David R Yarkony

List of Publications by Year
in descending order

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204 papers	10,329 citations	50170 46 h-index	42291 92 g-index
209 all docs	209 docs citations	209 times ranked	3618 citing authors

#	Article	IF	Citations
1	Conical Intersections. Advanced Series in Physical Chemistry, 2004, , .	1.5	864
2	Diabolical conical intersections. Reviews of Modern Physics, 1996, 68, 985-1013.	16.4	853
3	Role of Conical Intersections in Molecular Spectroscopy and Photoinduced Chemical Dynamics. Annual Review of Physical Chemistry, 2012, 63, 325-352.	4.8	401
4	Conical Intersections:â€‰ Diabolical and Often Misunderstood. Accounts of Chemical Research, 1998, 31, 511-518.	7.6	396
5	Conical Intersections:Â The New Conventional Wisdom. Journal of Physical Chemistry A, 2001, 105, 6277-6293.	1.1	335
6	Conical Intersections. Advanced Series in Physical Chemistry, 2011, , .	1.5	300
7	Analytic evaluation of nonadiabatic coupling terms at the MR-CI level. I. Formalism. Journal of Chemical Physics, 2004, 120, 7322-7329.	1.2	290
8	Nonadiabatic Quantum Chemistryâ€”Past, Present, and Future. Chemical Reviews, 2012, 112, 481-498.	23.0	254
9	Analytic evaluation of nonadiabatic coupling terms at the MR-CI level. II. Minima on the crossing seam: Formaldehyde and the photodimerization of ethylene. Journal of Chemical Physics, 2004, 120, 7330-7339.	1.2	216
10	Current Issues in Nonadiabatic Chemistryâ€. The Journal of Physical Chemistry, 1996, 100, 18612-18628.	2.9	179
11	Nuclear dynamics near conical intersections in the adiabatic representation: I. The effects of local topography on interstate transitions. Journal of Chemical Physics, 2001, 114, 2601-2613.	1.2	165
12	On the evaluation of nonadiabatic coupling matrix elements using SAâ€MCSCF/CI wave functions and analytic gradient methods. I. Journal of Chemical Physics, 1984, 81, 4549-4553.	1.2	158
13	On the intersection of two potential energy surfaces of the same symmetry. Systematic characterization using a Lagrange multiplier constrained procedure. Journal of Chemical Physics, 1993, 99, 5251-5256.	1.2	133
14	Nonadiabatic Tunneling in Photodissociation of Phenol. Journal of the American Chemical Society, 2016, 138, 7828-7831.	6.6	126
15	Energies and Derivative Couplings in the Vicinity of a Conical Intersection Using Degenerate Perturbation Theory and Analytic Gradient Techniques. 1. Journal of Physical Chemistry A, 1997, 101, 4263-4270.	1.1	119
16	On the consequences of nonremovable derivative couplings. I. The geometric phase and quasidiabatic states: A numerical study. Journal of Chemical Physics, 1996, 105, 10456-10461.	1.2	112
17	On the adiabatic to diabatic states transformation near intersections of conical intersections. Journal of Chemical Physics, 2000, 112, 2111-2120.	1.2	106
18	Accurate nonadiabatic dynamics. Physical Chemistry Chemical Physics, 2016, 18, 26335-26352.	1.3	104

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19	On the evaluation of non-adiabatic coupling matrix elements for large scale CI wavefunctions. Chemical Physics Letters, 1985, 113, 159-164.	1.2	96
20	Fitting coupled potential energy surfaces for large systems: Method and construction of a 3-state representation for phenol photodissociation in the full 33 internal degrees of freedom using multireference configuration interaction determined data. Journal of Chemical Physics, 2014, 140, 024112.	1.2	89
21	Spin-forbidden chemistry within the Breit-Pauli approximation. International Reviews in Physical Chemistry, 1992, 11, 195-242.	0.9	86
22	On the adiabatic to diabatic states transformation in the presence of a conical intersection: A most diabatic basis from the solution to a Poissonâ€™s equation. I. Journal of Chemical Physics, 1998, 109, 20-25.	1.2	86
23	Nonadiabatic Interactions Between Potential Energy Surfaces: Theory and Applications. Advances in Chemical Physics, 0, , 1-71.	0.3	82
