Jack Simons

List of Publications by Year in Descending Order

188 papers	7,225 citations	45 h-index	79 g-index
191 ext. papers	7,626 ext. citations	4.4 avg, IF	6.04 L-index

#	Paper	IF	Citations
188	Do not forget the Rydberg orbitals.. *Journal of Chemical Physics*, **2022**, 156, 100901	3.9	2
187	Tribute to Alexander I. Boldyrev. *Journal of Physical Chemistry A*, **2021**, 125, 9261-9263	2.8	
186	Analysis of Stabilization and Extrapolation Methods for Determining Energies and Lifetimes of Metastable Electronic States. *Journal of Physical Chemistry A*, **2021**, 125, 7735-7749	2.8	0
185	Caralumane Superacids of Lewis and Brønsted Character. *Journal of Physical Chemistry A*, **2021**, 125, 999-1011	2.8	1
184	Unusual and Conventional Dative Bond Formation by s Lone Pair Donation from Alkaline Earth Metal Atoms to BH, AlH, and GaH. *Journal of Physical Chemistry A*, **2020**, 124, 5369-5377	2.8	3
183	Fate of Dipole-Bound Anion States when Hydrated. *Journal of Physical Chemistry A*, **2020**, 124, 2064-2076	2.8	8
182	Ejecting Electrons from Molecular Anions via Shine, Shake/Rattle, and Roll. *Journal of Physical Chemistry A*, **2020**, 124, 8778-8797	2.8	9
181	Concluding remarks for advances in ion spectroscopy Faraday Discussion. *Faraday Discussions*, **2019**, 217, 623-643	3.6	
180	Selected boron, aluminum, and gallium trihalide and trihydride anions. *Chemical Physics*, **2017**, 482, 387-392	2.3	4
179	General-Order Many-Body Green's Function Method. *Journal of Chemical Theory and Computation*, **2015**, 11, 1595-606	6.4	43
178	Negative electron affinities from conventional electronic structure methods. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	46
177	Refinements to the Utah-Washington mechanism of electron capture dissociation. *Journal of Physical Chemistry B*, **2014**, 118, 7892-901	3.4	16
176	Thymine dimer repair by electron transfer from photo-excited 2?,3?,5?-tri-O-acetyl-8-oxo-7,8-dihydroguanosine or 2?,3?,5?-tri-O-acetyl-ribosyluric acid – a theoretical study. *Molecular Physics*, **2013**, 111, 1580-1588	1.7	1
175	Theoretical study of negative molecular ions. *Annual Review of Physical Chemistry*, **2011**, 62, 107-28	15.7	93
174	One-electron electron-molecule potentials consistent with ab initio Møller-Plesset theory. *Journal of Physical Chemistry A*, **2010**, 114, 8631-43	2.8	7
173	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, 7074-85	16.4	25
172	Mechanisms for S–S and N–C$_\alpha$ bond cleavage in peptide ECD and ETD mass spectrometry. *Chemical Physics Letters*, **2010**, 484, 81-95	2.5	79

