Jack Simons

List of Publications by Year
in descending order

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190 papers	8,038 citations	47004 47 h-index	54911 84 g-index
191 all docs	191 docs citations	191 times ranked	3585 citing authors

#	Article	IF	Citations
1	Molecular Anions. Journal of Physical Chemistry A, 2008, 112, 6401-6511.	2.5	364
2	Ab initio electronic structure of anions. Chemical Reviews, 1987, 87, 535-555.	47.7	336
3	How Do Low-Energy (0.1â^'2 eV) Electrons Cause DNA-Strand Breaks?. Accounts of Chemical Research, 2006, 39, 772-779.	15.6	331
4	First experimental photoelectron spectra of superhalogens and their theoretical interpretations. Journal of Chemical Physics, 1999, 110, 4763-4771.	3.0	269
5	Theory of electron affinities of small molecules. Journal of Chemical Physics, 1973, 58, 4899-4907.	3.0	267
6	Mechanism for Damage to DNA by Low-Energy Electronsâ€. Journal of Physical Chemistry B, 2002, 106, 7991-7994.	2.6	262
7	The Only Stable State of O2-Is the X2ÎgGround State and It (Still!) Has an Adiabatic Electron Detachment Energy of 0.45 eV. Journal of Physical Chemistry A, 2003, 107, 8521-8529.	2.5	240
8	Small Multiply Charged Anions as Building Blocks in Chemistry. Accounts of Chemical Research, 1996, 29, 497-502.	15.6	170
9	Contribution of electron correlation to the stability of dipole-bound anionic states. Physical Review A, 1996, 54, 1906-1909.	2.5	167
10	The coupled-cluster method with a multiconfiguration reference state. International Journal of Quantum Chemistry, 1981, 19, 207-216.	2.0	163
11	Ab initio analytical molecular gradients and Hessians. Journal of Chemical Physics, 1983, 79, 334-357.	3.0	159
12	A unitary multiconfigurational coupledâ€cluster method: Theory and applications. Journal of Chemical Physics, 1988, 88, 993-1002.	3.0	156
13	Resonance state lifetimes from stabilization graphs. Journal of Chemical Physics, 1981, 75, 2465-2467.	3.0	152
14	Comparison of the convergence characteristics of some iterative wave function optimization methods. Journal of Chemical Physics, 1982, 76, 543-557.	3.0	152
15	Tetracoordinated Planar Carbon in Pentaatomic Molecules. Journal of the American Chemical Society, 1998, 120, 7967-7972.	13.7	150
16	How to choose a one-electron basis set to reliably describe a dipole-bound anion. International Journal of Quantum Chemistry, 2000, 80, 1024-1038.	2.0	141
17	Propensity rules for vibration-induced electron detachment of anions. Journal of the American Chemical Society, 1981, 103, 3971-3976.	13.7	135
18	Adiabatic electron affinities of small superhalogens: LiF2, LiCl2, NaF2, and NaCl2. Journal of Chemical Physics, 1997, 107, 3867-3875.	3.0	122

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19	Theoretical Study of Negative Molecular Ions. Annual Review of Physical Chemistry, 2011, 62, 107-128.	10.8	106
20	Applications of multiconfigurational coupledâ€cluster theory. Journal of Chemical Physics, 1982, 76, 4548-4559.	3.0	105
21	Walking on potential energy surfaces. Journal of Chemical Physics, 1990, 92, 340-346.	3.0	105
22	Model Calculations Relevant to Disulfide Bond Cleavage via Electron Capture Influenced by Positively Charged Groups. Journal of Physical Chemistry B, 2003, 107, 13505-13511.	2.6	104
23	Damage to Model DNA Fragments by 0.25â^1.0 eV Electrons Attached to a Thymine Ï€* Orbital. Journal of Physical Chemistry B, 2004, 108, 5800-5805.	2.6	101
24	Electron Attachment Step in Electron Capture Dissociation (ECD) and Electron Transfer Dissociation (ETD). Journal of Physical Chemistry A, 2005, 109, 5801-5813.	2.5	92
