃ—E, 4EÃ—E and 5EÃ—E Jahnâ€“Teller Hamiltonians of trigonal systems. Chemical Physics, 2008, 352, 125-134.	1.9	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.	3.0	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.	3.1	58

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145	Computational Model of Photocatalytic Water Splitting. Journal of Physical Chemistry A, 2008, 112, 7311-7313.	2.5	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.	2.5	51
147	Nonradiative Decay Mechanisms of the Biologically Relevant Tautomer of Guanine. Journal of Physical Chemistry A, 2008, 112, 11965-11968.	2.5	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.	7.1	74
149	Ab initio characterization of the conical intersections involved in the photochemistry of phenol. Journal of Chemical Physics, 2008, 129, 224307.	3.0	105
150	Effects of intense femtosecond pumping on ultrafast electronic-vibrational dynamics in molecular systems with relaxation. Journal of Chemical Physics, 2008, 129, 214303.	3.0	45
151	Relativistic EÃ—T Jahnâ€“Teller effect in tetrahedral systems. Journal of Chemical Physics, 2008, 129, 224102.	3.0	32
152	Quasiclassical theory of the dynamicalEâ€‰Ã—â€‰EJahnâ€“Teller effect including spinâ€“orbit interaction. Molecular Physics, 2007, 105, 1471-1485.	1.7	8
153	Spin-orbit vibronic coupling in Î3 states of linear triatomic molecules. Journal of Chemical Physics, 2007, 126, 134312.	3.0	23
154	Computational Studies of the Photophysics of Hydrogen-Bonded Molecular Systems. Journal of Physical Chemistry A, 2007, 111, 11725-11735.	2.5	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.	2.8	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.	2.8	48
158	Photoinduced Electron and Proton Transfer in the Hydrogen-Bonded Pyridineâ‹¯Pyrrole System. Journal of Physical Chemistry B, 2007, 111, 6110-6112.	2.6	31
159	Photophysics of Eumelanin: Ab Initio Studies on the Electronic Spectroscopy and Photochemistry of 5,6-Dihydroxyindole. ChemPhysChem, 2007, 8, 756-762.	2.1	65
160	A study of spinâ€“orbit vibronic-coupling effects in the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si7.gif" display="inline" overflow="scroll"><mml:mrow><mml:mover accent="true"><mml:mrow><mml:mtext>A</mml:mtext></mml:mrow><mml:mrow><mml:mo stretchy="true">â‰¼</mml:mo></mml:mrow></mml:mover><mml:msup><mml:mrow /><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msup><mml:mi mathvariant="normal">Î</mml:	2.6	9
161	Quasistationary upper-well states of EÃ—E Jahnâ€“Teller systems with spin-orbit coupling. Chemical Physics, 2007, 332, 243-248.	1.9	8
162	Analysis of vibrational coherences in homodyne and two-dimensional heterodyne photon-echo spectra of Nile Blue. Chemical Physics, 2007, 341, 113-122.	1.9	22

#	Article	IF	Citations
163	Photoinduced multi-mode quantum dynamics of pyrrole at the â€“ conical intersections. Journal of Photochemistry and Photobiology A: Chemistry, 2007, 190, 177-189.	3.9	44
164	Multimode Molecular Dynamics Beyond the Born-Oppenheimer Approximation. Advances in Chemical Physics, 2007, , 59-246.	0.3	1,010
165	Resonance Raman Spectrum of the Solvated Electron in Methanol:Â Simulation within a Cluster Model. Journal of Physical Chemistry A, 2006, 110, 5613-5619.	2.5	6
166	Conical Intersections in Thymine. Journal of Physical Chemistry A, 2006, 110, 13238-13244.	2.5	200
167	Geometric phase effects in the coherent control of the branching ratio of photodissociation products of phenol. Journal of Chemical Physics, 2006, 124, 224316.	3.0	74
168	Photophysics of Organic Photostabilizers. Ab Initio Study of the Excited-State Deactivation Mechanisms of 2-(2â€˜-Hydroxyphenyl)benzotriazole. Journal of Physical Chemistry A, 2006, 110, 6301-6306.	2.5	107
169	Photoionization-induced dynamics of ammonia:Ab initiopotential energy surfaces and time-dependent wave packet calculations for the ammonia cation. Journal of Chemical Physics, 2006, 124, 214306.	3.0	77
170	Photophysics of intramolecularly hydrogen-bonded aromatic systems: ab initio exploration of the excited-state deactivation mechanisms of salicylic acid. Physical Chemistry Chemical Physics, 2006, 8, 3410.	2.8	131
171	Role of Electron-Driven Proton-Transfer Processes in the Excited-State Deactivation of the Adenineâ‹¯Thymine Base Pair. Journal of Physical Chemistry A, 2006, 110, 9031-9038.	2.5	180
172	The chemical physics of the photostability of life. Europhysics News, 2006, 37, 20-23.	0.3	93
173	Ab initio studies of the photophysics of 2-aminopurine. Molecular Physics, 2006, 104, 1113-1121.	1.7	46
174	The relativistic EÃ—E Jahnâ€“Teller effect revisited. Chemical Physics, 2006, 322, 405-410.	1.9	45
175	Simulation of the photodetachment spectrum of the pyrrolide anion. Chemical Physics, 2006, 329, 50-64.	1.9	20
176	Vibronic effects on resonant electron conduction through single molecule junctions. Chemical Physics Letters, 2006, 430, 355-360.	2.6	36
