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	Unified Description of the Jahnâ€“Teller Effect in Molecules with Only C_sSymmetry: Cyclohexoxy in Its Full 48-Dimensional Internal Coordinates. Journal of Physical Chemistry A, 2022, 126, 61-67.	1.1	2
2	Internal conversion and intersystem crossing dynamics based on coupled potential energy surfaces with full geometry-dependent spinâ€“orbit and derivative couplings. Nonadiabatic photodissociation dynamics of NH₃(A) leading to the NH(X³Î£^{â¯}, a¹Î”) + H₂ channel. Physical Chemistry Chemical Physics, 2022, 24, 15060-15067.	1.3	3
3	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
4	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
5	Vibrational energy levels of the S ₀ and S ₁ states of formaldehyde using an accurate ab initio based global diabatic potential energy matrix. Molecular Physics, 2021, 119, .	0.8	3
6	Enabling a Unified Description of Both Internal Conversion and Intersystem Crossing in Formaldehyde: A Global Coupled Quasi-Diabatic Hamiltonian for Its S₀, S₁, and T₁ States. Journal of Chemical Theory and Computation, 2021, 17, 4157-4168.	2.3	12
7	Full-dimensional quantum stereodynamics of the non-adiabatic quenching of OH(A2Î£+) by H2. Nature Chemistry, 2021, 13, 909-915.	6.6	17
8	Conical intersection seams in spinâ€“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.	1.2	6
9	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
10	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
11	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.	2.3	6
12	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
13	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.	2.1	2
14	Construction of Quasi-diabatic Hamiltonians That Accurately Represent ab Initio 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.	1.1	15
15	On the nonadiabatic collisional quenching of OH(A) by H₂: a four coupled quasi-diabatic state description. Physical Chemistry Chemical Physics, 2020, 22, 13516-13527.	1.3	15
16	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
17	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	1.2	42
18	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.	1.1	8

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19	Diabatic and adiabatic representations: Electronic structure caveats. Computational and Theoretical Chemistry, 2019, 1152, 41-52.	1.1	15
20	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
21	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
22	A Quasi-Diabatic Representation of the 1,2¹A States of Methylamine. Journal of Physical Chemistry A, 2019, 123, 5231-5241.	1.1	19
23	Nonadiabatic Dynamics in Photodissociation of Hydroxymethyl in the 32A(3px) Rydberg State: A Nine-Dimensional Quantum Study. Journal of Physical Chemistry A, 2019, 123, 1937-1944.	1.1	8
24	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
25	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
26	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
27	Determining whether diabolical singularities limit the accuracy of molecular property based diabatic representations: The 1,21A states of methylamine. Journal of Chemical Physics, 2018, 149, 154108.	1.2	7
28	Nonadiabatic tunneling via conical intersections and the role of the geometric phase. Physical Review A, 2017, 95, .	1.0	48
29	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
30	Nonadiabatic photodissociation dynamics of the hydroxymethyl radical via the 22A(3s) Rydberg state: A four-dimensional quantum study. Journal of Chemical Physics, 2017, 146, 224306.	1.2	13
31	Constructive and Destructive Interference in Nonadiabatic Tunneling via Conical Intersections. Journal of Chemical Theory and Computation, 2017, 13, 1902-1910.	2.3	34
32	Encoding of vinylidene isomerization in its anion photoelectron spectrum. Science, 2017, 358, 336-339.	6.0	55
33	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
34	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
35	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
36	Constructing diabatic representations using adiabatic and approximate diabatic data â€“ Coping with diabolical singularities. Journal of Chemical Physics, 2016, 144, 044104.	1.2	22