25	Theoretical Study of Damage to DNA by 0.2â^1.5 eV Electrons Attached to Cytosineâ€. Journal of Physical Chemistry A, 2004, 108, 2999-3005.	2.5	89
26	Energies of dipole-bound anionic states. International Journal of Quantum Chemistry, 1997, 64, 183-191.	2.0	86
27	Mechanisms for Sâ€“S and Nâ€“CÎ± bond cleavage in peptide ECD and ETD mass spectrometry. Chemical Physics Letters, 2010, 484, 81-95.	2.6	84
28	Direct Calculation of Firstâ€and Secondâ€Order Density Matrices. The Higher RPA Method. Journal of Chemical Physics, 1971, 55, 1218-1230.	3.0	78
29	A complete treatment of the electron propagator through third order. Journal of Chemical Physics, 1975, 63, 5302-5304.	3.0	76
30	Complex coordinate rotation of the electron propagator. Journal of Chemical Physics, 1980, 73, 2858-2866.	3.0	75
31	Doubleâ€Rydberg anions: Groundâ€state electronic and geometric stabilities. Journal of Chemical Physics, 1990, 93, 3874-3880.	3.0	74
32	Mo/llerâ€“Plesset perturbation theory for van der Waals complexes bound by electron correlation effects: Ground states of the Ar and Mg dimers. Journal of Chemical Physics, 1987, 87, 3569-3579.	3.0	70
33	Theoretical studies of molecular ions. Ionization potentials of CNâ^ and BOâ^. Journal of Chemical Physics, 1976, 64, 3610-3614.	3.0	66
34	Repulsive Coulomb Barriers in Compact Stable and Metastable Multiply Charged Anions. Journal of the American Chemical Society, 2000, 122, 11893-11899.	13.7	63
35	Effects of Base Ï€-Stacking on Damage to DNA by Low-Energy Electrons. Journal of Physical Chemistry A, 2004, 108, 11381-11387.	2.5	63
36	General-Order Many-Body Greenâ€™s Function Method. Journal of Chemical Theory and Computation, 2015, 11, 1595-1606.	5.3	61

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37	Vertical and adiabatical ionization potentials of MHâˆ’K+1 anions. Ab initio study of the structure and stability of hypervalent MHk+1 molecules. Journal of Chemical Physics, 1993, 99, 4628-4637.	3.0	60
38	Energyâ€Shift Theory of Lowâ€Lying Excited Electronic States of Molecules. Journal of Chemical Physics, 1972, 57, 3787-3792.	3.0	57
39	Electronic energies, geometries, and vibrational frequencies of the ground and lowâ€lying excited states of the boron trimer. Journal of Chemical Physics, 1991, 94, 2961-2967.	3.0	55
40	A direct ab initio dynamics study of the water-assisted tautomerization of formamide. International Journal of Quantum Chemistry, 1997, 63, 861-874.	2.0	54
41	Ab Initio Study of the Stabilization of Multiply Charged Anions in Water. Journal of Physical Chemistry B, 1998, 102, 4205-4208.	2.6	53
42	Stabilization calculation of the energy and lifetime of metastable SO42âˆ’. Journal of Chemical Physics, 2002, 116, 2848-2851.	3.0	51
43	Is TeF2âˆ’8the MX2âˆ’ndianion with the largest electron detachment energy (5 eV). Journal of Chemical Physics, 1992, 97, 2826-2827.	3.0	50
44	Theoretical search for large Rydberg molecules: NH3CH3, NH2(CH3)2, NH(CH3)3, and N(CH3)4. Journal of Chemical Physics, 1992, 97, 6621-6627.	3.0	50
45	Negative electron affinities from conventional electronic structure methods. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	50
46	Direct atomicâ€orbitalâ€based timeâ€dependent Hartreeâ€“Fock calculations of frequencyâ€dependent polarizabilities. Journal of Chemical Physics, 1992, 96, 2978-2987.	3.0	48
47	A combined experimental and theoretical study of the neutral, cationic, and anionic Si3N cluster molecule. Journal of Chemical Physics, 1994, 101, 2871-2879.	3.0	48
