Wolfgang Domcke

List of Publications by Year
in descending order

396 papers	24,044 citations	6233 80 h-index	11899 134 g-index
400 all docs	400 docs citations	400 times ranked	7948 citing authors

#	Article	IF	Citations
1	Multimode Molecular Dynamics Beyond the Born-Oppenheimer Approximation. Advances in Chemical Physics, 2007, , 59-246.	0.3	1,010
2	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.	1.3	881
3	Conical Intersections. Advanced Series in Physical Chemistry, 2004, , .	1.5	864
4	Role of Conical Intersections in Molecular Spectroscopy and Photoinduced Chemical Dynamics. Annual Review of Physical Chemistry, 2012, 63, 325-352.	4.8	401
5	Theory of resonance and threshold effects in electron-molecule collisions: The projection-operator approach. Physics Reports, 1991, 208, 97-188.	10.3	396
6	Efficient Deactivation of a Model Base Pair via Excited-State Hydrogen Transfer. Science, 2004, 306, 1765-1768.	6.0	330
7	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.	6.6	306
8	Conical Intersections. Advanced Series in Physical Chemistry, 2011, , .	1.5	300
9	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.	3.3	290
10	Theory of Ultrafast Nonadiabatic Excited-State Processes and their Spectroscopic Detection in Real Time. Advances in Chemical Physics, 2007, , 1-169.	0.3	282
11	Photoinduced Electron and Proton Transfer in Phenol and Its Clusters with Water and Ammonia. Journal of Physical Chemistry A, 2001, 105, 9275-9283.	1.1	273
12	Ab initio studies on the photophysics of the guanineâ€“cytosine base pair. Physical Chemistry Chemical Physics, 2004, 6, 2763-2771.	1.3	273
13	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.	1.2	256
14	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.	1.3	246
15	Many-body theory of core holes. Physical Review A, 1980, 22, 206-222.	1.0	238
16	Computational Studies of the Photophysics of Hydrogen-Bonded Molecular Systems. Journal of Physical Chemistry A, 2007, 111, 11725-11735.	1.1	227
17	Correlation effects in the ionization of hydrocarbons. Journal of Chemical Physics, 1978, 69, 1591-1603.	1.2	222
18	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.	0.9	221

#	Article	IF	Citations
19	Ab initio investigations on the photophysics of indole. Chemical Physics Letters, 1999, 315, 293-298.	1.2	213
20	Conical Intersections in Thymine. Journal of Physical Chemistry A, 2006, 110, 13238-13244.	1.1	200
21	A manyâ€body approach to the vibrational structure in molecular electronic spectra. I. Theory. Journal of Chemical Physics, 1976, 64, 603-611.	1.2	199
22	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.	0.6	198
23	Nonperturbative approach to femtosecond spectroscopy: General theory and application to multidimensional nonadiabatic photoisomerization processes. Journal of Chemical Physics, 1995, 103, 3998-4011.	1.2	197
24	Characterization of theS1â€“S2conical intersection in pyrazine usingabinitiomulticonfiguration selfâ€consistentâ€field and multireference configurationâ€interaction methods. Journal of Chemical Physics, 1994, 100, 1400-1413.	1.2	193
25	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.	1.1	180
26	Charge transfer in aminobenzonitriles: do they twist?. Chemical Physics Letters, 1996, 250, 428-436.	1.2	179
27	Time-dependent quantum wave-packet description of the Ï€1Ïƒ* photochemistry of phenol. Journal of Chemical Physics, 2005, 122, 224315.	1.2	177
28	Interplay of Jahnâ€“Teller and pseudoâ€Jahnâ€“Teller vibronic dynamics in the benzene cation. Journal of Chemical Physics, 1988, 89, 2023-2040.	1.2	173
29	Photostability of 9H-adenine: mechanisms of the radiationless deactivation of the lowest excited singlet states. Chemical Physics, 2005, 313, 107-112.	0.9	170
30	Ab initio study of the excited-state coupled electronâ€“proton-transfer process in the 2-aminopyridine dimer. Chemical Physics, 2003, 294, 73-83.	0.9	166
31	Vibronic coupling and symmetry breaking in core electron ionization. Chemical Physics, 1977, 25, 189-196.	0.9	162
32	CHEMISTRY: Unraveling the Molecular Mechanisms of Photoacidity. Science, 2003, 302, 1693-1694.	6.0	158
33	Spectroscopic effects of conical intersections of molecular potential energy surfaces. Molecular Physics, 1981, 43, 851-875.	0.8	155
34	Ab Initio Investigation of the Structure and Spectroscopy of Hydroniumâ‹¯Water Clusters. Journal of Physical Chemistry A, 2002, 106, 4158-4167.	1.1	154
35	Modeling of ultrafast electron-transfer processes: Validity of multilevel Redfield theory. Journal of Chemical Physics, 2003, 119, 2761-2773.	1.2	151
36	Promotion of intramolecular charge transfer in dimethylamino derivatives: twisting versus acceptor-group rehybridization. Chemical Physics Letters, 1996, 259, 119-127.	1.2	143

