Carlo Petrongolo

List of Publications by Year in descending order

88 papers	2,462 citations	159585 30 h-index	223800 46 g-index
92 all docs	92 docs citations	92 times ranked	986 citing authors

#	Article	IF	Citations
1	Nonadiabatic treatment of the intensity distribution in the Vâ€“N bands of ethylene. Journal of Chemical Physics, 1982, 76, 3655-3667.	3.0	148
2	Ab initiostudy of NO2. Molecular Physics, 1990, 70, 835-848.	1.7	120
3	Theoretical investigations on the solvation process. Theoretica Chimica Acta, 1971, 20, 331-342.	0.8	106
4	Theoretical prediction of the potential curves for the lowestâ€lying states of the C2+ molecular ion. Journal of Chemical Physics, 1981, 74, 4594-4602.	3.0	87
5	SCF Minimal Basis Set Calculations and Exclusive Orbitals for CNâ¯, HCN, N3â¯, HN3, NCOâ¯, and HNCO. Journal of Chemical Physics, 1968, 48, 1500-1508.	3.0	79
6	Abinitioâ€‰study of NO2. V. Nonadiabatic vibronic states and levels of theXÌƒâ€‰2A1/Ãƒâ€‰2B2conical intersection. Journal of Chemical Physics, 1996, 105, 9051-9067.	3.0	79
7	Diabatic representation of the Ãƒ²A₁[Btilde]²B₂conical intersection in NH₂. Molecular Physics, 1990, 70, 825-834.	1.7	75
8	Quantum Wave Packet Study of Nonadiabatic Effects in O(1D) + H2â† OH + H. Journal of Physical Chemistry A, 1999, 103, 9448-9459.	2.5	72
9	Nonadiabatic theory of triatomics: General formalism and application to Rennerâ€“Teller and conicalâ€intersection effects. Journal of Chemical Physics, 1988, 89, 1297-1308.	3.0	69
10	Ab initiostudy of NO2. Molecular Physics, 1991, 73, 1085-1099.	1.7	67
11	Internal rotation potential energy for the glycine molecule in its zwitterionic and neutral forms. A comparison among several methods. The Journal of Physical Chemistry, 1980, 84, 435-442.	2.9	50
12	Theoretical prediction of the potential curves for the lowestâ€lying states of the CSi+ and Si2+ molecular ions. Journal of Chemical Physics, 1981, 74, 4611-4620.	3.0	44
13	Nonadiabatic investigation of the Vâ€“N spectrum of ethylene in a new diabatic representation. Journal of Chemical Physics, 1983, 78, 7284-7289.	3.0	42
14	Trajectory-Surface-Hopping Study of the Rennerâ¯Teller Effect in the N(2D) + H2 Reaction. Journal of Physical Chemistry A, 2002, 106, 8276-8284.	2.5	42
15	Nonadiabatic wave packet dynamics of NO2 on the XÌƒâ€Š2Aâ€²/Ãƒâ€Š2Aâ€² conical intersection. Journal of Chemical Physics, 1999, 110, 4419-4427.	3.0	41
16	Minimalâ€Basisâ€Set LCAOâ€“SCFâ€“MO Calculations for the Ground State of O3, NO2â€“, NOF, and OF2 Molecules. Journal of Chemical Physics, 1968, 48, 407-411.	3.0	40
17	MRD-CI ground state geometry and vertical spectrum of N3. Journal of Molecular Structure, 1988, 175, 215-220.	3.6	40
18	Renner-Teller quantum dynamics of the N(D2)+H2â†NH+H reaction. Journal of Chemical Physics, 2006, 125, 064308.	3.0	40

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19	Nonadiabatic quantum dynamics of C(1D)+H2â†'CH+H: Coupled-channel calculations including Renner-Teller and Coriolis terms. Journal of Chemical Physics, 2011, 135, 114308.	3.0	38