48	Temperature Dependence of the Biotinâˆ’Avidin Bond-Rupture Force Studied by Atomic Force Microscopy. Journal of Physical Chemistry B, 2002, 106, 9847-9852.	2.6	48
49	Theoretical studies of molecular ions. Vertical ionization potentials of hydrogen fluoride. Journal of Chemical Physics, 1974, 61, 2670-2674.	3.0	47
50	Application of cholesky-like matrix decomposition methods to the evaluation of atomic orbital integrals and integral derivatives. International Journal of Quantum Chemistry, 1989, 36, 673-688.	2.0	47
51	The electron propagator and superoperator resolvent. Journal of Chemical Physics, 1976, 64, 4541-4543.	3.0	46
52	Modified rotationally adiabatic model for rotational autoionization of dipoleâ€bound molecular anions. Journal of Chemical Physics, 1989, 91, 6858-6865.	3.0	42
53	Ab initio studies of the structures and energies of the Hâˆ’(H2O) and Hâˆ’(H2O)2 complexes. Journal of Chemical Physics, 1987, 87, 2965-2975.	3.0	41
54	Theoretical study of C2 and Câˆ’2 : Xâ€‰1Î£+g , aâ€‰3Îu , Xâ€‰2Î£+g , and Bâ€‰2Î£+u potentials. Journal of Chemical Physics, 1987, 86, 6972-6981.	3.0	41

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55	A calculation of the electron detachment energy of NO2â¯. Journal of Chemical Physics, 1977, 66, 2427-2430.	3.0	40
56	Theoretical study of the dipole-bound anion (HPPH3)â¯. Journal of Chemical Physics, 1999, 110, 274-280.	3.0	40
57	Resonance state energies and lifetimes via analytic continuation of stabilization graphs. Journal of Chemical Physics, 1986, 84, 4462-4469.	3.0	39
58	Excess electrons in condensed media: Theory of optical absorption spectrum in molecular solutions. Journal of Chemical Physics, 1978, 68, 415-432.	3.0	38
59	Potential energy curves of M(npâ€‰2P)â‹…RG(2Î) excited states and M+â‹…RG ground states (M=Li, Na; RG=He, Ne). Journal of Chemical Physics, 1994, 100, 8212-8218.	3.0	38
60	An experimental and theoretical determination of the electron affinity of the ethynyl radical, HC2â‹…. Journal of Chemical Physics, 1979, 71, 2057.	3.0	37
61	Strategies for walking on potential energy surfaces using local quadratic approximations. International Journal of Quantum Chemistry, 1990, 38, 263-276.	2.0	35
62	A calculation of the electron affinity of the lithium molecule. Journal of Chemical Physics, 1976, 64, 4548-4550.	3.0	33
63	Perturbative solution of equations of motion for excitation and ionization processes. Journal of Chemical Physics, 1976, 64, 1413-1418.	3.0	32
64	Complex coordinate rotation calculation of branching ratios. International Journal of Quantum Chemistry, 1982, 21, 727-739.	2.0	32
65	Ab initio electronic structure of HCNâ¯ and HNCâ¯ dipole-bound anions and a description of electron loss upon tautomerization. Journal of Chemical Physics, 2001, 114, 7443-7449.	3.0	32
66	Dipole-Bound Anion of the HNNH3Isomer of Hydrazine. An Ab Initio Study. Journal of Physical Chemistry A, 1999, 103, 625-631.	2.5	31
67	Theoretical studies of molecular ions: Beâ¯2. Journal of Chemical Physics, 1976, 65, 1601-1602.	3.0	30
68	A potentially sizeâ€consistent multiconfiguration based coupled electron pair approximation. Journal of Chemical Physics, 1989, 90, 3671-3679.	3.0	30
69	Ab initio study of the internal rotation barrier of formamide and the formamide-H2O complex. International Journal of Quantum Chemistry, 1993, 45, 123-132.	2.0	30
70	A dipole-bound dianion. Journal of Chemical Physics, 2000, 112, 6563-6570.	3.0	30
71	Analysis of the equation-of-motion theory of electron affinities and ionization potentials. Chemical Physics, 1976, 14, 145-158.	1.9	28