177	Two-channel semiclassical S-matrix for the EÃ—E Jahnâ€“Teller problem including spinâ€“orbit coupling. Chemical Physics, 2006, 322, 349-353.	1.9	6
178	Generalized diatomics-in-molecule method applied to the anion. Chemical Physics, 2006, 325, 378-388.	1.9	12
179	Study of strong Î£â€“Î and spinâ€“orbit vibronic coupling effects in linear triatomic molecules. Chemical Physics, 2006, 327, 457-467.	1.9	12
180	Importance of Spin-Orbit Coupling for the Assignment of the Photodetachment Spectra of AuX2â‹¯ (X=Cl, Br, and I). ChemPhysChem, 2006, 7, 723-727.	2.1	15

#	Article	IF	Citations
181	Relevance of Electron-Driven Proton-Transfer Processes for the Photostability of Proteins. ChemPhysChem, 2006, 7, 561-564.	2.1	64
182	Calculation of the vibronic structure of the photodetachment spectra of CCClâ^' and CCBrâ^'. Journal of Chemical Physics, 2006, 125, 164327.	3.0	8
183	Calculation of the vibronic structure of the XÌƒÎ2 photoelectron spectra of XCN,X=F, Cl, and Br. Journal of Chemical Physics, 2006, 124, 044317.	3.0	18
184	A new method for the calculation of two-pulse time- and frequency-resolved spectra. Chemical Physics, 2005, 312, 135-143.	1.9	26
185	Photostability of 9H-adenine: mechanisms of the radiationless deactivation of the lowest excited singlet states. Chemical Physics, 2005, 313, 107-112.	1.9	170
186	Isotope effects in vibrational excitation and dissociative electron attachment of DCl and DBr. European Physical Journal D, 2005, 35, 225-230.	1.3	8
187	Charge transport through a flexible molecular junction. European Physical Journal D, 2005, 55, 189-202.	0.4	32
188	Efficient method for the calculation of time- and frequency-resolved four-wave mixing signals and its application to photon-echo spectroscopy. Journal of Chemical Physics, 2005, 123, 164112.	3.0	80
189	Photochemistry of water: The (H2O)5 cluster. Journal of Chemical Physics, 2005, 122, 184320.	3.0	25
190	Remarkable impact of intermode couplings on multimode vibronic dynamics: the photoelectron spectrum of CH3F. Journal of Chemical Physics, 2005, 123, 231103.	3.0	20
191	Experimental and Theoretical Evidence for Long-Lived Molecular Hydrogen AnionsH2â^'andD2â^'. Physical Review Letters, 2005, 94, 223003.	7.8	40
192	Photochemistry of pyrrole: Time-dependent quantum wave-packet description of the dynamics at the Ï€1Ïƒ*-S0 conical intersections. Journal of Chemical Physics, 2005, 123, 144307.	3.0	120
193	Spectroscopic effects of first-order relativistic vibronic coupling in linear triatomic molecules. Journal of Chemical Physics, 2005, 123, 124104.	3.0	20
194	Time- and frequency-resolved fluorescence spectra of nonadiabatic dissipative systems: What photons can tell us. Journal of Chemical Physics, 2005, 122, 134504.	3.0	44
195	Tautomeric selectivity of the excited-state lifetime of guanine/cytosine base pairs: The role of electron-driven proton-transfer processes. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 17903-17906.	7.1	290
196	Time-dependent quantum wave-packet description of the Ï€1Ïƒ* photochemistry of phenol. Journal of Chemical Physics, 2005, 122, 224315.	3.0	177
197	Photochemistry of MCl(H2O)4, M = H, Li, Na clusters: finite-size models of the photodetachment of the chloride anion in salt solutions. Physical Chemistry Chemical Physics, 2005, 7, 970.	2.8	25
198	Transient Phenomena in Time- and Frequency-Gated Spontaneous Emission. Journal of Physical Chemistry A, 2005, 109, 3587-3597.	2.5	5

#	Article	IF	Citations
199	Optimal control of ultrafastcis-transphotoisomerization of retinal in rhodopsin via a conical intersection. Journal of Chemical Physics, 2005, 123, 144508.	3.0	73
200	Ab Initio Studies on the Radiationless Decay Mechanisms of the Lowest Excited Singlet States of 9H-Adenine. Journal of the American Chemical Society, 2005, 127, 6257-6265.	13.7	306
201	Photoinduced dynamics of ethene in the N, V, and Z valence states: A six-dimensional nonadiabatic quantum dynamics investigation. Journal of Chemical Physics, 2004, 120, 11000-11010.	3.0	60
202	THE MULTI-MODE VIBRONIC-COUPLING APPROACH. Advanced Series in Physical Chemistry, 2004, , 323-367.	1.5	86
203	GENERIC ASPECTS OF THE DYNAMICS AT CONICAL INTERSECTIONS: INTERNAL CONVERSION, VIBRATIONAL RELAXATION AND PHOTOISOMERIZATION. Advanced Series in Physical Chemistry, 2004, , 395-427.	1.5	9
204	Ab initio studies on the photophysics of the guanineâ€“cytosine base pair. Physical Chemistry Chemical Physics, 2004, 6, 2763-2771.	2.8	273
205	Quantum dynamical simulations of ultrafast photoinduced electron-transfer processes. Journal of Photochemistry and Photobiology A: Chemistry, 2004, 166, 19-31.	3.9	22
206	Theoretical study of vibrational wave-packet dynamics in electron-transfer systems. Chemical Physics, 2004, 296, 217-229.	1.9	39
207	The relativistic Rennerâ€“Teller effect revisited. Chemical Physics, 2004, 301, 111-127.	1.9	27