20	Ab initio study of NO2. VI. Vibrational and vibronic coupling in the XÌƒ2A1/ÃƒB2 conical intersection up to 16â€‰000â€‰cmâ^'1. Journal of Chemical Physics, 1997, 106, 10066-10071.	3.0	37
21	Structure-activity relations of phenethylamine. Comparison of quantum mechanical SCF ab initio and semiempirical calculations. Journal of the American Chemical Society, 1975, 97, 1338-1347.	13.7	36
22	Rennerâ€"Teller coupled-channel dynamics of the N(D2)+H2 reaction and the role of the NH2â€^AÌƒâ€‰A21 electronic state. Journal of Chemical Physics, 2008, 129, 244307.	3.0	36
23	Rotational, Steric, and Coriolis Effects on the F + HCl â†' HF + Cl Reaction on the 12Aâ€² Ground-State Surface. Journal of Physical Chemistry A, 2009, 113, 4208-4212.	2.5	35
24	Quantum real wave-packet dynamics of the N(S4)+NO(XÌƒÎ2)â†'N2(XÌƒÎ£g+1)+O(P3) reaction on the ground and first excited triplet potential energy surfaces: Rate constants, cross sections, and product distributions. Journal of Chemical Physics, 2006, 124, 174303.	3.0	34
25	Ab initio study of Î²-lactam antibiotics. II. Potential energy surface for the amidic CN bond breaking in the 3-cephem + OHâ^' reaction and comparison with the Î²-lactam + OHâ^' reaction. Chemical Physics, 1980, 45, 291-304.	1.9	33
26	Product distributions, rate constants, and mechanisms of LiH+H reactions. Journal of Chemical Physics, 2005, 122, 214303.	3.0	33
27	Coriolis coupling effects on the initial-state-resolved dynamics of the N(D2)+H2â†'NH+H reaction. Journal of Chemical Physics, 2007, 127, 204311.	3.0	32
28	The protonation of organic molecules: electrostatic versus SCF CNDO calculations for three-membered ring molecules. Chemical Physics Letters, 1973, 20, 201-206.	2.6	31
29	Ab initio study of Î²-lactam antibiotics. I. Potential energy surface for the amidic CN bond breaking in the Î²-lactam + OHâ^' reaction. Chemical Physics, 1980, 45, 279-290.	1.9	31
30	Doubleâ€Î¶ LCAO SCF MO Calculations for NO2 and OF2. Journal of Chemical Physics, 1968, 48, 1497-1499.	3.0	30
31	Molecular orbital studies on the mechanism of drug-receptor interaction. 2. .beta.-Adrenergic drugs. An approach to explain the role of the aromatic moiety. Journal of Medicinal Chemistry, 1977, 20, 1645-1653.	6.4	30
32	Ab initiostudy of NO2. Molecular Physics, 1994, 82, 553-565.	1.7	30
33	Ab initioLCAO-MO-SCF calculation of the electrostatic molecular potential of chlorpromazine and promazine. International Journal of Quantum Chemistry, 1978, 13, 457-468.	2.0	29
34	Searching for resonances in the reaction Cl+CH4â†'HCl+CH3: Quantum versus quasiclassical dynamics and comparison with experiments. Journal of Chemical Physics, 2007, 127, 104302.	3.0	29
35	Molecular orbital studies on the mechanism of drug-receptor interaction. 1. Adrenergic drugs. Conformation and reactivity of isoproterenol and 1-(p-nitrophenyl)-2-isopropylaminoethanol. Journal of Medicinal Chemistry, 1974, 17, 501-507.	6.4	28
36	SCF wavefunction for the ground state of CNâ^' and the change of the correlation energy in some simple protonation processes. Chemical Physics Letters, 1969, 3, 473-475.	2.6	27