72	Comment on the electronic structure of small beryllium and magnesium clusters and their anions. Journal of Chemical Physics, 1980, 72, 2889-2890.	3.0	28

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73	Anionic states of LiFLi. Journal of Chemical Physics, 1994, 100, 1308-1311.	3.0	28
74	Why Are (MgO)nClusters and Crystalline MgO So Reactive?. The Journal of Physical Chemistry, 1996, 100, 8023-8030.	2.9	28
75	Low-energy (0.1 eV) electron attachment S?S bond cleavage assisted by Coulomb stabilization. International Journal of Quantum Chemistry, 2005, 102, 838-846.	2.0	28
76	Monte Carlo simulation of small hydrate clusters of NOâ^'2. Journal of Chemical Physics, 1980, 73, 1814-1826.	3.0	27
77	Geometrical derivatives of dipole moments and polarizabilities. International Journal of Quantum Chemistry, 1984, 25, 1135-1150.	2.0	27
78	Dissociative Recombination of H3O+. Journal of Physical Chemistry A, 1999, 103, 6552-6563.	2.5	27
79	Analytical Model for Rates of Electron Attachment and Intramolecular Electron Transfer in Electron Transfer Dissociation Mass Spectrometry. Journal of the American Chemical Society, 2010, 132, 7074-7085.	13.7	27
80	An excess electron bound to urea. I. Canonical and zwitterionic tautomers. Journal of Chemical Physics, 2001, 115, 8373-8380.	3.0	26
81	Peculiar Structures of Small Magnesium Carbide Clusters:Â MgC2, (MgC2)2, and (MgC2)4. Journal of Physical Chemistry A, 1997, 101, 2215-2217.	2.5	25
82	Rydberg bonding in ammonium dimer ((NH4)2). The Journal of Physical Chemistry, 1992, 96, 8840-8843.	2.9	23
83	Ab initio study of geometrically metastable multiprotonated species: MHk+n. Journal of Chemical Physics, 1992, 97, 4272-4281.	3.0	23
84	Two-photon ionization spectroscopy and all-electron ab initio study of LiCa. Journal of Chemical Physics, 1998, 109, 6655-6665.	3.0	23
85	Analysis of the â€™â€™charge resonanceâ€™â€™ transition in anthracene dimer anion. Journal of Chemical Physics, 1980, 72, 425-428.	3.0	22
86	Calculation of hyperfine coupling constants of the CN and CP ground state radicals. Journal of Chemical Physics, 1993, 98, 7012-7019.	3.0	22
87	Theoretical study of electron capture dissociation of [Mg(H2O)n]2+ clusters. International Journal of Mass Spectrometry, 2008, 277, 166-174.	1.5	22
88	Refinements to the Utahâ€“Washington Mechanism of Electron Capture Dissociation. Journal of Physical Chemistry B, 2014, 118, 7892-7901.	2.6	22
89	Excess electrons in condensed media. A model for migration in dilute molecular solutions. Journal of Chemical Physics, 1977, 67, 389-398.	3.0	20
90	Electronic structure of small metal clusters. II. Anions of Li2, LiNa, and Na2. Journal of Chemical Physics, 1978, 69, 1788-1789.	3.0	20

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91	Resolvent operator approach to manyâ€body perturbation theory. II. Open shells. Journal of Chemical Physics, 1982, 76, 1979-1994.	3.0	20
92	An excess electron bound to urea. III. The urea dimer as an electron trap. Journal of Chemical Physics, 2002, 116, 6118-6125.	3.0	20
93	Translational and rotational symmetries in integral derivatives. Journal of Chemical Physics, 1985, 82, 4566-4576.	3.0	19
94	Propensity rules for vibration-rotation-induced electron detachment of diatomic anions: application to amidogen(1-) ion .fwdarw. imidogen + electron. The Journal of Physical Chemistry, 1988, 92, 3086-3091.	2.9	19
95	Polarization Green's function with multiconfiguration self-consistent-field reference states. International Journal of Quantum Chemistry, 1979, 16, 1209-1237.	2.0	18