171	One-particle green's function with multiconfiguration reference states. *International Journal of Quantum Chemistry*, **2009**, 14, 389-404	2.1	4
170	The complex coordinate rotation method and exterior scaling: A simple example. *International Journal of Quantum Chemistry*, **2009**, 18, 113-121	2.1	3
169	Multiconfigurational wavefunction optimization using the unitary group method. *International Journal of Quantum Chemistry*, **2009**, 18, 211-228	2.1	6
168	The electronic structure of singlet cyclopentadienylidene. *International Journal of Quantum Chemistry*, **2009**, 18, 349-353	2.1	
167	Application of the coordinate rotation method to metastable atom-diatom scattering resonances. *International Journal of Quantum Chemistry*, **2009**, 18, 467-475	2.1	
166	Electron propagator studies of molecular anions. *International Journal of Quantum Chemistry*, **2009**, 22, 575-581	2.1	1
165	Effects of local Coulomb potentials on acid and base protonation□deprotonation rates and equilibria. *International Journal of Quantum Chemistry*, **2009**, 109, 3120-3130	2.1	2
164	Direct calculation of density matrices: Natural orbitals and occupation numbers of model conjugated molecules. *International Journal of Quantum Chemistry*, **2009**, 8, 323-333	2.1	2
163	Molecular anions. *Journal of Physical Chemistry A*, **2008**, 112, 6401-511	2.8	315
162	Theoretical study of electron capture dissociation of [Mg(H2O)n]2+ clusters. *International Journal of Mass Spectrometry*, **2008**, 277, 166-174	1.9	20
161	How do low-energy (0.1-2 eV) electrons cause DNA-strand breaks?. *Accounts of Chemical Research*, **2006**, 39, 772-9	24.3	303
160	Role of angular electron pair correlation in stabilizing C. *International Journal of Quantum Chemistry* , **2006**, 106, 507-513	2.1	3
159	F + H2 -jFH + 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	2.1	3
158	Electron attachment step in electron capture dissociation (ECD) and electron transfer dissociation (ETD). *Journal of Physical Chemistry A*, **2005**, 109, 5801-13	2.8	90
157	Low-energy (0.1 eV) electron attachment S?S bond cleavage assisted by Coulomb stabilization. *International Journal of Quantum Chemistry*, **2005**, 102, 838-846	2.1	27
156	Equations of motion methods for computing electron affinities and ionization potentials **2005**, 443-464		12
155	Effects of Base □Stacking on Damage to DNA by Low-Energy Electrons. *Journal of Physical Chemistry A*, **2004**, 108, 11381-11387	2.8	60
154	Damage to Model DNA Fragments by 0.25□1.0 eV Electrons Attached to a Thymine □ Orbital. *Journal of Physical Chemistry B*, **2004**, 108, 5800-5805	3.4	96

153	Theoretical Study of Damage to DNA by 0.2–1.5 eV Electrons Attached to Cytosine. *Journal of Physical Chemistry A*, **2004**, 108, 2999-3005	2.8	87
152	Dipole-bound anions supported by charge-transfer interaction: Anionic states of HnF3-nN -jBH3 and H3N -jBHnF3-n (n = 0, 1, 2, 3). *International Journal of Quantum Chemistry*, **2003**, 92, 367-375	2.1	10
151	The Only Stable State of O2- Is the X 2Πg Ground State and It (Still!) Has an Adiabatic Electron Detachment Energy of 0.45 eV. *Journal of Physical Chemistry A*, **2003**, 107, 8521-8529	2.8	216
150	Model Calculations Relevant to Disulfide Bond Cleavage via Electron Capture Influenced by Positively Charged Groups. *Journal of Physical Chemistry B*, **2003**, 107, 13505-13511	3.4	95
149	Are HBO2 and BOH2 electronically stable?. *Molecular Physics*, **2003**, 101, 1259-1265	1.7	7
148	Electron detachment energies in high-symmetry alkali halide solvated-electron anions. *Journal of Chemical Physics*, **2003**, 119, 902-908	3.9	7
147	An excess electron bound to urea. III. The urea dimer as an electron trap. *Journal of Chemical Physics*, **2002**, 116, 6118-6125	3.9	18
146	An analytical model for vibrational non-Born–Oppenheimer induced electron ejection in molecular anions. *Journal of Chemical Physics*, **2002**, 117, 9124-9132	3.9	4
145	Stabilization calculation of the energy and lifetime of metastable SO42. *Journal of Chemical Physics*, **2002**, 116, 2848-2851	3.9	46
144	Mechanism for Damage to DNA by Low-Energy Electrons. *Journal of Physical Chemistry B*, **2002**, 106, 7991-7994	3.4	247
143	Temperature Dependence of the Biotin–Avidin Bond-Rupture Force Studied by Atomic Force Microscopy. *Journal of Physical Chemistry B*, **2002**, 106, 9847-9852	3.4	45
142	Ab initio electronic structure of HCN2 and HNC2 dipole-bound anions and a description of electron loss upon tautomerization. *Journal of Chemical Physics*, **2001**, 114, 7443-7449	3.9	30
141	Is 9-acridinamine anion a dispersion-bound anion?. *Journal of Chemical Physics*, **2001**, 115, 11193-11199	3.9	16
140	An excess electron bound to urea oligomers. II. Chains and ribbons. *Journal of Chemical Physics*, **2001**, 115, 10731-10737	3.9	5
139	An excess electron bound to urea. I. Canonical and zwitterionic tautomers. *Journal of Chemical Physics*, **2001**, 115, 8373-8380	3.9	24
138	On the possibility of binding of two electrons to dipole potentials. *International Journal of Quantum Chemistry*, **2000**, 76, 197-204	2.1	13
137	How to choose a one-electron basis set to reliably describe a dipole-bound anion. *International Journal of Quantum Chemistry*, **2000**, 80, 1024-1038	2.1	127
136	A dipole-bound dianion. *Journal of Chemical Physics*, **2000**, 112, 6563-6570	3.9	28