208	Time-resolved spontaneous emission beyond the doorwayâ€“window approximation. Chemical Physics, 2004, 301, 129-139.	1.9	22
209	Coherent vibrational dynamics during ultrafast photoinduced electron-transfer reactions: quantum dynamical simulations within multilevel Redfield theory. Chemical Physics Letters, 2004, 384, 157-164.	2.6	24
210	Unified description of sequential and coherent contributions to time-resolved spontaneous emission signals: generalized doorwayâ€“window approach. Chemical Physics Letters, 2004, 391, 234-242.	2.6	16
211	Time-dependent quantum wave-packet description of the1ÏЀÏƒ* photochemistry of pyrrole. Faraday Discussions, 2004, 127, 283-293.	3.2	78
212	Simulation of the resonance Raman spectrum of the hydrated electron in the hydrated-hydronium cluster model. Physical Chemistry Chemical Physics, 2004, 6, 5297.	2.8	20
213	Efficient Deactivation of a Model Base Pair via Excited-State Hydrogen Transfer. Science, 2004, 306, 1765-1768.	12.6	330
214	Intramolecular Hydrogen Bonding in the S1(ÏЀÏ€*) Excited State of Anthranilic Acid and Salicylic Acid:â€‰TDDFT Calculation of Excited-State Geometries and Infrared Spectra. Journal of Physical Chemistry A, 2004, 108, 10917-10922.	2.5	100
215	Multimode Jahn?Teller and pseudo-Jahn?Teller coupling effects in the photoelectron spectrum of CH3F. Chemical Physics, 2004, 304, 17-17.	1.9	3
216	Conical Intersections. Advanced Series in Physical Chemistry, 2004, , .	1.5	864

#	Article	IF	Citations
217	FEMTOSECOND TIME-RESOLVED SPECTROSCOPY OF THE DYNAMICS AT CONICAL INTERSECTIONS. Advanced Series in Physical Chemistry, 2004, , 739-801.	1.5	3
218	The Sudden-Polarization Effect and its Role in the Ultrafast Photochemistry of Ethene. Angewandte Chemie - International Edition, 2003, 42, 3434-3436.	13.8	33
219	Ab initio study of the excited-state coupled electronâ€“proton-transfer process in the 2-aminopyridine dimer. Chemical Physics, 2003, 294, 73-83.	1.9	166
220	Quasiclassical quantization of the four-state vibronic problem associated with accidentally degenerate Î£+, Î and Î£â^' states. Chemical Physics, 2003, 293, 179-191.	1.9	3
221	Theoretical investigation of Jahnâ€“Teller and pseudo-Jahnâ€“Teller interactions in the ammonia cation. Journal of Chemical Physics, 2003, 118, 5880-5893.	3.0	31
222	Detection of Electronic and Vibrational Coherence Effects in Electron-Transfer Systems by Femtosecond Time-Resolved Fluorescence Spectroscopy:â€‰ Theoretical Aspects. Journal of Physical Chemistry A, 2003, 107, 2657-2666.	2.5	35
223	Photochemistry of HCl(H2O)4:Â Cluster Model of the Photodetachment of the Chloride Anion in Water. Journal of Physical Chemistry A, 2003, 107, 1557-1562.	2.5	40
224	Anionic water clusters with large vertical electron binding energies and their electronic spectra: (H2O)11â€“ and (H2O)14â€“. Physical Chemistry Chemical Physics, 2003, 5, 1130-1136.	2.8	30
225	A simple model for the calculation of nonlinear optical response functions and femtosecond time-resolved spectra. Journal of Chemical Physics, 2003, 118, 5287-5301.	3.0	35
226	Photoinduced dynamics of the valence states of ethene: A six-dimensional potential-energy surface of three electronic states with several conical intersections. Journal of Chemical Physics, 2003, 119, 1397-1411.	3.0	65
227	CHEMISTRY: Unraveling the Molecular Mechanisms of Photoacidity. Science, 2003, 302, 1693-1694.	12.6	158
228	Modeling of ultrafast electron-transfer processes: Validity of multilevel Redfield theory. Journal of Chemical Physics, 2003, 119, 2761-2773.	3.0	151
229	Vibrational excitation of hydrogen fluoride by low-energy electrons: theory and experiment. Journal of Physics B: Atomic, Molecular and Optical Physics, 2003, 36, 2837-2849.	1.5	34
230	Multilevel Redfield description of the dissipative dynamics at conical intersections. Journal of Chemical Physics, 2002, 116, 263.	3.0	119
231	Time- and frequency-gated spontaneous emission as a tool for studying vibrational dynamics in the excited state. Physical Review A, 2002, 65, .	2.5	34
232	Ab Initio Investigation of the Structure and Spectroscopy of Hydroniumâ^'Water Clusters. Journal of Physical Chemistry A, 2002, 106, 4158-4167.	2.5	154
233	Excited-state hydrogen detachment and hydrogen transfer driven by repulsive 1Ï€Ïƒ* states: A new paradigm for nonradiative decay in aromatic biomolecules. Physical Chemistry Chemical Physics, 2002, 4, 1093-1100.	2.8	881
234	Hydrated hydronium: a cluster model of the solvated electron?. Physical Chemistry Chemical Physics, 2002, 4, 4-10.	2.8	133

#	Article	IF	Citations
235	Four-channel semiclassical S-matrix for a Î£+â€“Îâ€“Î£â^'-type conical intersection in triatomic systems. Chemical Physics, 2002, 279, 215-228.	1.9	6
236	Development of an effective single-electron model of the electronic structure of hydronium and hydroniumâ€“water clusters. Chemical Physics Letters, 2002, 356, 556-562.	2.6	13