96	Ab initio potentialâ€energy surfaces for Cd(1P)+H2=CdH(Xâ€‰2Î£+)+H, HCdH(Xâ€‰1Î£+g), Cd(3P)+H2, and Cd(1S)+H+H. Journal of Chemical Physics, 1992, 96, 6555-6564.	3.0	18
97	Is 9-acridinamine anion a dispersion-bound anion?. Journal of Chemical Physics, 2001, 115, 11193-11199.	3.0	18
98	A calculation of the photodetachment energy of NH2â¯. Journal of Chemical Physics, 1976, 65, 5393-5397.	3.0	17
99	Calculation of hyperfine coupling constants of the ground state Xâ€‰3Î£â¯ of NH and B2. Journal of Chemical Physics, 1993, 99, 5995-6003.	3.0	17
100	Line shapes of chargeâ€transfer spectra. Journal of Chemical Physics, 1979, 70, 4974-4981.	3.0	16
101	Associative electron detachment: Oâ¯+Hâ†'OH+eâ¯. Journal of Chemical Physics, 1985, 83, 3888-3893.	3.0	16
102	Mixed valence/dipole-bound dianions. Journal of Chemical Physics, 1999, 111, 9469-9474.	3.0	16
103	On the Possibility of Mixed Rydberg-Valence Bonds. Journal of Physical Chemistry A, 1999, 103, 3575-3580.	2.5	16
104	On the lowest sigma and pi anion states of Be2 and Be3. Journal of Chemical Physics, 1982, 77, 5250-5252.	3.0	15
105	A multiconfiguration selfâ€consistentâ€field group function method for problems with repeating potentials. Journal of Chemical Physics, 1983, 79, 6104-6111.	3.0	15
106	Roles Played by Metastable States in Chemistry. ACS Symposium Series, 1984, , 3-16.	0.5	15
107	On the possibility of binding of two electrons to dipole potentials. International Journal of Quantum Chemistry, 2000, 76, 197-204.	2.0	15
108	First-Order geometrical response equations for state-averaged multiconfigurational self-consistent field (SA-MCSCF) wave functions. International Journal of Quantum Chemistry, 1991, 40, 361-378.	2.0	14

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109	Singletâ€toâ€triplet energy transfer via 1Î1/3Î£+1 curve crossings in group 2 and 12 metalâ€“atom/rareâ€gas systems. Journal of Chemical Physics, 1993, 99, 3815-3822.	3.0	14
110	Interaction of an aluminum atom with an alkaline earth atom: Spectroscopic and ab initio investigations of AlCa. Journal of Chemical Physics, 1994, 101, 5441-5453.	3.0	14
111	Inversion in the relative stabilities of HBO and BOH upon ionization. Journal of Chemical Physics, 1999, 110, 3765-3768.	3.0	14
112	Ejecting Electrons from Molecular Anions via Shine, Shake/Rattle, and Roll. Journal of Physical Chemistry A, 2020, 124, 8778-8797.	2.5	14
113	Fate of Dipole-Bound Anion States when Hydrated. Journal of Physical Chemistry A, 2020, 124, 2064-2076.	2.5	14
114	An analysis of the natural orbital theory of ionization potentials. Journal of Chemical Physics, 1977, 66, 1067-1069.	3.0	13
115	New anionic states of the lithium trimer. Journal of Chemical Physics, 1994, 101, 4867-4877.	3.0	13
116	Laser Photolysis of Matrix-Isolated Methyl Nitrate:â€‰ Experimental and Theoretical Characterization of the Infrared Spectrum of Imine Peroxide (HNOO). Journal of the American Chemical Society, 1998, 120, 12327-12333.	13.7	13
117	Direct analytical calculation of firstâ€order density matrix elements through third order. Journal of Chemical Physics, 1973, 59, 2436-2440.	3.0	12
118	Spectroscopy of binary solutions. The benzeneâ€“iodine chargeâ€transfer spectrum. Journal of Chemical Physics, 1978, 69, 1406-1417.	3.0	12
119	Dissociation of vibronic states ofCâ€“1Aâ€² DCN: Quantum treatment. Journal of Chemical Physics, 1984, 80, 176-185.	3.0	12
120	Dipole-bound anions supported by charge-transfer interaction: Anionic states of HnF3?nN ? BH3 and H3N ? BHnF3?n (n = 0, 1, 2, 3). International Journal of Quantum Chemistry, 2003, 92, 367-375.	2.0	12