135	Characterization of the Rydberg Bonding in (NH4)2-. *Journal of Physical Chemistry A*, **2000**, 104, 10855-10858	2.8	7
134	An Unstable Anion Stabilized in a Molecular Trap. *Journal of Physical Chemistry A*, **2000**, 104, 712-717	2.8	5
133	Repulsive Coulomb Barriers in Compact Stable and Metastable Multiply Charged Anions. *Journal of the American Chemical Society*, **2000**, 122, 11893-11899	16.4	59
132	Valence−Rydberg Bonding in Bimolecular RCa+−NH2R′ Complexes. *Journal of the American Chemical Society*, **2000**, 122, 369-377	16.4	3
131	How to choose a one-electron basis set to reliably describe a dipole-bound anion **2000**, 80, 1024		4
130	Reactive dynamics for Zn(3P)+H2/D2/HD→ZnH/ZnD+H/D: Rotational populations in ZnH/ZnD products. *Journal of Chemical Physics*, **1999**, 110, 229-240	3.9	7
129	First experimental photoelectron spectra of superhalogens and their theoretical interpretations. *Journal of Chemical Physics*, **1999**, 110, 4763-4771	3.9	243
128	Mixed valence/dipole-bound dianions. *Journal of Chemical Physics*, **1999**, 111, 9469-9474	3.9	14
127	Theoretical study of the dipole-bound anion (HPPH3)−. *Journal of Chemical Physics*, **1999**, 110, 274-280	3.9	38
126	Inversion in the relative stabilities of HBO and BOH upon ionization. *Journal of Chemical Physics*, **1999**, 110, 3765-3768	3.9	10
125	On the Possibility of Mixed Rydberg-Valence Bonds. *Journal of Physical Chemistry A*, **1999**, 103, 3575-3580	2.8	14
124	Time-Domain and Tunneling Pictures of Nonadiabatic Induced Electron Ejection in Molecular Anions. *Journal of Physical Chemistry A*, **1999**, 103, 9408-9416	2.8	8
123	Dipole-Bound Anion of the HNNH3 Isomer of Hydrazine. An Ab Initio Study. *Journal of Physical Chemistry A*, **1999**, 103, 625-631	2.8	29
122	Sponge Model for the Kinetics of Surface Thermal Decomposition of Microcrystalline Solids: Application to HMX. *Journal of Physical Chemistry B*, **1999**, 103, 8650-8656	3.4	6
121	Dissociative Recombination of H3O+. *Journal of Physical Chemistry A*, **1999**, 103, 6552-6563	2.8	24
120	Tetracoordinated Planar Carbon in Pentaatomic Molecules. *Journal of the American Chemical Society*, **1998**, 120, 7967-7972	16.4	134
119	Laser Photolysis of Matrix-Isolated Methyl Nitrate: Experimental and Theoretical Characterization of the Infrared Spectrum of Imine Peroxide (HNOO). *Journal of the American Chemical Society*, **1998**, 120, 12327-12333	16.4	11
118	Ab Initio Study of the Stabilization of Multiply Charged Anions in Water. *Journal of Physical Chemistry B*, **1998**, 102, 4205-4208	3.4	48