24	A theoretical treatment of the predissociation of the individual rovibronic levels of OH/OD(Aâ€‰2Î£+). Journal of Chemical Physics, 1992, 97, 1838-1849.	1.2	80
25	Beyond Two-State Conical Intersections. Three-State Conical Intersections in Low Symmetry Molecules:â€‰ the Allyl Radical. Journal of the American Chemical Society, 2003, 125, 10672-10676.	6.6	77
26	On the mechanism of the reaction CH(Xâ€‰2Î)+N2(Xâ€‰1Î£+g)â†'HCN(Xâ€‰1Î£+) +N(4Sâ€‰). I. A theoretical treatment of the electronic structure aspects of the intersystem crossing. Journal of Chemical Physics, 1991, 95, 1808-1816.	1.2	73
27	Toward eliminating the electronic structure bottleneck in nonadiabatic dynamics on the fly: An algorithm to fit nonlocal, quasidiabatic, coupled electronic state Hamiltonians based on ab initio electronic structure data. Journal of Chemical Physics, 2010, 132, 104101.	1.2	73
28	Accidental conical intersections of three states of the same symmetry. I. Location and relevance. Journal of Chemical Physics, 2002, 117, 6907-6910.	1.2	68
29	On the characterization of regions of avoided surface crossings using an analytic gradient based method. Journal of Chemical Physics, 1990, 92, 2457-2463.	1.2	65
30	Accurate first-derivative nonadiabatic couplings for the H3 system. Journal of Chemical Physics, 2001, 115, 4640-4659.	1.2	61
31	Permutation invariant polynomial neural network approach to fitting potential energy surfaces. IV. Coupled diabatic potential energy matrices. Journal of Chemical Physics, 2018, 149, 144107.	1.2	61
32	A theoretical analysis of the state-specific decomposition of OH(Aâ€‰2Î£+,vâ€²,Nâ€²,F1/F2) levels, including the effects of spinâ€“orbit and Coriolis interactions. Journal of Chemical Physics, 1999, 110, 363-376.	1.2	58
33	On the evaluation of nonadiabatic coupling matrix elements for MCSCF/CI wave functions using analytic derivative methods. III. Second derivative terms. Journal of Chemical Physics, 1986, 84, 348-353.	1.2	56
34	Encoding of vinylidene isomerization in its anion photoelectron spectrum. Science, 2017, 358, 336-339.	6.0	55
35	On the representation of coupled adiabatic potential energy surfaces using quasi-diabatic Hamiltonians: A distributed origins expansion approach. Journal of Chemical Physics, 2012, 136, 174110.	1.2	54
36	Interpolation of diabatic potential-energy surfaces: Quantum dynamics on ab initio surfaces. Journal of Chemical Physics, 2005, 123, 134110.	1.2	53

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37	On the electronic structure of the NH radical. The fine structure splitting of the Xâ€‰3Î£â^' state and the spinâ€forbidden (bâ€‰1Î£+, aâ€‰1Î")â†'Xâ€‰3Î£â^', and the spinâ€allowed Aâ€‰3Îâ†'Xâ€‰3Î£â^' and câ€‰1Îâ†'(bâ€‰1Î£+,aâ€ Chemical Physics, 1989, 91, 4745-4757.	1.2	52
38	Determining quasidiabatic coupled electronic state Hamiltonians using derivative couplings: A normal equations based method. Journal of Chemical Physics, 2008, 129, 124104.	1.2	52
39	The Reactions Al(2P) + H2 â†' AlH2(12Aâ€˜, 22Aâ€˜) â†' AlH2(X2A1) or AlH(XÎ£+) + H:â€‰ Unusual Conical Intersections and Possible Nonadiabatic Recrossing. Journal of Physical Chemistry A, 1997, 101, 7953-7959.	1.1	51
40	Full-Dimensional Quantum State-to-State Nonadiabatic Dynamics for Photodissociation of Ammonia in its A-Band. Journal of Physical Chemistry Letters, 2014, 5, 1055-1060.	2.1	50
41	Electronic structure of CaO. I. Journal of Chemical Physics, 1978, 68, 3990-3997.	1.2	49
42	Energies and derivative couplings in the vicinity of a conical intersection. II. CH2(2â€‰3Aâ€³,3â€‰3Aâ€³) and H2S(1â€‰1Aâ€³,2â€‰1Aâ€³), unexpected results in an ostensibly standard case. Journal of Chemical Physics, 1997, 107, 7825-7838.	1.2	48
43	Quasi-diabatic representations of adiabatic potential energy surfaces coupled by conical intersections including bond breaking: A more general construction procedure and an analysis of the diabatic representation. Journal of Chemical Physics, 2012, 137, 22A511.	1.2	48