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37	Strong Correlation Effects in inner Valence Ionization of N2 AND CO. Chemical Physics, 1977, 26, 149-153.	0.9	141
38	Aspects of dissipative electronic and vibrational dynamics of strongly vibronically coupled systems. Journal of Chemical Physics, 1990, 92, 1045-1061.	1.2	141
39	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.	1.2	141
40	On the nature and signatures of the solvated electron in water. Physical Chemistry Chemical Physics, 2012, 14, 22-34.	1.3	141
41	Ab initioinvestigation of potentialâ€energy surfaces involved in the photophysics of benzene and pyrazine. Journal of Chemical Physics, 1993, 98, 5627-5641.	1.2	140
42	Localized and delocalized core holes and their interrelation. Journal of Chemical Physics, 1977, 66, 5084-5086.	1.2	138
43	Theoretical studies of inner-valence-shell photoionization cross sections in N2 and CO. Chemical Physics, 1981, 58, 71-91.	0.9	137
44	Hydrated hydronium: a cluster model of the solvated electron?. Physical Chemistry Chemical Physics, 2002, 4, 4-10.	1.3	133
45	Strong vibronic coupling effects in ionization spectra: The â€œmystery bandâ€•of butatriene. Chemical Physics, 1977, 26, 169-177.	0.9	131
46	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.	1.3	131
47	Ab Initio Investigation of Reaction Pathways for Intramolecular Charge Transfer in Dimethylanilino Derivatives. Journal of Physical Chemistry A, 1998, 102, 2716-2722.	1.1	129
48	Many-Body Effects in Valence and Core Photoionization of Molecules. Physica Scripta, 1980, 21, 481-491.	1.2	125
49	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.	1.0	123
50	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.	1.2	120
51	Vibronic coupling effects in the photoelectron spectrum of ethylene. Journal of Chemical Physics, 1978, 69, 4252-4263.	1.2	119
52	Multilevel Redfield description of the dissipative dynamics at conical intersections. Journal of Chemical Physics, 2002, 116, 263.	1.2	119
53	Nuclear dynamics in resonant electron-molecule scattering beyond the local approximation: Vibrational excitation and dissociative attachment inH2andD2. Physical Review A, 1985, 32, 181-193.	1.0	116
54	Ab initio study of excited-state intramolecular proton dislocation in salicylic acid. Chemical Physics, 1998, 232, 257-265.	0.9	115

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55	Theory of the vibrational structure of resonances in electron-molecule scattering. Physical Review A, 1977, 16, 1465-1482.	1.0	114
56	Experimental and theoretical investigation of the complete valence shell ionization spectra of CO2and N2O. Chemical Physics, 1979, 40, 171-183.	0.9	113
57	Microscopic modelling of photoisomerization and internal-conversion dynamics. Chemical Physics, 1994, 186, 27-40.	0.9	112
58	Abinitiocharacterization of theS1â€“S2conical intersection in pyrazine and calculation of spectra. Journal of Chemical Physics, 1992, 96, 5298-5309.	1.2	110
59	Nonradiative Decay Mechanisms of the Biologically Relevant Tautomer of Guanine. Journal of Physical Chemistry A, 2008, 112, 11965-11968.	1.1	109
60	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.	1.1	107
61	Ab initio characterization of the conical intersections involved in the photochemistry of phenol. Journal of Chemical Physics, 2008, 129, 224307.	1.2	105
62	Photophysics of Malonaldehyde:Â An ab Initio Study. Journal of Physical Chemistry A, 1999, 103, 4494-4504.	1.1	104
63	Strong nonadiabatic effects and conical intersections in molecular spectroscopy and unimolecular decay: C2H4+. Journal of Chemical Physics, 1982, 77, 2014-2022.	1.2	102
64	On the vibrational structure in photoelectron spectra by the method of Green's functions. Journal of Chemical Physics, 1974, 60, 2878-2889.	1.2	101
65	Modeling of ultrafast electron-transfer dynamics: multi-level Redfield theory and validity of approximations. Chemical Physics, 2001, 268, 105-120.	0.9	101
66	Theoretical investigation of potential energy surfaces relevant for excited-state hydrogen transfer in o-hydroxybenzaldehyde. Chemical Physics, 1994, 184, 115-124.	0.9	100
67	Intramolecular Hydrogen Bonding in the S1(Ï€Ï€*) 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.	1.1	100
68	The chemical physics of the photostability of life. Europhysics News, 2006, 37, 20-23.	0.1	93
69	S1-S2 Conical intersection and ultrafast S2â†’S1 Internal conversion in pyrazine. Chemical Physics Letters, 1988, 150, 235-242.	1.2	92
70	Detection of ultrafast molecular-excited-state dynamics with time- and frequency-resolved pump-probe spectroscopy. Physical Review A, 1992, 45, 3032-3040.	1.0	90
71	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
72	The influence of finite lifetime of electronic states on the vibrational structure of molecular electronic spectra. Chemical Physics, 1979, 44, 33-44.	0.9	89