117	Semiquantum Expressions for Electronically Nonadiabatic Electron Ejection Rates. *Journal of Physical Chemistry A*, **1998**, 102, 6035-6042	2.8	9
116	Two-photon ionization spectroscopy and all-electron ab initio study of LiCa. *Journal of Chemical Physics*, **1998**, 109, 6655-6665	3.9	20
115	Adiabatic electron affinities of small superhalogens: LiF2, LiCl2, NaF2, and NaCl2. *Journal of Chemical Physics*, **1997**, 107, 3867-3875	3.9	112
114	Polyhedral Ionic Molecules. *Journal of the American Chemical Society*, **1997**, 119, 4618-4621	16.4	6
113	Ab Initio Predictions of New Carbon Hypermagnesium Species: Mg2C and Mg3C. *Journal of Physical Chemistry A*, **1997**, 101, 902-906	2.8	6
112	Peculiar Structures of Small Magnesium Carbide Clusters: MgC2, (MgC2)2, and (MgC2)4. *Journal of Physical Chemistry A*, **1997**, 101, 2215-2217	2.8	22
111	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	2.8	6
110	A direct ab initio dynamics study of the water-assisted tautomerization of formamide. *International Journal of Quantum Chemistry*, **1997**, 63, 861-874	2.1	47
109	13C carbonyl chemical shielding tensors: Comparing SCF, MBPT (2), and DFT predictions to experiment. *International Journal of Quantum Chemistry*, **1997**, 63, 875-894	2.1	3
108	Energies of dipole-bound anionic states. *International Journal of Quantum Chemistry*, **1997**, 64, 183-191	2.1	82
107	Small Multiply Charged Anions as Building Blocks in Chemistry. *Accounts of Chemical Research*, **1996** , 29, 497-502	24.3	156
106	Why Are (MgO)n Clusters and Crystalline MgO So Reactive?. *The Journal of Physical Chemistry*, **1996**, 100, 8023-8030		25
105	Contribution of electron correlation to the stability of dipole-bound anionic states. *Physical Review A*, **1996**, 54, 1906-1909	2.6	156
104	Potential energy surfaces and reactive dynamics of Zn(3P) with H2. *Journal of Chemical Physics*, **1996**, 105, 10919-10924	3.9	10
103	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		3
102	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	3.9	13
101	Combining doubly charged cations and anions to form new species. *Journal of Chemical Physics*, **1994**, 100, 5778-5784	3.9	1
100	New anionic states of the lithium trimer. *Journal of Chemical Physics*, **1994**, 101, 4867-4877	3.9	10