44	Nonadiabatic tunneling via conical intersections and the role of the geometric phase. Physical Review A, 2017, 95, .	1.0	48
45	On the reaction Na(2P)+H2â†'Na(2S)+H2nonadiabatic effects. Journal of Chemical Physics, 1986, 84, 3206-3211.	1.2	47
46	On the electronic structure aspects of spinâ€forbidden processes in N2O. Journal of Chemical Physics, 1993, 99, 6824-6831.	1.2	47
47	Conical Intersections of Three Electronic States Affect the Ground State of Radical Species with Little or No Symmetry:Â Pyrazolyl. Journal of the American Chemical Society, 2003, 125, 12428-12429.	6.6	47
48	On the reaction Mg+N2Oâ†'MgO+N2. Journal of Chemical Physics, 1983, 78, 6763-6772.	1.2	46
49	The role of conical intersections in the nonadiabatic quenching of OH(Aâ€Š2Î£+) by molecular hydrogen. Journal of Chemical Physics, 2000, 113, 10091-10099.	1.2	46
50	CONICAL INTERSECTIONS: THEIR DESCRIPTION AND CONSEQUENCES. Advanced Series in Physical Chemistry, 2004, , 41-127.	1.5	46
51	Computational determination of the Ãƒ state absorption spectrum of NH3 and of ND3 using a new quasi-diabatic representation of the $\skew3\tilde{X}$ and Ãƒ states and full six-dimensional quantum dynamics. Journal of Chemical Physics, 2012, 136, 234301.	1.2	46
52	On the simulation of photoelectron spectra in molecules with conical intersections and spin-orbit coupling: The vibronic spectrum of CH3S. Journal of Chemical Physics, 2007, 127, 104309.	1.2	45
53	Representation of coupled adiabatic potential energy surfaces using neural network based quasi-diabatic Hamiltonians: 1,2 ²Aâ€² states of LiFH. Physical Chemistry Chemical Physics, 2019, 21, 14205-14213.	1.3	45
54	Radiative and nonradiative decay of the NH(ND)Aâ€‰3Î electronic state: Predissociation induced by the5Î£â^'state. Journal of Chemical Physics, 1991, 94, 1913-1922.	1.2	44

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55	On the Construction of Diabatic Bases Using Molecular Properties. Rigorous Results in the Vicinity of a Conical Intersection. Journal of Physical Chemistry A, 1998, 102, 8073-8077.	1.1	43
56	On the vibronic coupling approximation: A generally applicable approach for determining fully quadratic quasidiabatic coupled electronic state Hamiltonians. Journal of Chemical Physics, 2007, 127, 094104.	1.2	43
57	Nonadiabatic processes involving three electronic states. I. Branch cuts and linked pairs of conical intersections. Journal of Chemical Physics, 2003, 119, 5058-5068.	1.2	42
58	Signatures of a Conical Intersection in Adiabatic Dissociation on the Ground Electronic State. Journal of the American Chemical Society, 2018, 140, 1986-1989.	6.6	42
59	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	1.2	42
60	First principles determination of the NH2/ND2($skew4ilde A, skew3ilde X$Ãƒ,XÌƒ) branching ratios for photodissociation of NH3/ND3 via full-dimensional quantum dynamics based on a new quasi-diabatic representation of coupled ab initio potential energy surfaces. Journal of Chemical Physics, 2012, 137, 22A541.	1.2	41
61	On the elimination of the electronic structure bottleneck in on the fly nonadiabatic dynamics for small to moderate sized (10-15 atom) molecules using fit diabatic representations based solely on ab initio electronic structure data: The photodissociation of phenol. Journal of Chemical Physics, 2016, 144, 024105.	1.2	40
62	Non-adiabaticity: the importance of conical intersections. Molecular Physics, 2016, 114, 1983-2013.	0.8	40
63	On the use of the Breitâ€“Pauli approximation for evaluating line strengths for spinâ€forbidden transitions: Application to NF. Journal of Chemical Physics, 1985, 83, 1168-1172.	1.2	39
64	Exploring molecular complexity: Conical intersections and NH3 photodissociation. Journal of Chemical Physics, 2004, 121, 628-631.	1.2	39