237	Title is missing!. European Physical Journal D, 2002, 52, 1057-1070.	0.4	18
238	On the mechanism of nonradiative decay of DNA bases: ab initio and TDDFT results for the excited states of 9H-adenine. European Physical Journal D, 2002, 20, 369-374.	1.3	198
239	Photoinduced Electron and Proton Transfer in Phenol and Its Clusters with Water and Ammonia. Journal of Physical Chemistry A, 2001, 105, 9275-9283.	2.5	273
240	Modeling of ultrafast electron-transfer dynamics: multi-level Redfield theory and validity of approximations. Chemical Physics, 2001, 268, 105-120.	1.9	101
241	Ab initio investigation of the potential energy surfaces involved in the photophysics of s-trans-1,3-butadiene. Chemical Physics, 2001, 269, 1-10.	1.9	43
242	Theoretical investigation of vibronic-coupling and ultrafast internal-conversion dynamics in the acetylene cation. Chemical Physics, 2001, 272, 1-14.	1.9	16
243	Generalized diatomics-in-molecules method for polyatomic anions. Physical Review A, 2001, 65, .	2.5	22
244	1â€“2 conical intersection in trans-butadiene: ultrafast dynamics and optical spectra. Chemical Physics Letters, 2000, 320, 535-541.	2.6	71
245	Effect of a dissipative environment on the dynamics at a conical intersection. Chemical Physics, 2000, 259, 227-236.	1.9	34
246	Conical intersections induced by repulsive 1Ï€Ïƒ* states in planar organic molecules: malonaldehyde, pyrrole and chlorobenzene as photochemical model systems. Chemical Physics, 2000, 259, 181-191.	1.9	221
247	Photoejection of electrons from pyrrole into an aqueous environment: ab initio results on pyrrole-water clusters. Chemical Physics Letters, 2000, 321, 479-484.	2.6	56
248	Photoinduced charge separation in indoleâ€“water clusters. Chemical Physics Letters, 2000, 329, 130-137.	2.6	68
249	Electron scattering in cooled HCl: boomerang structures and outer-well resonances in elastic and vibrational excitation cross sections. Journal of Physics B: Atomic, Molecular and Optical Physics, 2000, 33, L209-L213.	1.5	35
250	Molecular-dynamics simulations of solvent effects in the intramolecular charge transfer of 4-(N,N-dimethylamino)benzonitrile. Physical Chemistry Chemical Physics, 2000, 2, 4341-4353.	2.8	39
251	Associative detachment, dissociative attachment, and vibrational excitation of HCl by low-energy electrons. Physical Review A, 1999, 60, 2873-2881.	2.5	51
252	Ab initio study of the amino group twisting and wagging reaction paths in the intramolecular charge transfer of 4-(N,N-dimethylamino)benzonitrile. Chemical Physics, 1999, 240, 9-18.	1.9	54

#	Article	IF	Citations
253	On the mechanism of rapid non-radiative decay in intramolecularly hydrogen-bonded ÏЄ systems. Chemical Physics Letters, 1999, 300, 533-539.	2.6	53
254	Potential-energy function for intramolecular proton transfer in the malonaldehyde cation. Chemical Physics Letters, 1999, 310, 548-552.	2.6	5
255	Ab initio investigations on the photophysics of indole. Chemical Physics Letters, 1999, 315, 293-298.	2.6	213
256	Photophysics of Malonaldehyde:Â An ab Initio Study. Journal of Physical Chemistry A, 1999, 103, 4494-4504.	2.5	104
257	Ab initio potential-energy functions for excited state intramolecular proton transfer: a comparative study of o-hydroxybenzaldehyde, salicylic acid and 7-hydroxy-1-indanone. Physical Chemistry Chemical Physics, 1999, 1, 3065-3072.	2.8	246
258	Vibrational coherence in ultrafast electron-transfer dynamics of oxazine 1 in N,N-dimethylaniline: simulation of a femtosecond pump-probe experiment. Chemical Physics, 1998, 233, 323-334.	1.9	66
259	Generalization of the nonlocal resonance model for low-energy electron collisions with hydrogen halides: the variable threshold exponent. Theoretical Chemistry Accounts, 1998, 100, 31-35.	1.4	17
260	Ab initio study of excited-state intramolecular proton dislocation in salicylic acid. Chemical Physics, 1998, 232, 257-265.	1.9	115
261	Ab Initio Investigation of Reaction Pathways for Intramolecular Charge Transfer in Dimethylanilino Derivatives. Journal of Physical Chemistry A, 1998, 102, 2716-2722.	2.5	129
262	Theory of vibrational relaxation processes in resonant collisions of low-energy electrons with large molecules. Journal of Chemical Physics, 1998, 109, 6577-6595.	3.0	36
263	Nuclear dynamics of the H collision complex beyond the local approximation: associative detachment and dissociative attachment to rotationally and vibrationally excited molecules. Journal of Physics B: Atomic, Molecular and Optical Physics, 1998, 31, 2571-2583.	1.5	86
264	Effect of a thermal bath on electronic resonance decay: A numerical path-integral study. Physical Review A, 1998, 58, 1152-1161.	2.5	9
265	Photodissociation of ozone in the Chappuis band. III. Product state distributions. Journal of Chemical Physics, 1998, 109, 2680-2684.	3.0	21