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37	Quantum dynamics of the N(4S)+O2 reaction on the Xâ€‰2Aâ€² and aâ€‰4Aâ€² surfaces: Reaction probabilities, cross sections, rate constants, and product distributions. Journal of Chemical Physics, 2002, 117, 3647-3655.	3.0	26
38	Bornâ€“Oppenheimer quantum dynamics of the C(D1)+H2 reaction on the CH2 alƒâ€‰A11 and blƒâ€‰B11 surfaces. Journal of Chemical Physics, 2009, 131, 114303.	3.0	25
39	DYNAMICS OF THE N(2D)+H2 REACTION ON THE $ilde{X}^2 A^{primeprime}$ SURFACE, PROPAGATING REAL WAVE PACKETS WITH AN ARCCOS MAPPING OF THE HAMILTONIAN. Journal of Theoretical and Computational Chemistry, 2003, 02, 547-551.	1.8	24
40	Quantum dynamics of the C(D1)+HD and C(D1)+nâ^'D2 reactions on the alƒâ€‰A1â€² and blƒâ€‰A1â€³ surfaces. Journal of Chemical Physics, 2010, 132, 104306.	3.0	24
41	MRD-CI quartet potential surfaces for the collinear reactions N(4Su)+N2(X1Î£g+, A3Î£u+, and B3Îg). Computational and Theoretical Chemistry, 1989, 202, 135-142.	1.5	23
42	Configuration-interaction calculations for the ground state of OF2, NO 2 ? , CN?: Canonical orbitals and exclusive orbitals. Theoretica Chimica Acta, 1969, 15, 332-343.	0.8	22
43	Potential surfaces and vibronic coupling for the conical intersection of the Ãƒ2A1 and BÌƒ2B2 states of NH2. Chemical Physics Letters, 1985, 115, 249-252.	2.6	22
44	Quantum mechanical and quasiclassical Bornâ€“Oppenheimer dynamics of the reaction N2 on the N2O and surfaces. Chemical Physics, 2012, 398, 81-89.	1.9	22
45	Quantum wave packet dynamics of the 1â€Š3Aâ€³â€‰N(4S)+NO(XÌƒâ€Š2Î)â†'N2(XÌƒâ€Š1Î£g+)+O(3P) reaction. Journal of Chemical Physics, 2003, 119, 7156-7162.	3.0	20
46	Ab initio Study of ?-lactam antibiotics. Theoretica Chimica Acta, 1979, 54, 239-243.	0.8	19
47	AB initio study of the internal rotation in 2-furancarboxaldehyde. Chemical Physics Letters, 1976, 42, 512-516.	2.6	18
48	Ab initio study of NO2. VII. Ãƒâ^2B2â†Ìƒâ^2A1 nonadiabatic Franckâ€“Condon absorption spectrum. Chemical Physics, 1997, 225, 55-62.	1.9	18
49	Wave packet dynamics of the N(4S)+O2(Xâ€Š3Î£gâ^')â†'NO(Xâ€Š2Î)+O(3P) reaction on the Xâ€Š2Aâ€² potential energy surface. Journal of Chemical Physics, 2001, 115, 3208-3214.	3.0	17
50	Electric and magnetic properties of LiH molecule according to Hartree-Fock perturbation theory. Theoretica Chimica Acta, 1970, 18, 341-353.	0.8	16
51	Basis set superposition effect on difference electrostatic molecular potential contour maps. International Journal of Quantum Chemistry, 1980, 18, 165-171.	2.0	16
52	Renner-Teller Quantum Dynamics of NH(a¹Î") + H Reactions on the NH₂ Ãƒ²A₁ and XÌƒ²B₁ Coupled Surfaces. Journal of Physical Chemistry A, 2010, 114, 9749-9754.	2.5	16
53	On the nature of the reaction path from the2B2stationary point to the [Xtilde]2A1minimum on the lowest2Aâ€² potential energy surface of NO2. Molecular Physics, 1992, 76, 1261-1263.	1.7	15
54	Time- and frequency-resolved spontaneous emission: Theory and application to the NO2 XÌƒâ€Š2Aâ€²/Ãƒâ€Š2Aâ€² conical intersection. Journal of Chemical Physics, 2000, 113, 4073-4082.	3.0	15