65	Marching along Ridges. Efficient Location of Energy-Minimized Conical Intersections of Two States Using Extrapolatable Functions. Journal of Physical Chemistry A, 2004, 108, 3200-3205.	1.1	39
66	Up to a Sign. The Insidious Effects of Energetically Inaccessible Conical Intersections on Unimolecular Reactions. Accounts of Chemical Research, 2019, 52, 501-509.	7.6	39
67	Extending the Representation of Multistate Coupled Potential Energy Surfaces To Include Properties Operators Using Neural Networks: Application to the 1,2¹A States of Ammonia. Journal of Chemical Theory and Computation, 2020, 16, 302-313.	2.3	39
68	On the evaluation of nonâ€Bornâ€“Oppenheimer interactions for Bornâ€“Oppenheimer wave functions. V. A body fixed frame approach. Applications to isotope effects on equilibrium geometries and the adiabatic correction for the Xâ€‰1Î£+ state of LiH. Journal of Chemical Physics, 1988, 89, 975-982.	1.2	38
69	On the quenching of helium 2â€‰3S: Potential energy curves for, and nonadiabatic, relativistic, and radiative couplings between, the aâ€‰3Î£+u, Aâ€‰1Î£+u, bâ€‰3Îg, Bâ€‰1Îg, câ€‰3Î£+g, and Câ€‰1Î£+g states of He2. Journal of Physics, 1989, 90, 7164-7175.	1.2	38
70	Unusual conical intersections in the Jahnâ€“Teller effect: The electronically excited states of Li3. Journal of Chemical Physics, 1999, 110, 3639-3642.	1.2	38
71	Diabatic bases and molecular properties. International Journal of Quantum Chemistry, 2000, 76, 235-243.	1.0	38
72	Neural network based quasi-diabatic Hamiltonians with symmetry adaptation and a correct description of conical intersections. Journal of Chemical Physics, 2019, 150, 214101.	1.2	38

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73	MCSCF wave functions for excited states of polar molecules: Application to BeO. Journal of Chemical Physics, 1980, 72, 1138-1144.	1.2	37
74	An improved quasi-diabatic representation of the 1, 2, 31A coupled adiabatic potential energy surfaces of phenol in the full 33 internal coordinates. Journal of Chemical Physics, 2016, 144, 124312.	1.2	37
75	On the evaluation of nonadiabatic coupling matrix elements for MCSCF/CI wave functions. IV. Second derivative terms using analytic gradient methods. Journal of Chemical Physics, 1987, 86, 321-328.	1.2	36
76	On the electronic structure of the X, A, and B states of CaCl. Journal of Chemical Physics, 1983, 79, 4376-4381.	1.2	34
77	Constructive and Destructive Interference in Nonadiabatic Tunneling via Conical Intersections. Journal of Chemical Theory and Computation, 2017, 13, 1902-1910.	2.3	34
78	On the noncrossing rule in polyatomic systems: Determination of a seam of actual surface crossings relevant to the quenching of H2(Bâ€‰1Î£+u) by helium. Journal of Chemical Physics, 1990, 93, 4473-4474.	1.2	33
79	On the role of conical intersections of two potential energy surfaces of the same symmetry in photodissociation. I. CH3SHâ†'CH3S+H and CH3+SH. Journal of Chemical Physics, 1994, 100, 3639-3644.	1.2	33
80	Conical intersections of three states: Energies, derivative couplings, and the geometric phase effect in the neighborhood of degeneracy subspaces. Application to the allyl radical. Journal of Chemical Physics, 2003, 119, 11561-11569.	1.2	33
81	On the lowâ€lying states of MgO. II. Journal of Chemical Physics, 1981, 74, 2379-2383.	1.2	32
82	Intersecting Conical Intersection Seams:â€‰ Their Location, Representation, and Effect on Local Topography. Journal of Physical Chemistry A, 2002, 106, 2580-2591.	1.1	31
83	On the connectivity of seams of conical intersection: Seam curvature. Journal of Chemical Physics, 2005, 123, 204101.	1.2	31
84	The electronic structure of CaO. II. An MCSCF/CI treatment of the lowâ€lying 1Î£+ and 1Î states. Journal of Chemical Physics, 1982, 77, 5573-5580.	1.2	30
85	On the Mg(3P)â€“He(1S) interaction using SAâ€MCSCF/ICFâ€CI wave functions. Journal of Chemical Physics, 1984, 80, 5089-5094.	1.2	30