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73	Theoretical studies on the femtosecond realâ€time measurement of ultrafast electronic decay in polyatomic molecules. Journal of Chemical Physics, 1989, 90, 7184-7194.	1.2	87
74	Efficient Calculation of Time- and Frequency-Resolved Four-Wave-Mixing Signals. Accounts of Chemical Research, 2009, 42, 1290-1298.	7.6	87
75	Singletâ€“Triplet Inversion in Heptazine and in Polymeric Carbon Nitrides. Journal of Physical Chemistry A, 2019, 123, 8099-8108.	1.1	87
76	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.	0.6	86
77	THE MULTI-MODE VIBRONIC-COUPLING APPROACH. Advanced Series in Physical Chemistry, 2004, , 323-367.	1.5	86
78	Molecular mechanisms of the photostability of indigo. Physical Chemistry Chemical Physics, 2011, 13, 1618-1628.	1.3	86
79	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
80	Theory of vibronic coupling in linear molecules. Journal of Chemical Physics, 1981, 74, 2945-2968.	1.2	83
81	A comparison of different approaches to the calculation of franck-condon factors for polyatomic molecules. Molecular Physics, 1977, 34, 1759-1770.	0.8	81
82	Vibronic coupling of shortâ€lived electronic states. Journal of Chemical Physics, 1986, 84, 152-169.	1.2	81
83	Resonance Raman spectroscopy of theS1andS2states of pyrazine: Experiment and first principles calculation of spectra. Journal of Chemical Physics, 1995, 103, 6851-6860.	1.2	81
84	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.	1.2	80
85	Model studies on femtosecond time-resolved ionization spectroscopy of excited-state vibrational dynamics and vibronic coupling. Chemical Physics, 1991, 151, 59-72.	0.9	78
86	Time-dependent quantum wave-packet description of the1Ï€Ïƒ* photochemistry of pyrrole. Faraday Discussions, 2004, 127, 283-293.	1.6	78
87	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
88	Intrinsic and extrinsic plasmon coupling in x-ray photoemission from core states of adsorbed atoms. Physical Review B, 1977, 16, 1480-1488.	1.1	77
89	Diabatic CASSCF orbitals and wavefunctions. Chemical Physics Letters, 1994, 226, 257-262.	1.2	77
90	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.	1.2	77

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91	Mechanisms of Ultrafast Excited-State Deactivation in Adenosine. Journal of Physical Chemistry A, 2014, 118, 122-127.	1.1	76
92	Geometric phase effects in the coherent control of the branching ratio of photodissociation products of phenol. Journal of Chemical Physics, 2006, 124, 224316.	1.2	74
93	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
94	Pathâ€integral treatment of multiâ€mode vibronic coupling. Journal of Chemical Physics, 1994, 100, 926-937.	1.2	73
95	Optimal control of ultrafastcis-transphotoisomerization of retinal in rhodopsin via a conical intersection. Journal of Chemical Physics, 2005, 123, 144508.	1.2	73
96	1â€“2 conical intersection in trans-butadiene: ultrafast dynamics and optical spectra. Chemical Physics Letters, 2000, 320, 535-541.	1.2	71
97	Photoinduced charge separation in indoleâ€“water clusters. Chemical Physics Letters, 2000, 329, 130-137.	1.2	68
98	Electronic recoil effects in high-energy photoelectron spectroscopy. Journal of Electron Spectroscopy and Related Phenomena, 1978, 13, 161-173.	0.8	67
99	Vibronic coupling in linear molecules and linear-to-bent transitions: HCN. Chemical Physics, 1979, 37, 303-317.	0.9	67
100	Theory of resonance Raman scattering and fluorescence from strongly vibronically coupled excited states of polyatomic molecules. Journal of Chemical Physics, 1990, 93, 5496-5509.	1.2	67
101	Strong correlation effects in the ionisation of CS2. Chemical Physics Letters, 1979, 61, 30-35.	1.2	66
102	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.	0.9	66
103	Green's function calculations on the complete valence ionization spectra of HF, HCl, HBr AND HI. Chemical Physics, 1981, 56, 43-52.	0.9	65
104	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.	1.2	65
105	Photophysics of Eumelanin: Ab Initio Studies on the Electronic Spectroscopy and Photochemistry of 5,6-Dihydroxyindole. ChemPhysChem, 2007, 8, 756-762.	1.0	65
106	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
107	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.	1.2	64
108	Ab initio investigation of the multimode dynamical Jahn-Teller effect in the X̃ 2E1g state of the benzene cation. Chemical Physics Letters, 1991, 177, 345-351.	1.2	64

