David R Yarkony

List of Publications by Year in Descending Order

201 papers	8,911 citations	43 h-index	85 g-index
209 ext. papers	9,465 ext. citations	4.9 avg, IF	6.74 L-index

#	Paper	IF	Citations
201	Conical intersection seams in spin-orbit coupled systems with an even number of electrons: A numerical study based on neural network fit surfaces. *Journal of Chemical Physics*, **2021**, 155, 174115	3.9	1
200	Enabling complete multichannel nonadiabatic dynamics: A global representation of the two-channel coupled, 1,2A and 1A states of NH using neural networks. *Journal of Chemical Physics*, **2021**, 154, 094121	3.9	5
199	Enabling a Unified Description of Both Internal Conversion and Intersystem Crossing in Formaldehyde: A Global Coupled Quasi-Diabatic Hamiltonian for Its S, S, and T States. *Journal of Chemical Theory and Computation*, **2021**, 17, 4157-4168	6.4	2
198	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	3.6	3
197	Full-dimensional quantum stereodynamics of the non-adiabatic quenching of OH(A) by H. *Nature Chemistry*, **2021**, 13, 909-915	17.6	3
196	Construction of Quasi-diabatic Hamiltonians That Accurately Represent Determined Adiabatic Electronic States Coupled by Conical Intersections for Systems on the Order of 15 Atoms. Application to Cyclopentoxide Photoelectron Detachment in the Full 39 Degrees of Freedom. *Journal of Physical Chemistry A*, **2020**, 124, 4539-4548	2.8	9
195	On the nonadiabatic collisional quenching of OH(A) by H: a four coupled quasi-diabatic state description. *Physical Chemistry Chemical Physics*, **2020**, 22, 13516-13527	3.6	8
194	Accurate Neural Network Representation of the Ab Initio Determined Spin-Orbit Interaction in the Diabatic Representation Including the Effects of Conical Intersections. *Journal of Physical Chemistry Letters*, **2020**, 11, 1848-1858	6.4	21
193	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. *Journal of Chemical Physics*, **2020**, 152, 134110	3.9	22
192	Extending the Representation of Multistate Coupled Potential Energy Surfaces To Include Properties Operators Using Neural Networks: Application to the 1,2A States of Ammonia. *Journal of Chemical Theory and Computation*, **2020**, 16, 302-313	6.4	27
191	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	6.4	15
190	Impact of Diabolical Singular Points on Nonadiabatic Dynamics and a Remedy: Photodissociation of Ammonia in the First Band. *Journal of Chemical Theory and Computation*, **2020**, 16, 6776-6784	6.4	4
189	Neural Network Based Quasi-diabatic Representation for S and S States of Formaldehyde. *Journal of Physical Chemistry A*, **2020**, 124, 10132-10142	2.8	8
188	Compact Bases for Vibronic Coupling in Spectral Simulations: The Photoelectron Spectrum of Cyclopentoxide in the Full 39 Internal Modes. *Journal of Physical Chemistry Letters*, **2020**, 11, 7245-7252	6.4	0
187	Diabatic and adiabatic representations: Electronic structure caveats. *Computational and Theoretical Chemistry*, **2019**, 1152, 41-52	2	7
186	Up to a Sign. The Insidious Effects of Energetically Inaccessible Conical Intersections on Unimolecular Reactions. *Accounts of Chemical Research*, **2019**, 52, 501-509	24.3	27
185	Neural network based quasi-diabatic Hamiltonians with symmetry adaptation and a correct description of conical intersections. *Journal of Chemical Physics*, **2019**, 150, 214101	3.9	29

184	A Quasi-Diabatic Representation of the 1,2A States of Methylamine. *Journal of Physical Chemistry A*, **2019**, 123, 5231-5241	2.8	14
183	Nonadiabatic Dynamics in Photodissociation of Hydroxymethyl in the 3A(3p) Rydberg State: A Nine-Dimensional Quantum Study. *Journal of Physical Chemistry A*, **2019**, 123, 1937-1944	2.8	7
182	On the Impact of Singularities in the Two-State Adiabatic to Diabatic State Transformation: A Global Treatment. *Journal of Physical Chemistry A*, **2019**, 123, 9874-9880	2.8	6