86	On the radiative lifetimes of the bâ€‰1Î£+ and aâ€‰1Î” states in NCl. Journal of Chemical Physics, 1987, 86, 1642-1643.	1.2	30
87	Systematic location of intersecting seams of conical intersection in triatomic molecules: The 1â€‰2Aâ€²â€“2â€‰2Aâ€² conical intersections in BH2. Journal of Chemical Physics, 1998, 108, 5657-5659.	1.2	30
88	Full-Dimensional Quantum Dynamics of Vibrationally Mediated Photodissociation of NH₃ and ND₃ on Coupled Ab Initio Potential Energy Surfaces: Absorption Spectra and NH₂(Ãƒ²A₁)/NH₂(XÌƒ²B₁) Branching Ratios. Journal of Physical Chemistry A, 2014, 118, 11926-11934.	1.1	30
89	Communication: On the competition between adiabatic and nonadiabatic dynamics in vibrationally mediated ammonia photodissociation in its A band. Journal of Chemical Physics, 2015, 142, 091101.	1.2	30
90	Accurate Neural Network Representation of the Ab Initio Determined Spinâ€“Orbit Interaction in the Diabatic Representation Including the Effects of Conical Intersections. Journal of Physical Chemistry Letters, 2020, 11, 1848-1858.	2.1	30

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91	On the Mechanism of the Spin-Nonconserving Chemical Reaction O(3P) + HCCH â†' CH2(Ã£1A1) + CO(X1Î£+). I. Feasibility. Journal of Physical Chemistry A, 1998, 102, 5305-5311.	1.1	29
92	Determining the molecular Aharonovâ€"Bohm phase angle: A rigorous approach employing a molecular properties based adiabatic to diabatic states transformation. Journal of Chemical Physics, 1999, 110, 701-705.	1.2	29
93	Substituent effects and the noncrossing rule: The importance of reduced symmetry subspaces. I. The quenching of OH(Aâ€‰2Î£+) by H2. Journal of Chemical Physics, 1999, 111, 6661-6664.	1.2	29
94	On the Construction of Property Based Diabatizations: Diabolical Singular Points. Journal of Physical Chemistry A, 2015, 119, 12383-12391.	1.1	29
95	High-fidelity first principles nonadiabaticity: diabatization, analytic representation of global diabatic potential energy matrices, and quantum dynamics. Physical Chemistry Chemical Physics, 2021, 23, 24962-24983.	1.3	29
96	Nonadiabatic effects in the vicinity of multiple surface crossings. Evaluation of derivative couplings with respect to rotational and internal degrees of freedom. Application to the charge transfer reaction H++NOâ†'H+NO+. Journal of Chemical Physics, 1989, 90, 1657-1665.	1.2	28
97	Spinâ€"orbit effects in the decomposition reaction N3H(XÌƒ1Aâ€™)â†'N2(X1Î£+g)+NH(X3Ïƒâ^', a1Î"). Journal of Chemical Physics, 1990, 92, 320-323.	1.2	28
98	Electronic structure aspects of the spin-forbidden reaction CH3(Xâ€‰2A2â€³)+N(4S)â†'HCN(Xâ€‰1Î£+)+H2(Xâ€‰1Î£g+). Journal of Chemical Physics, 1997, 107, 4994-4999.	1.2	28
99	On the effects of spin-orbit coupling on conical intersection seams in molecules with an odd number of electrons. I. Locating the seam. Journal of Chemical Physics, 2001, 115, 2038-2050.	1.2	28
100	ELECTRONIC STRUCTURE ASPECTS OF NONADIABATIC PROCESSES IN POLYATOMIC SYSTEMS. Advanced Series in Physical Chemistry, 1995, , 642-721.	1.5	27
101	Theoretical studies of spinâ€forbidden radiationless decay in polyatomic systems. II. Radiationless decay of aâ€N2O2. Journal of Chemical Physics, 1993, 98, 3845-3849.	1.2	26
102	A criterion for the confluence of two seams of conical intersection in triatomic molecules. Theoretical Chemistry Accounts, 1998, 98, 197-201.	0.5	26
103	On the use of the Breitâ€"Pauli approximation for evaluating line strengths for spinâ€forbidden transitions. II. The symbolic matrix element method. Journal of Chemical Physics, 1986, 84, 2075-2078.	1.2	25
104	Spinâ€forbidden radiative decay involving quasidegenerate states. Application to the Bâ€‰1Î£+â†'aâ€‰3Î transition in MgO. Journal of Chemical Physics, 1988, 89, 7324-7333.	1.2	25