99	Anionic states of LiFLi. *Journal of Chemical Physics*, **1994**, 100, 1308-1311	3.9	27
98	Potential energy curves of M(np 2P)?RG(2)excited states and M+?RG ground states (M=Li, Na; RG=He, Ne). *Journal of Chemical Physics*, **1994**, 100, 8212-8218	3.9	34
97	Al3H stable and transition state structures. *Journal of Chemical Physics*, **1994**, 101, 10746-10752	3.9	6
96	A combined experimental and theoretical study of the neutral, cationic, and anionic Si3N cluster molecule. *Journal of Chemical Physics*, **1994**, 101, 2871-2879	3.9	42
95	Singlet-to-triplet energy transfer via 1/3 curve crossings in group 2 and 12 metalatom/rare-gas systems. *Journal of Chemical Physics*, **1993**, 99, 3815-3822	3.9	12
94	Collisional energy transfer in bimolecular ionmolecule dynamics M++(H2; D2; or HD)-(MH++H; MD++D; MH++D; or MD++H). *Journal of Chemical Physics*, **1993**, 99, 2601-2615	3.9	9
93	Vertical and adiabatical ionization potentials of MHK+1 anions. Ab initio study of the structure and stability of hypervalent MHk+1 molecules. *Journal of Chemical Physics*, **1993**, 99, 4628-4637	3.9	56
92	Calculation of hyperfine coupling constants of the ground state X 3of NH and B2. *Journal of Chemical Physics*, **1993**, 99, 5995-6003	3.9	16
91	Graphical description of the symmetries of potential energy surfaces. *Journal of Chemical Physics*, **1993**, 98, 8801-8809	3.9	9
90	Calculation of hyperfine coupling constants of the CN and CP ground state radicals. *Journal of Chemical Physics*, **1993**, 98, 7012-7019	3.9	21
89	Interpretation of the hyperfine coupling constants of the boron trimer in rare-gas matrices. *Journal of Chemical Physics*, **1993**, 98, 3060-3065	3.9	8
88	Ab initio study of the internal rotation barrier of formamide and the formamideH2O complex. *International Journal of Quantum Chemistry*, **1993**, 45, 123-132	2.1	28
87	Finding transition states when second-order JahnTeller instability occurs. *International Journal of Quantum Chemistry*, **1993**, 48, 211-218	2.1	6
86	Second-order JahnTeller instability and the activation energy for Al+(1S) + H2 -jAlH+(2) + H. *International Journal of Quantum Chemistry*, **1993**, 48, 309-317	2.1	3
85	Rydberg bonding in ammonium dimer ((NH4)2). *The Journal of Physical Chemistry*, **1992**, 96, 8840-8843		19
84	Ab initio potential-energy surfaces for Cd(1P)+H2=CdH(X 2)+H, HCdH(X 1g), Cd(3P)+H2, and Cd(1S)+H+H. *Journal of Chemical Physics*, **1992**, 96, 6555-6564	3.9	17
83	The B3Li moleculeselectronic and geometrical structure. *Journal of Chemical Physics*, **1992**, 97, 8357-8360	3.9	3
82	Direct atomic-orbital-based time-dependent HartreeFock calculations of frequency-dependent polarizabilities. *Journal of Chemical Physics*, **1992**, 96, 2978-2987	3.9	42

81	Interactions of the B3 cluster with H atoms and H2 molecules. *Journal of Chemical Physics*, **1992**, 96, 8251-8257	3.9	9
80	Ab initio study of geometrically metastable multiprotonated species: MHk+n. *Journal of Chemical Physics*, **1992**, 97, 4272-4281	3.9	21
79	Is TeF2 the MX2 dianion with the largest electron detachment energy (5 eV). *Journal of Chemical Physics*, **1992**, 97, 2826-2827	3.9	46
78	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	3.9	46
77	Self-Consistent-Field potential-energy surfaces for hydrogen atom pairs within small palladium clusters. *International Journal of Quantum Chemistry*, **1992**, 41, 793-810	2.1	2
76	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	2.1	12
75	Electronic energies, geometries, and vibrational frequencies of the ground and low-lying excited states of the boron trimer. *Journal of Chemical Physics*, **1991**, 94, 2961-2967	3.9	51
74	A rigorous upper bound energy for the unitary coupled electron pair approximation method. *Journal of Chemical Physics*, **1991**, 94, 5252-5252	3.9	1
73	Strategies for walking on potential energy surfaces using local quadratic approximations. *International Journal of Quantum Chemistry*, **1990**, 38, 263-276	2.1	32
72	Double-Rydberg anions: Ground-state electronic and geometric stabilities. *Journal of Chemical Physics*, **1990**, 93, 3874-3880	3.9	66
71	Lifetimes of electronically metastable double-Rydberg anions: FH2. *Journal of Chemical Physics*, **1990**, 93, 2546-2553	3.9	7
70	Walking on potential energy surfaces. *Journal of Chemical Physics*, **1990**, 92, 340-346	3.9	97
69	A potentially size-consistent multiconfiguration based coupled electron pair approximation. *Journal of Chemical Physics*, **1989**, 90, 3671-3679	3.9	29
68	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	2.1	44
67	Modified rotationally adiabatic model for rotational autoionization of dipole-bound molecular anions. *Journal of Chemical Physics*, **1989**, 91, 6858-6865	3.9	40
66	A unitary multiconfigurational coupled-cluster method: Theory and applications. *Journal of Chemical Physics*, **1988**, 88, 993-1002	3.9	132
65	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		16
64	Ab initio studies of the structures and energies of the H(H2O) and H(H2O)2 complexes. *Journal of Chemical Physics*, **1987**, 87, 2965-2975	3.9	37