181	Representation of coupled adiabatic potential energy surfaces using neural network based quasi-diabatic Hamiltonians: 1,2 A' states of LiFH. *Physical Chemistry Chemical Physics*, **2019**, 21, 14205-14213	3.6	34
180	Signatures of a Conical Intersection in Adiabatic Dissociation on the Ground Electronic State. *Journal of the American Chemical Society*, **2018**, 140, 1986-1989	16.4	31
179	Permutation invariant polynomial neural network approach to fitting potential energy surfaces. IV. Coupled diabatic potential energy matrices. *Journal of Chemical Physics*, **2018**, 149, 144107	3.9	43
178	Determining whether diabolical singularities limit the accuracy of molecular property based diabatic representations: The 1,2A states of methylamine. *Journal of Chemical Physics*, **2018**, 149, 154108	3.9	6
177	Nonadiabatic tunneling via conical intersections and the role of the geometric phase. *Physical Review A*, **2017**, 95,	2.6	35
176	Multistate, multichannel coupled diabatic state representations of adiabatic states coupled by conical intersections. CHOH photodissociation. *Journal of Chemical Physics*, **2017**, 146, 134302	3.9	14
175	Nonadiabatic photodissociation dynamics of the hydroxymethyl radical via the 2A(3s) Rydberg state: A four-dimensional quantum study. *Journal of Chemical Physics*, **2017**, 146, 224306	3.9	11
174	Constructive and Destructive Interference in Nonadiabatic Tunneling via Conical Intersections. *Journal of Chemical Theory and Computation*, **2017**, 13, 1902-1910	6.4	28
173	Encoding of vinylidene isomerization in its anion photoelectron spectrum. *Science*, **2017**, 358, 336-339	33.3	36
172	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	3.9	19
171	Accurate nonadiabatic dynamics. *Physical Chemistry Chemical Physics*, **2016**, 18, 26335-26352	3.6	75
170	An improved quasi-diabatic representation of the 1, 2, 3(1)A coupled adiabatic potential energy surfaces of phenol in the full 33 internal coordinates. *Journal of Chemical Physics*, **2016**, 144, 124312	3.9	33
169	Non-adiabaticity: the importance of conical intersections. *Molecular Physics*, **2016**, 114, 1983-2013	1.7	31
168	Nonadiabatic Tunneling in Photodissociation of Phenol. *Journal of the American Chemical Society*, **2016**, 138, 7828-31	16.4	102
167	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	3.9	35

166	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	3.9	24
165	Constructing diabatic representations using adiabatic and approximate diabatic data--Coping with diabolical singularities. *Journal of Chemical Physics*, **2016**, 144, 044104	3.9	20
164	On the electronic structure of the ground state of cyclopentoxy. The case for a two coupled state description. *Journal of Molecular Spectroscopy*, **2015**, 311, 36-41	1.3	4
163	Nonadiabatic Photodissociation of the Hydroxymethyl Radical from the 2(2)A State. Surface Hopping Simulations Based on a Full Nine-Dimensional Representation of the 1,2,3(2)A Potential Energy Surfaces Coupled by Conical Intersections. *Journal of Physical Chemistry A*, **2015**, 119, 7498-509	2.8	13
162	On the Construction of Property Based Diabatizations: Diabolical Singular Points. *Journal of Physical Chemistry A*, **2015**, 119, 12383-91	2.8	25
161	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	3.9	26
160	Full-Dimensional Quantum State-to-State Nonadiabatic Dynamics for Photodissociation of Ammonia in its A-Band. *Journal of Physical Chemistry Letters*, **2014**, 5, 1055-60	6.4	44
159	Full-dimensional quantum dynamics of vibrationally mediated photodissociation of NH3 and ND3 on coupled ab initio potential energy surfaces: absorption spectra and NH2(□(2)A1)/NH2(X (2)B1) branching ratios. *Journal of Physical Chemistry A*, **2014**, 118, 11926-34	2.8	25
158	On the description of conical intersections--a continuous representation of the local topography of seams of conical intersection of three or more electronic states: a generalization of the two state result. *Journal of Chemical Physics*, **2014**, 141, 174109	3.9	7
157	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	3.9	80