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109	Relevance of Electron-Driven Proton-Transfer Processes for the Photostability of Proteins. ChemPhysChem, 2006, 7, 561-564.	1.0	64
110	Symmetry Breaking and Non-Born-Oppenheimer Effects in Radical Cations. Angewandte Chemie International Edition in English, 1983, 22, 210-224.	4.4	62
111	Projection-operator calculations for molecular shape resonances: TheÎ£u+2resonance in electron-hydrogen scattering. Physical Review A, 1985, 31, 641-651.	1.0	61
112	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
113	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.	1.2	60
114	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.	0.8	58
115	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
116	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
117	Computational Studies of the Photophysics of Neutral and Zwitterionic Amino Acids in an Aqueous Environment: Tyrosineâˆ™(H2O)2 and Tryptophanâˆ™(H2O)2 Clusters. Journal of Physical Chemistry A, 2009, 113, 542-550.	1.1	57
118	Negative shake-up energy in core ionization. Chemical Physics, 1979, 39, 149-157.	0.9	56
119	Photodissociation of ozone in the Chappuis band. I. Electronic structure calculations. Journal of Chemical Physics, 1997, 107, 7282-7295.	1.2	56
120	Femtosecond pump-probe spectroscopy of electron-transfer systems: a nonperturbative approach. Chemical Physics, 1997, 217, 275-287.	0.9	56
121	Photoejection of electrons from pyrrole into an aqueous environment: ab initio results on pyrrole-water clusters. Chemical Physics Letters, 2000, 321, 479-484.	1.2	56
122	Ionization potentials of ethylene, allene and butatriene by a green function method. Chemical Physics, 1976, 18, 469-476.	0.9	55
123	High-order expansion of T2Ã—t2 Jahnâ€“Teller potential-energy surfaces in tetrahedral molecules. Journal of Chemical Physics, 2010, 132, 154108.	1.2	55
124	A difficult assignment problem. Molecular Physics, 1977, 34, 381-396.	0.8	54
125	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.	0.9	54
126	Multi-mode vibronic coupling with dissipation. Application of the Monte Carlo wavefunction propagation method. Chemical Physics Letters, 1995, 235, 370-376.	1.2	53

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127	On the mechanism of rapid non-radiative decay in intramolecularly hydrogen-bonded Ï€ systems. Chemical Physics Letters, 1999, 300, 533-539.	1.2	53
128	A theoretical photoelectron spectrum of cyanogen by a Green-function method. Chemical Physics, 1975, 10, 459-470.	0.9	52
129	Jahnâ€"Teller effect induced by non-degenerate vibrational modes in cumulenes. Chemical Physics, 1978, 33, 319-326.	0.9	52
130	Manyâ€body calculations on molecules with secondâ€row atoms: H2S and H2CS. Journal of Chemical Physics, 1977, 66, 4893-4899.	1.2	51
131	On the adequacy of the molecular-orbital picture for describing ionization processes. International Journal of Quantum Chemistry, 1978, 14, 593-601.	1.0	51
132	Associative detachment, dissociative attachment, and vibrational excitation of HCl by low-energy electrons. Physical Review A, 1999, 60, 2873-2881.	1.0	51
133	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
134	Computational investigation of the photoinduced homolytic dissociation of water in the pyridineâ€"water complex. Physical Chemistry Chemical Physics, 2013, 15, 5957.	1.3	51
135	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
136	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.	1.2	50
137	Time-dependent wave-packet description of dissociative electron attachment. Physical Review A, 1993, 47, 1031-1044.	1.0	49
138	Computational studies of aqueous-phase photochemistry and the hydrated electron in finite-size clusters. Physical Chemistry Chemical Physics, 2007, 9, 3818.	1.3	48
139	Evidence for the need of a non-Bornâ€"Oppenheimer description of excited-state hydrogen transfer. Chemical Physics Letters, 1993, 211, 82-87.	1.2	46
140	Ab initio studies of the photophysics of 2-aminopurine. Molecular Physics, 2006, 104, 1113-1121.	0.8	46
141	Nonadiabatic nuclear dynamics of the ammonia cation studied by surface hopping classical trajectory calculations. Journal of Chemical Physics, 2015, 142, 104307.	1.2	46
142	The EâŠ—(Ïµ + Ïµ) Jahn-Teller effect. Molecular Physics, 1980, 41, 1291-1315.	0.8	45
143	Model calculation on the pump-probe measurement of ultrafast electronic population decay in polyatomic molecules. Chemical Physics Letters, 1987, 140, 133-141.	1.2	45
144	The relativistic EÃ—E Jahnâ€"Teller effect revisited. Chemical Physics, 2006, 322, 405-410.	0.9	45