266	Photodissociation of ozone in the Chappuis band. II. Time-dependent wave-packet calculations and interpretation of diffuse vibrational structures. Journal of Chemical Physics, 1997, 107, 7296-7313.	3.0	40
267	Photodissociation of ozone in the Chappuis band. I. Electronic structure calculations. Journal of Chemical Physics, 1997, 107, 7282-7295.	3.0	56
268	Model study of near-threshold photoionization of large molecules: The effect of vibrational relaxation. Journal of Chemical Physics, 1997, 106, 3174-3185.	3.0	5
269	Mechanism of photoinduced intramolecular charge transfer in aminobenzethynes: an ab initio study. Journal of Photochemistry and Photobiology A: Chemistry, 1997, 105, 325-328.	3.9	6
270	Femtosecond pump-probe spectroscopy of electron-transfer systems: a nonperturbative approach. Chemical Physics, 1997, 217, 275-287.	1.9	56

#	Article	IF	Citations
271	Intramolecular electron-transfer dynamics in the inverted regime: quantum mechanical multi-mode model including dissipation. Chemical Physics Letters, 1996, 259, 113-118.	2.6	44
272	Promotion of intramolecular charge transfer in dimethylamino derivatives: twisting versus acceptor-group rehybridization. Chemical Physics Letters, 1996, 259, 119-127.	2.6	143
273	Charge transfer in aminobenzonitriles: do they twist?. Chemical Physics Letters, 1996, 250, 428-436.	2.6	179
274	Real-time path-integral approach for general two-state multi-mode vibronic-coupling models. Chemical Physics, 1996, 206, 63-72.	1.9	7
275	Calculation of cross sections for vibrational excitation and dissociative attachment in electron collisions with HBr and DBr. Physical Review A, 1996, 53, 2262-2271.	2.5	31
276	Calculation of dissociative electron attachment and vibrational excitation cross-section of HBr. Chemical Physics Letters, 1995, 234, 304-308.	2.6	7
277	Multi-mode vibronic coupling with dissipation. Application of the Monte Carlo wavefunction propagation method. Chemical Physics Letters, 1995, 235, 370-376.	2.6	53
278	Recursive evaluation of the real-time path integral for dissipative systems. The spin-boson model. Chemical Physics Letters, 1995, 236, 445-450.	2.6	30
279	A model for the quantum dynamics of Rydberg states of large molecules. Chemical Physics Letters, 1995, 245, 364-370.	2.6	3
280	Path-integral treatment of the real-time dynamics of few-mode spin-boson models. Chemical Physics, 1995, 200, 11-21.	1.9	8
281	Pathâ€integral treatment of multiâ€mode vibronic coupling. II. Correlation expansion of class averages. Journal of Chemical Physics, 1995, 102, 6499-6510.	3.0	29
282	Resonance Raman spectroscopy of theS1andS2states of pyrazine: Experiment and first principles calculation of spectra. Journal of Chemical Physics, 1995, 103, 6851-6860.	3.0	81
283	Nonperturbative approach to femtosecond spectroscopy: General theory and application to multidimensional nonadiabatic photoisomerization processes. Journal of Chemical Physics, 1995, 103, 3998-4011.	3.0	197
284	Pathâ€integral treatment of multiâ€mode vibronic coupling. Journal of Chemical Physics, 1994, 100, 926-937.	3.0	73
285	Characterization of theS1â€“S2conical intersection in pyrazine usingabinitiomulticonfiguration selfâ€consistentâ€field and multireference configurationâ€interaction methods. Journal of Chemical Physics, 1994, 100, 1400-1413.	3.0	193
286	Diabatic CASSCF orbitals and wavefunctions. Chemical Physics Letters, 1994, 226, 257-262.	2.6	77
287	Model studies on femtosecond spectroscopy of multidimensional photoisomerization and internal-conversion dynamics. A nonperturbative approach. Chemical Physics Letters, 1994, 228, 665-671.	2.6	19
288	Theoretical investigation of potential energy surfaces relevant for excited-state hydrogen transfer in o-hydroxybenzaldehyde. Chemical Physics, 1994, 184, 115-124.	1.9	100

#	Article	IF	Citations
289	Microscopic modelling of photoisomerization and internal-conversion dynamics. Chemical Physics, 1994, 186, 27-40.	1.9	112
290	Evidence for the need of a non-Bornâ€"Oppenheimer description of excited-state hydrogen transfer. Chemical Physics Letters, 1993, 211, 82-87.	2.6	46
291	XÌƒ2AGâ€"Ãƒ 2B1g conical intersection in the pyrazine cation and its effect on the photoelectron spectrum. Chemical Physics Letters, 1993, 205, 117-122.	2.6	24
292	Internal conversion funnel in benzene and pyrazine: adiabatic and diabatic representation. Chemical Physics Letters, 1993, 203, 220-226.	2.6	38
293	Vibronic coupling in the pEâ€³ Rydberg series of NH3. Chemical Physics Letters, 1993, 204, 505-510.	2.6	5
294	Direct construction of diabatic states in the CASSCF approach. Application to the conical intersection of the 1A2 and 1B1 excited states of ozone. Chemical Physics Letters, 1993, 216, 362-368.	2.6	141
295	Time-dependent wave-packet description of dissociative electron attachment. Physical Review A, 1993, 47, 1031-1044.	2.5	49