156	Seams of conical intersections relevant to the quenching of OH(A(2)□+)) by collisions with H2. *Journal of Physical Chemistry A*, **2013**, 117, 7344-55	2.8	12
155	On the photoionization spectrum of propyne: a fully ab initio simulation of the low-energy spectrum including the Jahn-Teller effect and the spin-orbit interaction. *Journal of Physical Chemistry A*, **2013**, 117, 12002-10	2.8	9
154	On the mechanism for the nonadiabatic reactive quenching of OH(A2□) by H2(1□g+): the role of the 2(2)A state. *Journal of Chemical Physics*, **2013**, 139, 064314	3.9	9
153	A Lippmann□Schwinger approach for the determination of photoionization and photodetachment cross sections based on a partial wave Green's function expansion and configuration interaction wave functions. *Molecular Physics*, **2012**, 110, 845-859	1.7	6
152	Role of conical intersections in molecular spectroscopy and photoinduced chemical dynamics. *Annual Review of Physical Chemistry*, **2012**, 63, 325-52	15.7	332
151	Nonadiabatic quantum chemistry--past, present, and future. *Chemical Reviews*, **2012**, 112, 481-98	68.1	205
150	First principles determination of the NH2□ND2(□□X) 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	3.9	37
149	Nonadiabatic effects in substitutional isomers of Jahn-Teller molecules: the strange case of hydroxymethoxy. *Journal of Chemical Physics*, **2012**, 137, 154315	3.9	8

148	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	3.9	42
147	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	3.9	43
146	Computational determination of the state absorption spectrum of NH3 and of ND3 using a new quasi-diabatic representation of the X and states and full six-dimensional quantum dynamics. *Journal of Chemical Physics*, **2012**, 136, 234301	3.9	42
145	Conical Intersections in Electron Photodetachment Spectroscopy: Theory and Applications. *Advanced Series in Physical Chemistry*, **2011**, 197-248		1
144	Determining partial differential cross sections for low-energy electron photodetachment involving conical intersections using the solution of a Lippmann-Schwinger equation constructed with standard electronic structure techniques. *Journal of Chemical Physics*, **2011**, 134, 174104	3.9	7
143	On the determination of partial differential cross sections for photodetachment and photoionization processes producing polyatomic molecules with electronic states coupled by conical intersections. *Journal of Chemical Physics*, **2011**, 134, 134110	3.9	8
142	Conical Intersections. *Advanced Series in Physical Chemistry*, **2011**,		233
141	On the determination of intensities for electron photodetachment and photoionization spectra involving states coupled by conical intersections: total integral cross sections for polyatomic molecules. *Journal of Chemical Physics*, **2010**, 133, 194107	3.9	8
140	The Photoelectron Spectrum of Pyrrolide: Nonadiabatic Effects due to Conical Intersections *Journal of Physical Chemistry C*, **2010**, 114, 5312-5320	3.8	11
139	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	3.9	62
138	On the representation of coupled adiabatic potential energy surfaces using quasi-diabatic Hamiltonians: description of accidental seams of conical intersection. *Molecular Physics*, **2010**, 108, 2611-2619	1.7	16
137	On the role of conical intersections and their local topography in the photodissociation of the 1-hydroxyethyl radical. *Chemical Physics*, **2010**, 378, 110-117	2.3	2
136	The simulated photoelectron spectrum of 1-propynide. *Journal of Chemical Physics*, **2009**, 130, 064306	3.9	13
135	The photoelectron spectrum of the ethoxide anion: conical intersections, the spin-orbit interaction, and sequence bands. *Journal of Chemical Physics*, **2009**, 131, 134303	3.9	18
134	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	3.9	19
133	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	3.9	18
132	A simulation of the photoelectron spectrum of pyrazolide. *Journal of Chemical Physics*, **2008**, 129, 064304	3.9	16