121	Equations of motion methods for computing electron affinities and ionization potentials. , 2005, , 443-464.		12
122	Dynamics of molecules in contact with an external medium at equilibrium. International Journal of Quantum Chemistry, 1978, 13, 553-562.	2.0	11
123	Coordinate rotation studies of H?, He?, Be?, Mg? resonances: Basis set and configuration list dependence. International Journal of Quantum Chemistry, 1983, 23, 1723-1738.	2.0	11
124	Translationâ€rotation invariance for Nâ€particle systems: Internal coordinates and search for stationary points in reduced spaces. Journal of Chemical Physics, 1985, 83, 3500-3506.	3.0	11
125	Interactions of the B3 cluster with H atoms and H2 molecules. Journal of Chemical Physics, 1992, 96, 8251-8257.	3.0	11
126	Collisional energy transfer in bimolecular ionâ€“molecule dynamics M++(H2; D2; or HD)â†'(MH++H;) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	3.0	11

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127	Potential energy surfaces and reactive dynamics of Zn(3P) with H2. Journal of Chemical Physics, 1996, 105, 10919-10924.	3.0	11
128	Time-Domain and Tunneling Pictures of Nonadiabatic Induced Electron Ejection in Molecular Anions. Journal of Physical Chemistry A, 1999, 103, 9408-9416.	2.5	11
129	Firstâ€•and Secondâ€Order Density Matrices of Symmetryâ€Projected Singleâ€Determinant Wavefunctions. Journal of Chemical Physics, 1969, 51, 296-301.	3.0	10
130	Graphical description of the symmetries of potential energy surfaces. Journal of Chemical Physics, 1993, 98, 8801-8809.	3.0	10
131	Interpretation of the hyperfine coupling constants of the boron trimer in rareâ€gas matrices. Journal of Chemical Physics, 1993, 98, 3060-3065.	3.0	10
132	Semiquantum Expressions for Electronically Nonadiabatic Electron Ejection Rates. Journal of Physical Chemistry A, 1998, 102, 6035-6042.	2.5	10
133	Characterization of the Rydberg Bonding in (NH4)2-. Journal of Physical Chemistry A, 2000, 104, 10855-10858.	2.5	10
134	A Note on Differences Between Operator-Level and Function-Level Equations of Motion. International Journal of Quantum Chemistry, 1977, 12, 227-229.	2.0	9
135	Lifetimes of electronically metastable doubleâ€Rydberg anions: FHâ^'2. Journal of Chemical Physics, 1990, 93, 2546-2553.	3.0	9
136	Polyhedral Ionic Molecules. Journal of the American Chemical Society, 1997, 119, 4618-4621.	13.7	9
137	Analysis of Stabilization and Extrapolation Methods for Determining Energies and Lifetimes of Metastable Electronic States. Journal of Physical Chemistry A, 2021, 125, 7735-7749.	2.5	9
138	Resolvent operator approach to manyâ€body perturbation theory. I. Closed shells. Journal of Chemical Physics, 1982, 76, 1972-1978.	3.0	8
139	Resolvent operator approach to manyâ€body perturbation theory. III. Applications. Journal of Chemical Physics, 1982, 76, 1995-2002.	3.0	8
140	Reactive dynamics for Zn(3P)+H2/D2/HDâ†'ZnH/ZnD+H/D: Rotational populations in ZnH/ZnD products. Journal of Chemical Physics, 1999, 110, 229-240.	3.0	8
141	Are HBOâ^'and BOHâ^'electronically stable?. Molecular Physics, 2003, 101, 1259-1265.	1.7	8
142	Electron detachment energies in high-symmetry alkali halide solvated-electron anions. Journal of Chemical Physics, 2003, 119, 902-908.	3.0	8
143	One-Electron Electronâ^'Molecule Potentials Consistent with ab Initio MÃ¸llerâ^'Plesset Theory^{â€}. Journal of Physical Chemistry A, 2010, 114, 8631-8643.	2.5	8
144	Semiclassical vibrational wave functions for electronically excited DCN: A highly quantum mechanical system. Journal of Chemical Physics, 1985, 82, 4199-4220.	3.0	7