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55	Nonadiabatic dynamics of O(1D) + N2$({X{}^1Sigma _g^ + })ightarrow $(XÎ£g+1)â†'O(3<i>P</i>) + N2$ ({X{}^1Sigma _g^ + })$(XÎ£g+1) on three coupled potential surfaces: Symmetry, Coriolis, spin-orbit, and Renner-Teller effects. Journal of Chemical Physics, 2012, 136, 054308.	3.0	15
56	Bornâ€"Oppenheimer and Rennerâ€"Teller coupled-channel quantum reaction dynamics of O(³P) + H₂⁺(X²Î£_g⁺) collisions. Physical Chemistry Chemical Physics, 2015, 17, 23392-23402.	2.8	15
57	Electrostatic Molecular Potential Contour Maps from Ab-initio Calculations. 1. Biologically Significant Molecules. 2. Mechanism of Cationic Polymerization. , 1981, , 335-380.		15
58	Conformational studies of molecules partially oriented in nematic phase: nuclear magnetic resonance and theoretical investigation of 2,2â€²-bifuryl. Journal of the Chemical Society Perkin Transactions II, 1977, , 314-318.	0.9	14
59	Ab initio study of the internal rotation in peroxyformic acid. Chemical Physics, 1977, 26, 243-249.	1.9	14
60	Quantum dynamics of NH(aÎ")1)+H reactions on the NH2 AÌƒâ€‰A21 surface. Journal of Chemical Physics, 2008, 129, 174307.	3.0	14
61	Adiabatic Quantum Dynamics of CH(X²Î) + H(²S) Reactions on the CH₂(XÌƒ³Aâ€³) Surface and Role of the Excited Electronic States. Journal of Physical Chemistry A, 2012, 116, 8291-8296.	2.5	14
62	Molecular calculations with the nonempiricalab initioMODPOT,VRDDO, andMODPOT/VRDDO procedures. XI. Theoretical study of the [C6H5OH?OC6H5]? molecular complex:Ab initioMODPOT/VRDDO calculations and electrostatic molecular potential contour maps. International Journal of Quantum Chemistry, 1980, 18, 173-184.	2.0	13
63	MRD-CI Stationary Points, Dissociation Energies, and Conical-Intersection Potentials of the Four Lowest Doublet States of NH2. Journal of Physical Chemistry A, 1997, 101, 5696-5699.	2.5	11
64	Nonadiabatic radiative lifetimes and fluorescence spectra of NO2. Journal of Chemical Physics, 1999, 111, 9651-9657.	3.0	11
65	Quantum and semiclassical dynamics of the Franckâ€"Condon wave packet on the coupled potential surfaces of the conical intersection. Chemical Physics, 2000, 259, 193-200.	1.9	11
66	Quantum Dynamics of the Reaction H(²S) + HeH⁺(X¹Î£⁺) â†' H₂⁺(X²Î£_g⁺) + He(¹S) from Cold to Hyperthermal Energies: Time-Dependent Wavepacket Study and Comparison with Time-Independent Calculations. Journal of Physical Chemistry A, 2014, 118, 6451-6456.	2.5	11
67	Conical-intersection quantum dynamics of OH(A2Î£+) + H(2S) collisions. Journal of Chemical Physics, 2013, 139, 094303.	3.0	10
68	Nematic phase nuclear magnetic resonance, ultrasonic relaxation, and theoretical ab initio investigation of internal rotation in pyridine-2-carbaldehyde. Journal of the Chemical Society Perkin Transactions II, 1975, , 1673.	0.9	9
69	Ab initio study of the internal rotation and of the electrostatic molecular potential of a model compound of tazolol and comparison with similar compounds. The Journal of Physical Chemistry, 1980, 84, 105-109.	2.9	9