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37	Accurate nonadiabatic dynamics. Physical Chemistry Chemical Physics, 2016, 18, 26335-26352.	1.3	104
38	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
39	Non-adiabaticity: the importance of conical intersections. Molecular Physics, 2016, 114, 1983-2013.	0.8	40
40	Nonadiabatic Tunneling in Photodissociation of Phenol. Journal of the American Chemical Society, 2016, 138, 7828-7831.	6.6	126
41	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
42	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.	0.4	4
43	Nonadiabatic Photodissociation of the Hydroxymethyl Radical from the 22A State. Surface Hopping Simulations Based on a Full Nine-Dimensional Representation of the 1,2,32A Potential Energy Surfaces Coupled by Conical Intersections. Journal of Physical Chemistry A, 2015, 119, 7498-7509.	1.1	14
44	On the Construction of Property Based Diabatizations: Diabolical Singular Points. Journal of Physical Chemistry A, 2015, 119, 12383-12391.	1.1	29
45	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
46	On the description of conical intersectionsâ€"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.	1.2	7
47	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
48	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
49	Seams of Conical Intersections Relevant to the Quenching of OH(A²Î£⁺) by Collisions with H₂. Journal of Physical Chemistry A, 2013, 117, 7344-7355.	1.1	15
50	On the Photoionization Spectrum of Propyne: A Fully ab Initio Simulation of the Low-Energy Spectrum Including the Jahnâ€"Teller Effect and the Spinâ€"Orbit Interaction. Journal of Physical Chemistry A, 2013, 117, 12002-12010.	1.1	11
51	On the mechanism for the nonadiabatic reactive quenching of OH(A2Î£+) by H2(1$Sigma _{m g}^+$Î£g+): The role of the 22A state. Journal of Chemical Physics, 2013, 139, 064314.	1.2	12
52	First principles determination of the NH2/ND2($skew4ilde A, skew3ilde X$AÌƒ,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
53	Nonadiabatic effects in substitutional isomers of Jahn-Teller molecules: The strange case of hydroxymethoxy. Journal of Chemical Physics, 2012, 137, 154315.	1.2	9
54	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

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55	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
56	Computational determination of the Ãƒ state absorption spectrum of NH3 and of ND3 using a new quasi-diabatic representation of the $skew3ilde{X}$XÌƒ and Ãƒ states and full six-dimensional quantum dynamics. Journal of Chemical Physics, 2012, 136, 234301.	1.2	46
57	A Lippmannâ€“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.	0.8	6
58	Role of Conical Intersections in Molecular Spectroscopy and Photoinduced Chemical Dynamics. Annual Review of Physical Chemistry, 2012, 63, 325-352.	4.8	401
59	Nonadiabatic Quantum Chemistryâ€”Past, Present, and Future. Chemical Reviews, 2012, 112, 481-498.	23.0	254
60	Conical Intersections in Electron Photodetachment Spectroscopy: Theory and Applications. Advanced Series in Physical Chemistry, 2011, , 197-248.	1.5	1
61	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.	1.2	7
62	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.	1.2	8
63	Conical Intersections. Advanced Series in Physical Chemistry, 2011, , .	1.5	300
64	On the role of conical intersections and their local topography in the photodissociation of the 1-hydroxyethyl radical. Chemical Physics, 2010, 378, 110-117.	0.9	3
65	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.	1.2	8
66	The Photoelectron Spectrum of Pyrrolide: Nonadiabatic Effects due to Conical Intersections. Journal of Physical Chemistry C, 2010, 114, 5312-5320.	1.5	13
67	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
68	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.	0.8	16
69	The simulated photoelectron spectrum of 1-propynide. Journal of Chemical Physics, 2009, 130, 064306.	1.2	13
70	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
71	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
72	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

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73	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
74	A simulation of the photoelectron spectrum of pyrazolide. Journal of Chemical Physics, 2008, 129, 064304.	1.2	16
75	Determining quasidiabatic coupled electronic state Hamiltonians using derivative couplings: A normal equations based method. Journal of Chemical Physics, 2008, 129, 124104.	1.2	52
76	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
77	On the locus of points of conical intersection: Seams near seams. Journal of Chemical Physics, 2007, 126, 044104.	1.2	8
78	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
79	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
80	On the characterization of three state conical intersections using a group homomorphism approach: Mapping the full Nâˆ’5 dimensional seam space. Journal of Chemical Physics, 2006, 124, 244103.	1.2	14
81	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
82	Interpolation of diabatic potential-energy surfaces: Quantum dynamics on ab initio surfaces. Journal of Chemical Physics, 2005, 123, 134110.	1.2	53
83	Statistical and nonstatistical nonadiabatic photodissociation from the first excited state of the hydroxymethyl radical. Journal of Chemical Physics, 2005, 122, 084316.	1.2	22
84	Escape from the double cone: Optimized descriptions of the seam space using gateway modes. Journal of Chemical Physics, 2005, 123, 134106.	1.2	15
85	On the connectivity of seams of conical intersection: Seam curvature. Journal of Chemical Physics, 2005, 123, 204101.	1.2	31
86	DETERMINATION OF POTENTIAL ENERGY SURFACE INTERSECTIONS AND DERIVATIVE COUPLINGS IN THE ADIABATIC REPRESENTATION. Advanced Series in Physical Chemistry, 2004, , 129-173.	1.5	12
87	CONICAL INTERSECTIONS: THEIR DESCRIPTION AND CONSEQUENCES. Advanced Series in Physical Chemistry, 2004, , 41-127.	1.5	46
88	Exploring molecular complexity: Conical intersections and NH3 photodissociation. Journal of Chemical Physics, 2004, 121, 628-631.	1.2	39
89	Marching along ridges. An extrapolatable approach to locating conical intersections. Faraday Discussions, 2004, 127, 325.	1.6	22
90	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