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145	Finding transition states when second-order Jahn-Teller instability occurs. International Journal of Quantum Chemistry, 1993, 48, 211-218.	2.0	7
146	Al3H stable and transition state structures. Journal of Chemical Physics, 1994, 101, 10746-10752.	3.0	7
147	Ab Initio Study of the Mechanism of Photolytic Deazatization of 2,3-Diazabicyclo[2.2.2]oct-2-ene and 2,3-Diazabicyclo[2.2.1]hept-2-ene. Journal of Physical Chemistry A, 1997, 101, 2379-2383.	2.5	7
148	Sponge Model for the Kinetics of Surface Thermal Decomposition of Microcrystalline Solids:â€‰ Application to HMX. Journal of Physical Chemistry B, 1999, 103, 8650-8656.	2.6	7
149	An excess electron bound to urea oligomers. II. Chains and ribbons. Journal of Chemical Physics, 2001, 115, 10731-10737.	3.0	7
150	One-particle green's function with multiconfiguration reference states. International Journal of Quantum Chemistry, 1978, 14, 389-404.	2.0	7
151	Nature of the autodetaching sub2PÂ½threshold states of the alkali anions. International Journal of Quantum Chemistry, 1978, 14, 333-336.	2.0	6
152	Electronic spectrocopy in condensed media: Spectra of styrene and cycloâ€octatetraene anions. Journal of Chemical Physics, 1978, 69, 5538-5544.	3.0	6
153	Electronic spectroscopy in condensed media: The lowestnâ€Ï€* transition of the solvated nitrite anion. Journal of Chemical Physics, 1979, 71, 60-67.	3.0	6
154	Application of spectral quantization to metastable states of Câ€‰1Aâ€™DCN. Journal of Chemical Physics, 1986, 85, 5826-5837.	3.0	6
155	Ab Initio Predictions of New Carbon Hypermagnesium Species:â€‰ Mg2C and Mg3C. Journal of Physical Chemistry A, 1997, 101, 902-906.	2.5	6
156	An Unstable Anion Stabilized in a Molecular Trap. Journal of Physical Chemistry A, 2000, 104, 712-717.	2.5	6
157	An analytical model for vibrational non-Bornâ€“Oppenheimer induced electron ejection in molecular anions. Journal of Chemical Physics, 2002, 117, 9124-9132.	3.0	6
158	Multiconfigurational wavefunction optimization using the unitary group method. International Journal of Quantum Chemistry, 1980, 18, 211-228.	2.0	6
159	Do not forget the Rydberg orbitals. Journal of Chemical Physics, 2022, 156, 100901.	3.0	6
160	The Siegert methods in resonance scattering: Relation toL2 methods. International Journal of Quantum Chemistry, 1981, 20, 779-780.	2.0	5
161	The B3Li moleculeâ€™s electronic and geometrical structure. Journal of Chemical Physics, 1992, 97, 8357-8360.	3.0	5
162	Valenceâ€’Rydberg Bonding in Bimolecular Râ€’Ca+â€¢NH2â€’Râ€˜ Complexes. Journal of the American Chemical Society, 2000, 122, 369-377.	13.7	5

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163	A survey of some theoretical studies of negative ions. International Journal of Quantum Chemistry, 1977, 11, 971-978.	2.0	4
164	Should one use complex basis functions in coordinate rotation calculations on molecules?. Journal of Chemical Physics, 1980, 73, 992-993.	3.0	4
165	Coordinate rotatedTDHF excitation energies Li? 1S ?1P. International Journal of Quantum Chemistry, 1982, 22, 275-288.	2.0	4
166	Reply to â€˜â€˜Comment on: â€˜Translationâ€“rotation invariance for Nâ€particle systems: Internal coordinates and search for stationary points in reduced spacesâ€™â€‰â€™. Journal of Chemical Physics, 1986, 84, 3581-3581.	3.0	4
167	A two-dimensional model for collisional energy transfer in bimolecular ion-molecule dynamics: M++(H2; D2; or HD)?(MH++H; MD++D; MH++D; or MD++H). Theoretica Chimica Acta, 1995, 90, 357-381.	0.8	4