131	Determining quasidiabatic coupled electronic state Hamiltonians using derivative couplings: A normal equations based method. *Journal of Chemical Physics*, **2008**, 129, 124104	3.9	48

130	On the multimode quadratic vibronic coupling problem: An open-ended solution using a parallel Lanczos algorithm. *Chemical Physics*, **2008**, 347, 57-64	2.3	16
129	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	3.9	35
128	On the locus of points of conical intersection: seams near seams. *Journal of Chemical Physics*, **2007**, 126, 044104	3.9	8
127	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	3.9	40
126	On the characterization of three state conical intersections using a group homomorphism approach: mapping the full N-5 dimensional seam space. *Journal of Chemical Physics*, **2006**, 124, 244103	3.9	14
125	On the characterization of three state conical intersections: a quasianalytic theory using a group homomorphism approach. *Journal of Chemical Physics*, **2006**, 124, 124109	3.9	20
124	On the characterization of three-state conical intersections using a group homomorphism approach: the two-state degeneracy spaces. *Journal of Physical Chemistry B*, **2006**, 110, 19031-9	3.4	15
123	Interpolation of diabatic potential-energy surfaces: quantum dynamics on ab initio surfaces. *Journal of Chemical Physics*, **2005**, 123, 134110	3.9	50
122	Statistical and nonstatistical nonadiabatic photodissociation from the first excited state of the hydroxymethyl radical. *Journal of Chemical Physics*, **2005**, 122, 84316	3.9	21
121	Escape from the double cone: optimized descriptions of the seam space using gateway modes. *Journal of Chemical Physics*, **2005**, 123, 134106	3.9	13
120	On the connectivity of seams of conical intersection: seam curvature. *Journal of Chemical Physics*, **2005**, 123, 204101	3.9	30
119	DETERMINATION OF POTENTIAL ENERGY SURFACE INTERSECTIONS AND DERIVATIVE COUPLINGS IN THE ADIABATIC REPRESENTATION. *Advanced Series in Physical Chemistry*, **2004**, 129-173		12
118	CONICAL INTERSECTIONS: THEIR DESCRIPTION AND CONSEQUENCES. *Advanced Series in Physical Chemistry*, **2004**, 41-127		38
117	Exploring molecular complexity: conical intersections and NH3 photodissociation. *Journal of Chemical Physics*, **2004**, 121, 628-31	3.9	37
116	Marching along ridges. An extrapolatable approach to locating conical intersections. *Faraday Discussions*, **2004**, 127, 325-36	3.6	21
115	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, 7330-9	3.9	208
114	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	2.8	34
113	Analytic evaluation of nonadiabatic coupling terms at the MR-CI level. I. Formalism. *Journal of Chemical Physics*, **2004**, 120, 7322-9	3.9	270

112	Conical Intersections. *Advances in Physical Chemistry*, **2004**,		679
111	Conical Intersections and the Spin-Orbit Interaction. *Advances in Chemical Physics*, **2003**, 557-581		6
110	Conical intersections of three electronic states affect the ground state of radical species with little or no symmetry: pyrazolyl. *Journal of the American Chemical Society*, **2003**, 125, 12428-9	16.4	45
109	Beyond two-state conical intersections. Three-state conical intersections in low symmetry molecules: the allyl radical. *Journal of the American Chemical Society*, **2003**, 125, 10672-6	16.4	65
108	On the properties of the seam and branching spaces of conical intersections in molecules with an odd number of electrons: A group homomorphism approach. *Journal of Chemical Physics*, **2003**, 118, 9952-9962	3.9	10
107	Nonadiabatic processes involving three electronic states. I. Branch cuts and linked pairs of conical intersections. *Journal of Chemical Physics*, **2003**, 119, 5058-5068	3.9	36
106	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	3.9	29
105	Intersecting Conical Intersection Seams: Their Location, Representation, and Effect on Local Topography. *Journal of Physical Chemistry A*, **2002**, 106, 2580-2591	2.8	29