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91	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
92	Analytic evaluation of nonadiabatic coupling terms at the MR-CI level. I. Formalism. Journal of Chemical Physics, 2004, 120, 7322-7329.	1.2	290
93	Conical Intersections. Advanced Series in Physical Chemistry, 2004, , .	1.5	864
94	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
95	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
96	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.	1.2	11
97	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
98	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
99	Conical Intersections and the Spin-Orbit Interaction. Advances in Chemical Physics, 2003, , 557-581.	0.3	8
100	Conical intersections and the nonadiabatic reactions H2O+O(3P)â†”OH(Aâ€Š2Î£+)+OH(Xâ€Š2Î). Journal of Chemical Physics, 2002, 117, 3733-3740.	1.2	12
101	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
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.	1.2	25
103	Photodissociation of the vinoxy radical through conical, and avoided, intersections. Journal of Chemical Physics, 2002, 117, 7198-7206.	1.2	23
104	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
105	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
106	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
107	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
108	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

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109	Conical Intersections:Â The New Conventional Wisdom. Journal of Physical Chemistry A, 2001, 105, 6277-6293.	1.1	335
110	Intersecting conical intersection seams in tetra-atomic molecules: the S1â€“S0internal conversion in HNCO. Molecular Physics, 2001, 99, 1463-1467.	0.8	6
111	Symmetry Friend or Foe:Â Confluences of Conical Intersection Seams in Tetra-Atomic Moleculesâ€. Journal of Physical Chemistry A, 2001, 105, 2642-2645.	1.1	12
112	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
113	Characterizing the local topography of conical intersections using orthogonality constrained parameters: Application to the internal conversion S1â†'S0 in HNCO. Journal of Chemical Physics, 2001, 114, 2614-2622.	1.2	14
114	Accurate first-derivative nonadiabatic couplings for the H3 system. Journal of Chemical Physics, 2001, 115, 4640-4659.	1.2	61
115	Diabatic bases and molecular properties. International Journal of Quantum Chemistry, 2000, 76, 235-243.	1.0	38
116	Perspective on "Some recent developments in the theory of molecular energy levels". Theoretical Chemistry Accounts, 2000, 103, 242-247.	0.5	4
117	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
118	On the adiabatic to diabatic states transformation near intersections of conical intersections. Journal of Chemical Physics, 2000, 112, 2111-2120.	1.2	106
119	On the strongly bound Bâ€‰3Î state of the CAr van der Waals complex: Bonding and predissociation. Journal of Chemical Physics, 1999, 111, 3070-3076.	1.2	9
120	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
121	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
122	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
123	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
124	S1â^'S0 Internal Conversion in Ketene. 1. The Role of Conical Intersections. Journal of Physical Chemistry A, 1999, 103, 6658-6668.	1.1	23
125	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
126	Conical Intersections:â€‰ Diabolical and Often Misunderstood. Accounts of Chemical Research, 1998, 31, 511-518.	7.6	396

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127	A criterion for the confluence of two seams of conical intersection in triatomic molecules. Theoretical Chemistry Accounts, 1998, 98, 197-201.	0.5	26
128	Quenching of Li (2 P) by H 2 : potential energy surfaces, conical intersection seam, and diabatic bases. Theoretical Chemistry Accounts, 1998, 100, 154-170.	0.5	11
129	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
130	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
131	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
132	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
133	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
134	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
135	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
136	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
137	A theoretical investigation of the spinâ€“orbit-induced predissociation of Bar C2Î”. Journal of Chemical Physics, 1997, 106, 6607-6611.	1.2	11
138	Resonances in the predissociation of the Aâ€‰2Î© state of MgBr. Journal of Chemical Physics, 1997, 106, 4091-4101.	1.2	13
139	On the Relation between Bonding and the Spinâ^'Orbit Interaction in BNe:Â the C2Î” and 14Î States. Journal of Physical Chemistry A, 1997, 101, 9520-9524.	1.1	7
140	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
141	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
142	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
143	New and Unusual Bonding in Open Shell van der Waals Molecules Revealed by the Heavy Atom Effect:â€‰ The Case of BAr. Journal of Physical Chemistry A, 1997, 101, 3166-3173.	1.1	14
144	Diabolical conical intersections. Reviews of Modern Physics, 1996, 68, 985-1013.	16.4	853

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145	Current Issues in Nonadiabatic Chemistryâ€. The Journal of Physical Chemistry, 1996, 100, 18612-18628.	2.9	179
146	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
147	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
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