296	Femtosecond spectroscopy of ultrafast nonadiabatic excited-state dynamics on the basis of ab initio potential-energy surfaces: the S2 state of pyrazine. The Journal of Physical Chemistry, 1993, 97, 12466-12472.	2.9	42
297	Systematically improved local complex potential approximation for the dynamics of electron-molecule collision complexes. Journal of Physics B: Atomic, Molecular and Optical Physics, 1993, 26, 2927-2942.	1.5	13
298	Path-integral approach to resonant electron-molecule scattering. Physical Review A, 1993, 47, 2838-2855.	2.5	24
299	Path-integral approach to resonant electron-molecule scattering. II. Second-order cumulant approximation and multimode applications. Physical Review A, 1993, 48, 4272-4285.	2.5	12
300	Ab initioinvestigation of potentialâ€energy surfaces involved in the photophysics of benzene and pyrazine. Journal of Chemical Physics, 1993, 98, 5627-5641.	3.0	140
301	Detection of ultrafast molecular-excited-state dynamics with time- and frequency-resolved pump-probe spectroscopy. Physical Review A, 1992, 45, 3032-3040.	2.5	90
302	Theoretische Chemie 1991. Nachrichten Aus Der Chemie, 1992, 40, 204-209.	0.0	0
303	Abinitiocharacterization of theS1â€“S2conical intersection in pyrazine and calculation of spectra. Journal of Chemical Physics, 1992, 96, 5298-5309.	3.0	110
304	Perturbation of the Jahn-Teller effect by partial isotopic substitution: multi-mode vibronic coupling in the X 2E1g and B 2E2g states of 1,4-C6H4D+2. Chemical Physics, 1992, 163, 133-147.	1.9	18
305	Theoretical study of the photoelectron spectrum of allene. Chemical Physics, 1992, 162, 349-358.	1.9	26
306	Model study on the real-time detection of ultrafast nonadiabatic dynamics associated with the Wulf-Chappuis bands of ozone. Chemical Physics Letters, 1992, 200, 163-172.	2.6	15

#	Article	IF	Citations
307	Model studies on femtosecond time-resolved ionization spectroscopy of excited-state vibrational dynamics and vibronic coupling. Chemical Physics, 1991, 151, 59-72.	1.9	78
308	Vibronic coupling in Rydberg series of linear molecules. Chemical Physics, 1991, 156, 21-31.	1.9	4
309	Theory of resonance and threshold effects in electron-molecule collisions: The projection-operator approach. Physics Reports, 1991, 208, 97-188.	25.6	396
310	Femtosecond timeâ€resolved ionization spectroscopy of ultrafast internalâ€conversion dynamics in polyatomic molecules: Theory and computational studies. Journal of Chemical Physics, 1991, 95, 7806-7822.	3.0	256
311	Ab initio investigation of the multimode dynamical Jahn-Teller effect in the XÌƒ 2E1g state of the benzene cation. Chemical Physics Letters, 1991, 177, 345-351.	2.6	64
312	Jahnâ€"Teller effect of the 2e2g level of chemisorbed benzene. Chemical Physics Letters, 1991, 180, 133-138.	2.6	19
313	Photophysically relevant potential energy functions of low-lying singlet states of benzene, pyridine and pyrazine: an ab initio study. Chemical Physics Letters, 1991, 180, 381-386.	2.6	50
314	Friction in dissociative attachment. Journal of Physics B: Atomic, Molecular and Optical Physics, 1991, 24, L367-L374.	1.5	7
315	Jahnâ€"Teller coupling in Rydberg series of benzene. Journal of Chemical Physics, 1991, 94, 5402-5413.	3.0	12
316	Threshold phenomena in low-energy electronâ€"polarâ€"molecule collisions: The nonlocal resonance model. AIP Conference Proceedings, 1990, , .	0.4	1
317	Theory of resonance Raman scattering and fluorescence from strongly vibronically coupled excited states of polyatomic molecules. Journal of Chemical Physics, 1990, 93, 5496-5509.	3.0	67
318	Aspects of dissipative electronic and vibrational dynamics of strongly vibronically coupled systems. Journal of Chemical Physics, 1990, 92, 1045-1061.	3.0	141
319	Non-Markovian dynamics of electron-molecule collision complexes. Physical Review A, 1989, 40, 1262-1278.	2.5	19
320	MQDT analysis of radiationless decay rates of autoionizing rydberg states of polyatomic molecules. Chemical Physics Letters, 1989, 162, 336-341.	2.6	12
321	Surface-hopping-induced femtosecond vibrational dephasing in strongly vibronically coupled systems. Chemical Physics Letters, 1989, 159, 61-65.	2.6	22
322	Theoretical studies on the femtosecond realâ€time measurement of ultrafast electronic decay in polyatomic molecules. Journal of Chemical Physics, 1989, 90, 7184-7194.	3.0	87
323	S1-S2 Conical intersection and ultrafast S2â†'S1 Internal conversion in pyrazine. Chemical Physics Letters, 1988, 150, 235-242.	2.6	92
324	Model studies on the time-resolved measurement of excited-state vibrational dynamics and vibronic coupling. Chemical Physics, 1988, 124, 227-238.	1.9	36

#	Article	IF	Citations
325	Interplay of Jahnâ€“Teller and pseudoâ€Jahnâ€“Teller vibronic dynamics in the benzene cation. Journal of Chemical Physics, 1988, 89, 2023-2040.	3.0	173
326	Resonances in molecular photoionization. IV. Theory of oneâ€color and twoâ€color nearâ€threshold photoionization of molecules. Journal of Chemical Physics, 1988, 89, 6209-6219.	3.0	14