104	Conical intersections and the nonadiabatic reactions H2O+O(3P)<-ρOH(A 2Σ)+OH(X 2Π). *Journal of Chemical Physics*, **2002**, 117, 3733-3740	3.9	8
103	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	3.9	22
102	Photodissociation of the hydroxymethyl radical. I. The role of conical intersections in line broadening and decomposition pathways. *Journal of Chemical Physics*, **2002**, 116, 8300	3.9	24
101	Photodissociation of the vinoxy radical through conical, and avoided, intersections. *Journal of Chemical Physics*, **2002**, 117, 7198-7206	3.9	23
100	Spin□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 Case□ *Journal of Physical Chemistry B*, **2002**, 106, 8108-8116	3.4	18
99	Accidental conical intersections of three states of the same symmetry. I. Location and relevance. *Journal of Chemical Physics*, **2002**, 117, 6907-6910	3.9	60
98	On the effects of spin□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	3.9	20
97	Characterizing the local topography of conical intersections using orthogonality constrained parameters: Application to the internal conversion S1-S0 in HNCO. *Journal of Chemical Physics*, **2001**, 114, 2614-2622	3.9	11
96	Accurate first-derivative nonadiabatic couplings for the H3 system. *Journal of Chemical Physics*, **2001**, 115, 4640-4659	3.9	59
95	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	3.9	27

94	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	3.9	141
93	Conical Intersections: The New Conventional Wisdom. *Journal of Physical Chemistry A*, **2001**, 105, 6277-6293	2.8	300
92	Intersecting conical intersection seams in tetra-atomic molecules: the S1–S0 internal conversion in HNCO. *Molecular Physics*, **2001**, 99, 1463-1467	1.7	3
91	Symmetry Friend or Foe: Confluences of Conical Intersection Seams in Tetra-Atomic Molecules *Journal of Physical Chemistry A*, **2001**, 105, 2642-2645	2.8	12
90	Diabatic bases and molecular properties. *International Journal of Quantum Chemistry*, **2000**, 76, 235-243	2.1	37
89	Perspective on Some recent developments in the theory of molecular energy levels *Theoretical Chemistry Accounts*, **2000**, 103, 242-247	1.9	4
88	The role of conical intersections in the nonadiabatic quenching of OH(A 2Σ) by molecular hydrogen. *Journal of Chemical Physics*, **2000**, 113, 10091-10099	3.9	44
87	On the adiabatic to diabatic states transformation near intersections of conical intersections. *Journal of Chemical Physics*, **2000**, 112, 2111-2120	3.9	90
86	On the strongly bound B 3state of the CAr van der Waals complex: Bonding and predissociation. *Journal of Chemical Physics*, **1999**, 111, 3070-3076	3.9	8
85	A theoretical analysis of the state-specific decomposition of OH(A 2Σ,v?,N?,F1/F2) levels, including the effects of spin–orbit and Coriolis interactions. *Journal of Chemical Physics*, **1999**, 110, 363-376	3.9	52
84	Determining the molecular Aharonov–Bohm phase angle: A rigorous approach employing a molecular properties based adiabatic to diabatic states transformation. *Journal of Chemical Physics*, **1999**, 110, 701-705	3.9	29
83	Substituent effects and the noncrossing rule: The importance of reduced symmetry subspaces. I. The quenching of OH(A 2Σ) by H2. *Journal of Chemical Physics*, **1999**, 111, 6661-6664	3.9	28
82	Unusual conical intersections in the Jahn–Teller effect: The electronically excited states of Li3. *Journal of Chemical Physics*, **1999**, 110, 3639-3642	3.9	35
81	S1–S0 Internal Conversion in Ketene. 1. The Role of Conical Intersections. *Journal of Physical Chemistry A*, **1999**, 103, 6658-6668	2.8	19
80	Suppressing the geometric phase effect: Closely spaced seams of the conical intersection in Na3(2 2E?). *Journal of Chemical Physics*, **1999**, 111, 4906-4912	3.9	19
79	Conical Intersections: Diabolical and Often Misunderstood. *Accounts of Chemical Research*, **1998**, 31, 511-518	24.3	364
78	A criterion for the confluence of two seams of conical intersection in triatomic molecules. *Theoretical Chemistry Accounts*, **1998**, 98, 197-201	1.9	24