105	On the role of conical intersections in photodissociation. V. Conical intersections and the geometric phase in the photodissociation of methyl mercaptan. Journal of Chemical Physics, 1996, 104, 7866-7881.	1.2	25
106	Photodissociation of the hydroxymethyl radical. I. The role of conical intersections in line broadening and decomposition pathways. Journal of Chemical Physics, 2002, 116, 8300.	1.2	25
107	On the incorporation of the geometric phase in general single potential energy surface dynamics: A removable approximation to ab initio data. Journal of Chemical Physics, 2016, 145, 234111.	1.2	25
108	Dynamic mapping of conical intersection seams: A general method for incorporating the geometric phase in adiabatic dynamics in polyatomic systems. Journal of Chemical Physics, 2017, 147, 044109.	1.2	25

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109	Insights into the Mechanism of Nonadiabatic Photodissociation from Product Vibrational Distributions. The Remarkable Case of Phenol. Journal of Physical Chemistry Letters, 2020, 11, 191-198.	2.1	25
110	On the quenching of Na(2P) by HCl: Nonadiabatic effects. Journal of Chemical Physics, 1987, 86, 4990-4996.	1.2	23
111	S1â^'S0 Internal Conversion in Ketene. 1. The Role of Conical Intersections. Journal of Physical Chemistry A, 1999, 103, 6658-6668.	1.1	23
112	Spin-orbit coupling and conical intersections in molecules with an odd number of electrons. III. A perturbative determination of the electronic energies, derivative couplings and a rigorous diabatic representation near a conical intersection. Journal of Chemical Physics, 2002, 116, 2825-2835.	1.2	23
113	Photodissociation of the vinoxy radical through conical, and avoided, intersections. Journal of Chemical Physics, 2002, 117, 7198-7206.	1.2	23
114	Suppressing the geometric phase effect: Closely spaced seams of the conical intersection in Na3(2â€Š2Eâ€²). Journal of Chemical Physics, 1999, 111, 4906-4912.	1.2	22
115	Marching along ridges. An extrapolatable approach to locating conical intersections. Faraday Discussions, 2004, 127, 325.	1.6	22
116	Statistical and nonstatistical nonadiabatic photodissociation from the first excited state of the hydroxymethyl radical. Journal of Chemical Physics, 2005, 122, 084316.	1.2	22
117	On the characterization of three state conical intersections: A quasianalytic theory using a group homomorphism approach. Journal of Chemical Physics, 2006, 124, 124109.	1.2	22
118	Constructing diabatic representations using adiabatic and approximate diabatic data â€“ Coping with diabolical singularities. Journal of Chemical Physics, 2016, 144, 044104.	1.2	22
119	Electronic structure and vertical excitation spectrum of methylene amidogen CH2N. International Journal of Quantum Chemistry, 1983, 23, 437-446.	1.0	21
120	A theoretical description of the radiative decay processes (bâ€‰1Î£+, aâ€‰1Î”)â†'Xâ€‰3Î£â^' in NF. Journal of Chemical Physics, 1986, 85, 7261-7267.	1.2	21
121	On the electronic structure and dynamical aspects of the predissociation of theAâ€‰2Î ©states of MgCl. A rigorous quantum mechanical treatment incorporating spinâ€“orbit and derivative coupling effects. Journal of Chemical Physics, 1990, 93, 6403-6418.	1.2	21
122	On the origin of the heavy atom effect in the fine-structure splitting of the 1â€‰2Î state of alkali metal 2P-rare gas van der Waals molecules. Journal of Chemical Physics, 1997, 107, 7690-7694.	1.2	21
123	The photoelectron spectrum of the isopropoxide anion: Nonadiabatic effects due to conical intersections and the spin-orbit interaction. Journal of Chemical Physics, 2009, 130, 154312.	1.2	21
124	Neural Network Based Quasi-diabatic Representation for S₀ and S₁ States of Formaldehyde. Journal of Physical Chemistry A, 2020, 124, 10132-10142.	1.1	21
125	On the perturbation of the BÌƒâ€‰2Aâ€™ state of HCO by the 1â€‰4Aâ€˜ and 1â€‰4Aâ€™ states: Surfaces of intersection and spinâ€“orbit interactions. Journal of Chemical Physics, 1994, 100, 473-480.	1.2	20