168	13C carbonyl chemical shielding tensors: Comparing SCF, MBPT (2), and DFT predictions to experiment. International Journal of Quantum Chemistry, 1997, 63, 875-894.	2.0	4
169	The complex coordinate rotation method and exterior scaling: A simple example. International Journal of Quantum Chemistry, 1980, 18, 113-121.	2.0	4
170	Selected boron, aluminum, and gallium trihalide and trihydride anions. Chemical Physics, 2017, 482, 387-392.	1.9	4
171	Unusual and Conventional Dative Bond Formation by s² Lone Pair Donation from Alkaline Earth Metal Atoms to BH₃, AlH₃, and GaH₃. Journal of Physical Chemistry A, 2020, 124, 5369-5377.	2.5	4
172	How to choose a oneâ€electron basis set to reliably describe a dipoleâ€bound anion. International Journal of Quantum Chemistry, 2000, 80, 1024-1038.	2.0	4
173	Diffusion of excess electrons in oneâ€and twoâ€component molecular solutions. A theoretical model. Journal of Chemical Physics, 1978, 68, 1695-1700.	3.0	3
174	Self-Consistent-Field potential-energy surfaces for hydrogen atom pairs within small palladium clusters. International Journal of Quantum Chemistry, 1992, 41, 793-810.	2.0	3
175	Second-order Jahn-Teller instability and the activation energy for Al+(1S) + H2 ? AlH+(2?+) + H. International Journal of Quantum Chemistry, 1993, 48, 309-317.	2.0	3
176	Role of angular electron pair correlation in stabilizing C2â^'60. International Journal of Quantum Chemistry, 2006, 106, 507-513.	2.0	3
177	F + H2 â†' FH + H potential energy surface: Construction of the reference configuration state function space and MR-ACPF-2 results. International Journal of Quantum Chemistry, 2006, 106, 1516-1527.	2.0	3
178	Finding Valence Antibonding Levels while Avoiding Rydberg, Pseudo-continuum, and Dipole-Bound Orbitals. Journal of the American Chemical Society, 0, , .	13.7	3
179	Combining doubly charged cations and anions to form new species. Journal of Chemical Physics, 1994, 100, 5778-5784.	3.0	2
180	Effects of local Coulomb potentials on acid and base protonation-deprotonation rates and equilibria. International Journal of Quantum Chemistry, 2009, 109, 3120-3130.	2.0	2

#	Article	IF	Citations
181	Direct calculation of density matrices: Natural orbitals and occupation numbers of model conjugated molecules. International Journal of Quantum Chemistry, 2009, 8, 323-333.	2.0	2
182	Caralumane Superacids of Lewis and BrÃ¸nsted Character. Journal of Physical Chemistry A, 2021, 125, 999-1011.	2.5	2
183	A rigorous upper bound energy for the unitary coupled electron pair approximation method. Journal of Chemical Physics, 1991, 94, 5252-5252.	3.0	1
184	Application of the coordinate rotation method to metastable atom-diatom scattering resonances. International Journal of Quantum Chemistry, 2009, 18, 467-475.	2.0	1
185	Electron propagator studies of molecular anions. International Journal of Quantum Chemistry, 2009, 22, 575-581.	2.0	1
186	Thymine dimer repair by electron transfer from photo-excited 2â€²,3â€²,5â€²-tri-O-acetyl-8-oxo-7,8-dihydroguanosine or 2â€²,3â€²,5â€²-tri-O-acetyl-ribosyluric acid â€“ a theoretical study. Molecular Physics, 2013, 111, 1580-1588.	1.7	1
187	How Do Low-energy (0.1â€“2 eV) Electrons Cause DNA Strand Breaks?. AIP Conference Proceedings, 2007, , .	0.4	0
188	The electronic structure of singlet cyclopentadienylidene. International Journal of Quantum Chemistry, 1980, 18, 349-353.	2.0	0
189	Concluding remarks for advances in ion spectroscopy Faraday Discussion. Faraday Discussions, 2019, 217, 623-643.	3.2	0
190	Tribute to Alexander I. Boldyrev. Journal of Physical Chemistry A, 2021, 125, 9261-9263.	2.5	0