77	Quenching of Li (2P) by H2: potential energy surfaces, conical intersection seam, and diabatic bases. *Theoretical Chemistry Accounts*, **1998**, 100, 154-170	1.9	11

76	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	2.8	42
75	On the Mechanism of the Spin-Nonconserving Chemical Reaction O(3P) + HCCH -p CH2(1A1) + CO(X1). I. Feasibility. *Journal of Physical Chemistry A*, **1998**, 102, 5305-5311	2.8	24
74	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	3.9	15
73	Systematic location of intersecting seams of conical intersection in triatomic molecules: The 1 2A? 2 2A? conical intersections in BH2. *Journal of Chemical Physics*, **1998**, 108, 5657-5659	3.9	26
72	On the adiabatic to diabatic states transformation in the presence of a conical intersection: A most diabatic basis from the solution to a Poisson equation. I. *Journal of Chemical Physics*, **1998**, 109, 20-25	3.9	82
71	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	1.7	12
70	On the origin of the heavy atom effect in the fine-structure splitting of the 1 2 state of alkali metal 2P-rare gas van der Waals molecules. *Journal of Chemical Physics*, **1997**, 107, 7690-7694	3.9	21
69	Electronic structure aspects of the spin-forbidden reaction CH3(X 2A2?)+N(4S)-p HCN(X 1)+H2(X 1 g+). *Journal of Chemical Physics*, **1997**, 107, 4994-4999	3.9	23
68	A theoretical investigation of the spin rbit-induced predissociation of Bar C2 . *Journal of Chemical Physics*, **1997**, 106, 6607-6611	3.9	10
67	Resonances in the predissociation of the A 2 state of MgBr. *Journal of Chemical Physics*, **1997**, 106, 4091-4101	3.9	13
66	On the Relation between Bonding and the Spin Orbit Interaction in BNe: the C2 and 14 States. *Journal of Physical Chemistry A*, **1997**, 101, 9520-9524	2.8	7
65	Energies and derivative couplings in the vicinity of a conical intersection. II. CH2(2 3A?,3 3A?) and H2S(1 1A?,2 1A?), unexpected results in an ostensibly standard case. *Journal of Chemical Physics*, **1997**, 107, 7825-7838	3.9	47
64	The Reactions Al(2P) + H2 -p AlH2(12A ,22A) -p AlH2(X2A1) or AlH(X1) + H: Unusual Conical Intersections and Possible Nonadiabatic Recrossing. *Journal of Physical Chemistry A*, **1997**, 101, 7953-7959	2.8	45
63	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	2.8	106
62	New and Unusual Bonding in Open Shell van der Waals Molecules Revealed by the Heavy Atom Effect: The Case of BAr. *Journal of Physical Chemistry A*, **1997**, 101, 3166-3173	2.8	14
61	Radiative and Nonradiative Decay of the BH(b3) State: A Joint Experimental and Theoretical Study. *The Journal of Physical Chemistry*, **1996**, 100, 5649-5653		8
60	Quenching of CH(a4) by CO(X1): Surfaces of Intersection, Spin Orbit Interactions, and the Incorporation of Kramers' Degeneracy. *The Journal of Physical Chemistry*, **1996**, 100, 17439-17445		12
59	Diabolical conical intersections. *Reviews of Modern Physics*, **1996**, 68, 985-1013	40.5	735

58	Current Issues in Nonadiabatic Chemistry *The Journal of Physical Chemistry*, **1996**, 100, 18612-18628		166
57	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	3.9	23
56	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	3.9	109
55	Radiationless decay of the 1,2,3 3g states of Al2: A fully first principles treatment using adiabatic and rigorous diabatic states. *Journal of Chemical Physics*, **1995**, 102, 1955-1964	3.9	19
54	On the spin-orbit induced radiationless decay of the b3state of BH. *Molecular Physics*, **1995**, 84, 611-618	1.7	5
53	On the role of conical intersections in photodissociation. III. The case of hydroxylamine. *Journal of Chemical Physics*, **1995**, 102, 8431-8439	3.9	17
52	Radiative and radiationless decay of resonances resulting from electronically nonadiabatic interactions: A computational approach valid for both narrow and broad linewidths and large energy shifts. *Journal of Chemical Physics*, **1995**, 103, 7336-7346	3.9	11
51	ELECTRONIC STRUCTURE ASPECTS OF NONADIABATIC PROCESSES IN POLYATOMIC SYSTEMS. *Advanced Series in Physical Chemistry*, **1995**, 642-721		25