327	Resonances in molecular photoionization. III. Multichannel extension and application to polyatomic molecules. Journal of Chemical Physics, 1988, 88, 5571-5579.	3.0	18
328	Friction and memory effects in the dynamics of short-lived negative ions. Journal of Physics B: Atomic, Molecular and Optical Physics, 1988, 21, L205-L211.	1.5	18
329	Resonances in molecular photoionization. I. Model calculations and analysis of general phenomena. Journal of Chemical Physics, 1987, 86, 176-187.	3.0	18
330	Model calculation on the pump-probe measurement of ultrafast electronic population decay in polyatomic molecules. Chemical Physics Letters, 1987, 140, 133-141.	2.6	45
331	Analytic expressions for the matrix elements of the morse green function with morse wavefunctions. Chemical Physics, 1986, 105, 137-143.	1.9	6
332	Direct calculation of complex resonance poles using separable expansions of the potential: Application to theÎ£u+2shape resonance in electron-H2scattering. Physical Review A, 1986, 33, 222-232.	2.5	12
333	Vibronic coupling of shortâ€lived electronic states. Journal of Chemical Physics, 1986, 84, 152-169.	3.0	81
334	Projection-operator calculations for molecular shape resonances: TheÎ£u+2resonance in electron-hydrogen scattering. Physical Review A, 1985, 31, 641-651.	2.5	61
335	Nuclear dynamics in resonant electron-molecule scattering beyond the local approximation: Vibrational excitation and dissociative attachment inH2andD2. Physical Review A, 1985, 32, 181-193.	2.5	116
336	Projection-operator calculations for shape resonances: A new method based on the many-body optical-potential approach. Physical Review A, 1984, 29, 2485-2496.	2.5	42
337	An accurate potential energy function of the H2â¯ ion at large internuclear distances. Chemical Physics Letters, 1984, 111, 211-214.	2.6	41
338	Strong non-adiabatic effects in C2D4+. Chemical Physics Letters, 1984, 110, 469-473.	2.6	7
339	Symmetry Breaking and Non-Born-Oppenheimer Effects in Radical Cations. Angewandte Chemie International Edition in English, 1983, 22, 210-224.	4.4	62
340	Theoretical study of electron transmission through N2. Chemical Physics Letters, 1983, 97, 352-356.	2.6	4
341	Theory of resonance and threshold effects in the electronic excitation of molecules by electron impact. Physical Review A, 1983, 28, 3315-3327.	2.5	7
342	Nuclear dynamics in resonant electron-molecule scattering beyond the local approximation: The 2.3-eV shape resonance inN2. Physical Review A, 1983, 28, 1363-1381.	2.5	123

#	Article	IF	Citations
343	Projection-operator approach to potential scattering. Physical Review A, 1983, 28, 2777-2791.	2.5	43
344	Strong nonadiabatic effects and conical intersections in molecular spectroscopy and unimolecular decay: C2H4+. Journal of Chemical Physics, 1982, 77, 2014-2022.	3.0	102
345	Strong non-condon effects induced by electron correlation: N2O+. Chemical Physics, 1982, 69, 175-183.	1.9	43
346	The effect of a resonance on vibrational structure in the photoelectron spectrum of acetylene. Chemical Physics Letters, 1981, 77, 242-245.	2.6	44
347	On the valence shell binding energy spectrum of carbonyl sulphide. Journal of Electron Spectroscopy and Related Phenomena, 1981, 22, 261-270.	1.7	35
348	Theoretical studies of inner-valence-shell photoionization cross sections in N2 and CO. Chemical Physics, 1981, 58, 71-91.	1.9	137
349	Green's function calculations on the complete valence ionization spectra of HF, HCl, HBr AND HI. Chemical Physics, 1981, 56, 43-52.	1.9	65
350	Theory of vibronic coupling in linear molecules. Journal of Chemical Physics, 1981, 74, 2945-2968.	3.0	83
351	Spectroscopic effects of conical intersections of molecular potential energy surfaces. Molecular Physics, 1981, 43, 851-875.	1.7	155
352	Photon energy dependence of satelite line intensity in the photoelectron spectrum of acetylene. Chemical Physics Letters, 1980, 70, 36-40.	2.6	42
353	Two-mode jahn-teller effect in nh+3. Chemical Physics Letters, 1980, 72, 427-431.	2.6	26
354	Effective single-mode Hamiltonian for the calculation of multi-mode Jahn-Teller band shapes. Solid State Communications, 1980, 35, 879-881.	1.9	19
355	The EâŠ—(Ïµ + Ïµ) Jahn-Teller effect. Molecular Physics, 1980, 41, 1291-1315.	1.7	45
356	Jahn-Teller effect for very strong coupling. Molecular Physics, 1980, 41, 669-677.	1.7	32
357	Many-Body Effects in Valence and Core Photoionization of Molecules. Physica Scripta, 1980, 21, 481-491.	2.5	125
358	Dynamical calculation of satellite intensities. Journal of Chemical Physics, 1980, 72, 1348-1358.	3.0	25
359	Many-body theory of core holes. Physical Review A, 1980, 22, 206-222.	2.5	238
360	Vibrational State Dependence of the Photoelectron Angular Asymmetry Parameter caused by Vibronic Coupling. Physica Scripta, 1979, 19, 11-15.	2.5	31

#	Article	IF	Citations
361	Strong correlation effects in the ionisation of CS2. Chemical Physics Letters, 1979, 61, 30-35.	2.6	66