70	Quantum scattering study of collisional energy transfer in He+NO2: The importance of the vibronic mixing. Journal of Chemical Physics, 2000, 112, 5672-5678.	3.0	9
71	Bornâ€"Oppenheimer and Rennerâ€"Teller Quantum Dynamics of CH(X²Î) + D(²S) Reactions on Three CHD Potential Surfaces. Journal of Physical Chemistry A, 2015, 119, 11254-11264.	2.5	9
72	Relaxation of NH(a1Î", v = 1) in Collisions with H(2S): An Experimental and Theoretical Study. Journal of Physical Chemistry A, 2009, 113, 14458-14464.	2.5	8

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73	Quantum dynamics of Rennerâ€“Teller and isotopic effects in NH(a1Î”) + D(2S) reactions. Physical Chemistry Chemical Physics, 2011, 13, 8470.	2.8	8
74	AB-INITIO MODPOT/VRDDO/MERGE CALCULATIONS ON LARGE BIOMEDICAL MOLECULES AND ELECTROSTATIC MOLECULAR POTENTIAL CONTOUR MAPS. Annals of the New York Academy of Sciences, 1981, 367, 452-477.	3.8	7
75	On the energy dependence of the hyperfine interaction in excited states of NO2. Journal of Chemical Physics, 2001, 115, 8868-8875.	3.0	7
76	Non-adiabatic Quantum Dynamics of the Dissociative Charge Transfer He++H2 â†' He+H+H+. Frontiers in Chemistry, 2019, 7, 249.	3.6	7
77	Absorption cross sections and correlation functions of the NH2 AÌƒA12â^'XÌƒB12 Rennerâ€“Teller system. Journal of Chemical Physics, 2005, 122, 234315.	3.0	6
78	The use of the electrostatic molecular potential in quantum pharmacology. I. Ab initio results. International Journal of Quantum Chemistry, 1975, 9, 181-190.	2.0	5
79	Nonadiabatic Rennerâ€“Teller quantum dynamics of OH(X²Î) + H⁺ reactive collisions. Physical Chemistry Chemical Physics, 2017, 19, 4454-4461.	2.8	5
80	Lanczos calculation of the <mml:math altimg="si11.gif" overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" xmlns:sb="http://www.elsevier.com/xml/common/struct-bib/dtd" xmlns:ce="http://www.elsevier.com/x	0.8	4
81	Fluorescence spectra of NH2 XÌƒâ€Š2B1â†Ãƒâ€Š2A1 Î£ bands: Experiment and theory. Journal of Chemical Physics, 2003, 119, 2614-2617.	3.0	4
82	An iterative extended Hï¿½ckel calculation for some amino acids containing sulphur and selenium. Theoretica Chimica Acta, 1971, 20, 31-40.	0.8	3
83	Quantum calculations of nonadiabatic 2A1â€“2B2 conical-intersection effects in the reactions and N(4S)+O2(A3Î”u). Chemical Physics, 2010, 375, 46-51.	1.9	3
84	Non-adiabatic quantum dynamics of the electronic quenching OH(A²Î£⁺) + Kr. Physical Chemistry Chemical Physics, 2020, 22, 17091-17105.	2.8	3
85	Quantum Dynamics of Nonadiabatic Rennerâ€“Teller Effects in Atom + Diatom Collisions. Journal of Physical Chemistry A, 2021, 125, 6637-6652.	2.5	3
86	Configuration interaction study of the lowest Ï€ and Ïƒ states in the succinimidyl radical. Computational and Theoretical Chemistry, 1986, 138, 69-76.	1.5	2
87	Nonadiabatic theory of triatomics: Formalism for1?u/1?g interaction, for electronic spin, and for2? Renner-Teller effect. International Journal of Quantum Chemistry, 1992, 42, 907-916.	2.0	2
88	Recent Theoretical Developments in Conical-Intersection Effects in Triatomic Spectra. Advances in Quantum Chemistry, 1998, , 127-144.	0.8	0