50	On the role of conical intersections of two potential energy surfaces of the same symmetry in photodissociation. I. CH3SH-CH3S+H and CH3+SH. *Journal of Chemical Physics*, **1994**, 100, 3639-3644	3.9	31
49	On the perturbation of the B 2Astate of HCO by the 1 4And 1 4Astates: Surfaces of intersection and spinorbit interactions. *Journal of Chemical Physics*, **1994**, 100, 473-480	3.9	18
48	Nonadiabatic perturbations and fine structure splittings in the 1,2 3g states of B2: An analysis based on adiabatic and rigorous diabatic states. *Journal of Chemical Physics*, **1994**, 100, 8204-8211	3.9	12
47	On the radiative lifetime of the (a 4v,N,Fi) levels of the CH radical: An ab initio treatment. *Journal of Chemical Physics*, **1994**, 100, 8991-8998	3.9	15
46	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	3.9	112
45	Theoretical studies of spin-forbidden radiationless decay in polyatomic systems. II. Radiationless decay of a-N2O2. *Journal of Chemical Physics*, **1993**, 98, 3845-3849	3.9	23
44	On the electronic structure aspects of spin-forbidden processes in N2O. *Journal of Chemical Physics*, **1993**, 99, 6824-6831	3.9	41
43	A theoretical treatment of the predissociation of the individual rovibronic levels of OH/OD(A 2). *Journal of Chemical Physics*, **1992**, 97, 1838-1849	3.9	76
42	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(X 2-H(2S)+NO+(X 1). *Journal of Chemical Physics*, **1992**, 97, 715-717	3.9	15
41	Spin-forbidden chemistry within the Breit-Pauli approximation. *International Reviews in Physical Chemistry*, **1992**, 11, 195-242	7	75

40	Radiative and nonradiative decay of the NH(ND) A 3Π electronic state: Predissociation induced by the 5Σ state. *Journal of Chemical Physics*, **1991**, 94, 1913-1922	3.9	41
39	A theoretical treatment of thea 3Π+ -p X1Σ++ spin-forbidden dipole-allowed radiative transition in NO+. *Journal of Chemical Physics*, **1991**, 95, 6562-6566	3.9	19
38	Predissociation of the c 1Π state of NH (ND): The role of dipolar spin-spin coupling. *Journal of Chemical Physics*, **1991**, 94, 2364-2367	3.9	16
37	On the mechanism of the reaction CH(X 2Π)+N2(X 1Σg)-pHCN(X 1Σ) +N(4S). I. A theoretical treatment of the electronic structure aspects of the intersystem crossing. *Journal of Chemical Physics*, **1991**, 95, 1808-1816	3.9	68
36	Spin-forbidden decay of the dication HS2+. *Journal of Chemical Physics*, **1991**, 94, 7208-7211	3.9	10
35	On the characterization of regions of avoided surface crossings using an analytic gradient based method. *Journal of Chemical Physics*, **1990**, 92, 2457-2463	3.9	62
34	Spin-orbit effects in the decomposition reaction N3H(X 1A')-pN2(X1Σg)+NH(X3Σa1Δ). *Journal of Chemical Physics*, **1990**, 92, 320-323	3.9	25
33	On the electronic structure and dynamical aspects of the predissociation of the A 2Σ states of MgCl. A rigorous quantum mechanical treatment incorporating spin-orbit and derivative coupling effects. *Journal of Chemical Physics*, **1990**, 93, 6403-6418	3.9	20
32	On the noncrossing rule in polyatomic systems: Determination of a seam of actual surface crossings relevant to the quenching of H2(B 1Σu) by helium. *Journal of Chemical Physics*, **1990**, 93, 4473-4474	3.9	28
31	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++NO-pH+NO+. *Journal of Chemical Physics*, **1989**, 90, 1657-1665	3.9	23
30	On the quenching of helium 2 3S: Potential energy curves for, and nonadiabatic, relativistic, and radiative couplings between, the a 3Σu, A 1Σu, b 3Πg, B 1Πg, c 3Σg, and C 1Σg states of He2. *Journal of Chemical Physics*, **1989**, 90, 7164-7175	3.9	33
29	On the electronic structure of the NH radical. The fine structure splitting of the X 3Σ state and the spin-forbidden (b 1Σ, a 1Δ)-pX 3Σ and the spin-allowed A 3Π-pX 3Σ and c 1Π-p(b 1Σ, a 1Δ) radiative transitions. *Journal of Chemical Physics*, **1989**, 91, 4745-4757	3.9	50