362	The influence of finite lifetime of electronic states on the vibrational structure of molecular electronic spectra. Chemical Physics, 1979, 44, 33-44.	1.9	89
363	Vibronic coupling in linear molecules and linear-to-bent transitions: HCN. Chemical Physics, 1979, 37, 303-317.	1.9	67
364	Experimental and theoretical investigation of the complete valence shell ionization spectra of CO2and N2O. Chemical Physics, 1979, 40, 171-183.	1.9	113
365	Negative shake-up energy in core ionization. Chemical Physics, 1979, 39, 149-157.	1.9	56
366	On the adequacy of the molecular-orbital picture for describing ionization processes. International Journal of Quantum Chemistry, 1978, 14, 593-601.	2.0	51
367	Jahnâ€"Teller effect induced by non-degenerate vibrational modes in cumulenes. Chemical Physics, 1978, 33, 319-326.	1.9	52
368	Electronic recoil effects in high-energy photoelectron spectroscopy. Journal of Electron Spectroscopy and Related Phenomena, 1978, 13, 161-173.	1.7	67
369	Breakdown of the molecular orbital picture of ionization for inner valence electrons: experimental and theoretical study of H2S and PH3. Journal of Electron Spectroscopy and Related Phenomena, 1978, 14, 59-72.	1.7	58
370	Complete breakdown of the quasiparticle picture for inner-valence electrons: Hydrogen cyanide and formic acid. Chemical Physics Letters, 1978, 57, 582-587.	2.6	24
371	Correlation effects in the ionization of hydrocarbons. Journal of Chemical Physics, 1978, 69, 1591-1603.	3.0	222
372	Vibronic coupling effects in the photoelectron spectrum of ethylene. Journal of Chemical Physics, 1978, 69, 4252-4263.	3.0	119
373	The Jahn-Teller effect in NH3+. Molecular Physics, 1978, 35, 1283-1299.	1.7	25
374	Localized and delocalized core holes and their interrelation. Journal of Chemical Physics, 1977, 66, 5084-5086.	3.0	138
375	Ionization potentials and vibrational structure in photoelectron spectra by a Greenâ€™s function method:transâ€HNNH,cisâ€HNNH, and 1,1â€dihydrodiazine (H2NN). Journal of Chemical Physics, 1977, 67, 44-51.	3.0	29
376	Manyâ€body calculations on molecules with secondâ€row atoms: H2S and H2CS. Journal of Chemical Physics, 1977, 66, 4893-4899.	3.0	51
377	Intrinsic and extrinsic plasmon coupling in x-ray photoemission from core states of adsorbed atoms. Physical Review B, 1977, 16, 1480-1488.	3.2	77
378	A comparison of different approaches to the calculation of franck-condon factors for polyatomic molecules. Molecular Physics, 1977, 34, 1759-1770.	1.7	81

#	Article	IF	Citations
379	A difficult assignment problem. Molecular Physics, 1977, 34, 381-396.	1.7	54
380	Radiative electron-attachment spectra of O3and SO2. Molecular Physics, 1977, 33, 1399-1406.	1.7	22
381	Theory of the vibrational structure of resonances in electron-molecule scattering. Physical Review A, 1977, 16, 1465-1482.	2.5	114
382	On the photoelectron spectrum of PN. Journal of Electron Spectroscopy and Related Phenomena, 1977, 11, 239-243.	1.7	6
383	Strong vibronic coupling effects in ionization spectra: The â€œmystery bandâ€•of butatriene. Chemical Physics, 1977, 26, 169-177.	1.9	131
384	Vibronic coupling and symmetry breaking in core electron ionization. Chemical Physics, 1977, 25, 189-196.	1.9	162
385	Strong Correlation Effects in inner Valence Ionization of N2 AND CO. Chemical Physics, 1977, 26, 149-153.	1.9	141
386	Ionization potentials of HCN and HNC by a Green's function method. Molecular Physics, 1976, 32, 1057-1061.	1.7	33
387	Calculation of the HeI photoelectron spectrum of CS including satellite lines. Chemical Physics Letters, 1976, 43, 258-262.	2.6	24
388	Ionization potentials of ethylene, allene and butatriene by a green function method. Chemical Physics, 1976, 18, 469-476.	1.9	55
389	A manyâ€body approach to the vibrational structure in molecular electronic spectra. I. Theory. Journal of Chemical Physics, 1976, 64, 603-611.	3.0	199
390	A manyâ€body approach to the vibrational structure in molecular electronic spectra. II. Application to nitrogen, carbon monoxide, and formaldehyde. Journal of Chemical Physics, 1976, 64, 612-625.	3.0	64
391	On the controversial assignment of the ionization potentials of formaldehyde. Chemical Physics Letters, 1975, 34, 60-62.	2.6	37
392	On the vibrational structure in inner-shell ionization spectra by a many-body approach. Chemical Physics Letters, 1975, 31, 582-587.	2.6	41
393	A theoretical photoelectron spectrum of cyanogen by a Green-function method. Chemical Physics, 1975, 10, 459-470.	1.9	52
394	On the vibrational structure in photoelectron spectra by the method of Green's functions. Journal of Chemical Physics, 1974, 60, 2878-2889.	3.0	101
395	Plasmon coupling to core hole excitations in carbon. Journal of Physics C: Solid State Physics, 1974, 7, 4503-4512.	1.5	36
396	Chemical Reactivity in the Ground and the Excited State. , 0, , 313-497.		1