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145	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
146	Theoretical analysis of photoinduced H-atom elimination in thiophenol. Journal of Chemical Physics, 2012, 136, 174312.	1.2	45
147	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
148	The effect of a resonance on vibrational structure in the photoelectron spectrum of acetylene. Chemical Physics Letters, 1981, 77, 242-245.	1.2	44
149	Intramolecular electron-transfer dynamics in the inverted regime: quantum mechanical multi-mode model including dissipation. Chemical Physics Letters, 1996, 259, 113-118.	1.2	44
150	Time- and frequency-resolved fluorescence spectra of nonadiabatic dissipative systems: What photons can tell us. Journal of Chemical Physics, 2005, 122, 134504.	1.2	44
151	Photoinduced multi-mode quantum dynamics of pyrrole at the â€“ conical intersections. Journal of Photochemistry and Photobiology A: Chemistry, 2007, 190, 177-189.	2.0	44
152	Assessing the performance of trajectory surface hopping methods: Ultrafast internal conversion in pyrazine. Journal of Chemical Physics, 2019, 150, 154119.	1.2	44
153	Strong non-condon effects induced by electron correlation: N2O+. Chemical Physics, 1982, 69, 175-183.	0.9	43
154	Projection-operator approach to potential scattering. Physical Review A, 1983, 28, 2777-2791.	1.0	43
155	Ab initio investigation of the potential energy surfaces involved in the photophysics of s-trans-1,3-butadiene. Chemical Physics, 2001, 269, 1-10.	0.9	43
156	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
157	Photon energy dependence of satelite line intensity in the photoelectron spectrum of acetylene. Chemical Physics Letters, 1980, 70, 36-40.	1.2	42
158	Projection-operator calculations for shape resonances: A new method based on the many-body optical-potential approach. Physical Review A, 1984, 29, 2485-2496.	1.0	42
159	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
160	Jahnâ€“Teller and spinâ€“orbit coupling effects in transition-metal trifluorides. Chemical Physics, 2011, 387, 56-65.	0.9	42
161	On the vibrational structure in inner-shell ionization spectra by a many-body approach. Chemical Physics Letters, 1975, 31, 582-587.	1.2	41
162	An accurate potential energy function of the H2â¯ ion at large internuclear distances. Chemical Physics Letters, 1984, 111, 211-214.	1.2	41

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163	Ultrafast non-adiabatic dynamics of ethylene including Rydberg states. Molecular Physics, 2013, 111, 2439-2450.	0.8	41
164	Photocatalytic Water Splitting with the Acridine Chromophore: A Computational Study. Journal of Physical Chemistry B, 2015, 119, 10664-10672.	1.2	41
165	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.	1.2	40
166	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.	1.1	40
167	Experimental and Theoretical Evidence for Long-Lived Molecular Hydrogen AnionsH2â^'andD2â^'. Physical Review Letters, 2005, 94, 223003.	2.9	40
168	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.	1.3	39
169	Theoretical study of vibrational wave-packet dynamics in electron-transfer systems. Chemical Physics, 2004, 296, 217-229.	0.9	39
170	Dissipative dynamics at conical intersections: simulations with the hierarchy equations of motion method. Faraday Discussions, 2016, 194, 61-80.	1.6	39
171	Internal conversion funnel in benzene and pyrazine: adiabatic and diabatic representation. Chemical Physics Letters, 1993, 203, 220-226.	1.2	38
172	On the controversial assignment of the ionization potentials of formaldehyde. Chemical Physics Letters, 1975, 34, 60-62.	1.2	37
173	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
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