28	Spin-forbidden radiative decay involving quasidegenerate states. Application to the B 1Σ-p 3Π transition in MgO. *Journal of Chemical Physics*, **1988**, 89, 7324-7333	3.9	25
27	On the electronic structure of the He+H2 system: Characterization of, and nonadiabatic interactions between, the 1 1A' and 2 1A' potential energy surfaces. *Journal of Chemical Physics*, **1988**, 89, 4945-4953	3.9	17
26	On the evaluation of non-Born-Oppenheimer interactions for Born-Oppenheimer wave functions. V. A body fixed frame approach. Applications to isotope effects on equilibrium geometries and the adiabatic correction for the X 1Σ state of LiH. *Journal of Chemical Physics*, **1988**, 89, 975-982	3.9	35
25	On the evaluation of lifetimes for spin-forbidden radiative transitions originating in coupling to states embedded in a continuum. Application to CH. *Journal of Chemical Physics*, **1988**, 88, 3853-3860	3.9	7
24	On the radiative lifetimes of the b 1Σ and a 1Δ states in NCl. *Journal of Chemical Physics*, **1987**, 86, 1642-1643	3.9	26
23	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	3.9	33

22	On the quenching of Na(2P) by HCl: Nonadiabatic effects. *Journal of Chemical Physics*, **1987**, 86, 4990-4996	3.9	22
21	On the quenching of Li(2p) by HCl: Nonadiabatic effects. *International Journal of Quantum Chemistry*, **1987**, 31, 91-97	2.1	14
20	A theoretical description of the radiative decay processes (b 1Σ+, a 1Δ)→X 3Σ− in NF. *Journal of Chemical Physics*, **1986**, 85, 7261-7267	3.9	21
19	On the use of the Breit-Pauli approximation for evaluating line strengths for spin-forbidden transitions. II. The symbolic matrix element method. *Journal of Chemical Physics*, **1986**, 84, 2075-2078	3.9	25
18	On the reaction Na(2P)+H2→Na(2S)+H2 nonadiabatic effects. *Journal of Chemical Physics*, **1986**, 84, 3206-3211	3.9	45
17	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	3.9	52
16	On the evaluation of non-adiabatic coupling matrix elements for large scale CI wavefunctions. *Chemical Physics Letters*, **1985**, 113, 159-164	2.5	91
15	On the use of the Breit-Pauli approximation for evaluating line strengths for spin-forbidden transitions: Application to NF. *Journal of Chemical Physics*, **1985**, 83, 1168-1172	3.9	37
14	On the Mg(3P)-He(1S) interaction using SA-MCSCF/ICF-CI wave functions. *Journal of Chemical Physics*, **1984**, 80, 5089-5094	3.9	28
13	On the evaluation of nonadiabatic coupling matrix elements using SA-MCSCF/CI wave functions and analytic gradient methods. I. *Journal of Chemical Physics*, **1984**, 81, 4549-4553	3.9	143
12	Electronic structure and vertical excitation spectrum of methylene amidogen CH2N. *International Journal of Quantum Chemistry*, **1983**, 23, 437-446	2.1	19
11	On the electronic structure of the X, A, and B states of CaCl. *Journal of Chemical Physics*, **1983**, 79, 4376-4381	3.9	33
10	On the reaction Mg+N2O→MgO+N2. *Journal of Chemical Physics*, **1983**, 78, 6763-6772	3.9	46
9	The electronic structure of CaO. II. An MCSCF/CI treatment of the low-lying 1Σ+ and 1Δ states. *Journal of Chemical Physics*, **1982**, 77, 5573-5580	3.9	30
8	On the low-lying states of MgO. II. *Journal of Chemical Physics*, **1981**, 74, 2379-2383	3.9	31
7	MCSCF wave functions for excited states of polar molecules: Application to BeO. *Journal of Chemical Physics*, **1980**, 72, 1138-1144	3.9	33
6	On the low lying singlet states of BeO. *Journal of Chemical Physics*, **1980**, 73, 5702-5705	3.9	14
5	Electronic structure of CaO. I. *Journal of Chemical Physics*, **1978**, 68, 3990-3997	3.9	47

4	On the electronic structure of the 2 1A1 state of methylene. *Journal of Chemical Physics*, **1978**, 69, 3875-3877	3.9	16
3	Vibrational energy levels of the S0 and S1 states of formaldehyde using an accurate ab initio based global diabatic potential energy matrix. *Molecular Physics*,e1918775	1.7	2
2	Diabatic bases and molecular properties		1
1	Nonadiabatic Interactions Between Potential Energy Surfaces: Theory and Applications. *Advances in Chemical Physics*,1-71		70