126	Radiationless decay of the 1,2,3â€‰3Îg states of Al2: A fully first principles treatment using adiabatic and rigorous diabatic states. Journal of Chemical Physics, 1995, 102, 1955-1964.	1.2	20

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127	On the effects of spinâ€“orbit coupling on conical intersection seams in molecules with an odd number of electrons. II. Characterizing the local topography of the seam. Journal of Chemical Physics, 2001, 115, 5066-5075.	1.2	20
128	The photoelectron spectrum of the ethoxide anion: Conical intersections, the spin-orbit interaction, and sequence bands. Journal of Chemical Physics, 2009, 131, 134303.	1.2	20
129	A theoretical treatment of theaâ€‰3Î£1+â€‰â†'X1Î£0++ spinâ€forbidden dipoleâ€allowed radiative transition in NO+. Journal of Chemical Physics, 1991, 95, 6562-6566.	1.2	19
130	A Quasi-Diabatic Representation of the 1,2¹A States of Methylamine. Journal of Physical Chemistry A, 2019, 123, 5231-5241.	1.1	19
131	Enabling complete multichannel nonadiabatic dynamics: A global representation of the two-channel coupled, 1,21A and 13A states of NH3 using neural networks. Journal of Chemical Physics, 2021, 154, 094121.	1.2	19
132	On the electronic structure of the 2 1A1 state of methylene. Journal of Chemical Physics, 1978, 69, 3875-3877.	1.2	18
133	On the electronic structure of the He+H2 system: Characterization of, and nonadiabatic interactions between, the 1â€‰1Aâ€™ and 2â€‰1Aâ€™ potential energy surfaces. Journal of Chemical Physics, 1988, 89, 4945-4953.	1.2	18
134	On the intersection of potential energy surfaces in charge transfer reactions: A crossing seam for two states of the same symmetry in the reaction H++NO(Xâ€‰2Î)â†'H(2S)+NO+(Xâ€‰1Î£+). Journal of Chemical Physics, 1992, 97, 715-717.	1.2	18
135	On the role of conical intersections in photodissociation. III. The case of hydroxylamine. Journal of Chemical Physics, 1995, 102, 8431-8439.	1.2	18
136	Spinâ^'Orbit Coupling and Conical Intersections. IV. A Perturbative Determination of the Electronic Energies, Derivative Couplings, and a Rigorous Diabatic Representation near a Conical Intersection. The General Caseâ€. Journal of Physical Chemistry B, 2002, 106, 8108-8116.	1.2	18
137	On the Characterization of Three-State Conical Intersections Using a Group Homomorphism Approach:Â The Two-State Degeneracy Spacesâ€. Journal of Physical Chemistry B, 2006, 110, 19031-19039.	1.2	18
138	A method to reduce the size of the vibronic basis employed in the simulation of spectra using the multimode vibronic coupling approximation. Journal of Chemical Physics, 2008, 128, 044119.	1.2	18
139	Predissociation of the câ€‰1Î state of NH (ND): The role of dipolar spinâ€“spin coupling. Journal of Chemical Physics, 1991, 94, 2364-2367.	1.2	17
140	Unanticipated confluences of seams of conical intersection: Reinvestigating intersecting potential-energy surfaces using new tools. I. C(3P)+H2. Journal of Chemical Physics, 1998, 109, 7047-7050.	1.2	17
141	On the multimode quadratic vibronic coupling problem: An open-ended solution using a parallel Lanczos algorithm. Chemical Physics, 2008, 347, 57-64.	0.9	17
142	Multistate, multichannel coupled diabatic state representations of adiabatic states coupled by conical intersections. CH2OH photodissociation. Journal of Chemical Physics, 2017, 146, 134302.	1.2	17
143	Full-dimensional quantum stereodynamics of the non-adiabatic quenching of OH(A2Î£+) by H2. Nature Chemistry, 2021, 13, 909-915.	6.6	17
144	On the description of potential energy surfaces exhibiting conical intersections: a compact representation of the energies and derivative couplings and locally diabatic bases for the HOH and OHH portions of the 11A'-21A' seam of conical intersection in water. Molecular Physics, 1998, 93, 971-983.	0.8	17

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