63	Mo/ller□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	3.9	68
62	Theoretical study of C2 and C□2 : X 1□g , a 3□ , X 2□g , and B 2□u potentials. *Journal of Chemical Physics*, **1987**, 86, 6972-6981	3.9	36
61	Ab initio electronic structure of anions. *Chemical Reviews*, **1987**, 87, 535-555	68.1	317
60	Reply to □Comment on: □Translation□otation invariance for N-particle systems: Internal coordinates and search for stationary points in reduced spaces□□*Journal of Chemical Physics*, **1986**, 84, 3581-3581	3.9	4
59	Resonance state energies and lifetimes via analytic continuation of stabilization graphs. *Journal of Chemical Physics*, **1986**, 84, 4462-4469	3.9	32
58	Application of spectral quantization to metastable states of C 1A□DCN. *Journal of Chemical Physics*, **1986**, 85, 5826-5837	3.9	5
57	Translation-rotation invariance for N-particle systems: Internal coordinates and search for stationary points in reduced spaces. *Journal of Chemical Physics*, **1985**, 83, 3500-3506	3.9	10
56	Semiclassical vibrational wave functions for electronically excited DCN: A highly quantum mechanical system. *Journal of Chemical Physics*, **1985**, 82, 4199-4220	3.9	6
55	Associative electron detachment: O□H-□DH+e□*Journal of Chemical Physics*, **1985**, 83, 3888-3893	3.9	15
54	Translational and rotational symmetries in integral derivatives. *Journal of Chemical Physics*, **1985**, 82, 4566-4576	3.9	17
53	Roles Played by Metastable States in Chemistry. *ACS Symposium Series*, **1984**, 3-16	0.4	13
52	Dissociation of vibronic states of C□A? DCN: Quantum treatment. *Journal of Chemical Physics*, **1984**, 80, 176-185	3.9	11
51	Geometrical derivatives of dipole moments and polarizabilities. *International Journal of Quantum Chemistry*, **1984**, 25, 1135-1150	2.1	27
50	Coordinate rotation studies of H□He□Be□Mg□resonances: Basis set and configuration list dependence. *International Journal of Quantum Chemistry*, **1983**, 23, 1723-1738	2.1	10
49	Ab initio analytical molecular gradients and Hessians. *Journal of Chemical Physics*, **1983**, 79, 334-357	3.9	145
48	A multiconfiguration self-consistent-field group function method for problems with repeating potentials. *Journal of Chemical Physics*, **1983**, 79, 6104-6111	3.9	15
47	Resolvent operator approach to many-body perturbation theory. I. Closed shells. *Journal of Chemical Physics*, **1982**, 76, 1972-1978	3.9	5
46	On the lowest sigma and pi anion states of Be2 and Be3. *Journal of Chemical Physics*, **1982**, 77, 5250-5253	3.9	14

45	Resolvent operator approach to many-body perturbation theory. II. Open shells. *Journal of Chemical Physics*, **1982**, 76, 1979-1994	3.9	17
44	Resolvent operator approach to many-body perturbation theory. III. Applications. *Journal of Chemical Physics*, **1982**, 76, 1995-2002	3.9	8
43	Applications of multiconfigurational coupled-cluster theory. *Journal of Chemical Physics*, **1982**, 76, 4548-4559	3.9	102
42	Comparison of the convergence characteristics of some iterative wave function optimization methods. *Journal of Chemical Physics*, **1982**, 76, 543-557	3.9	147
41	Complex coordinate rotation calculation of branching ratios. *International Journal of Quantum Chemistry*, **1982**, 21, 727-739	2.1	30
40	Coordinate rotated TDHF excitation energies Li□1S -j1P. *International Journal of Quantum Chemistry*, **1982**, 22, 275-288	2.1	4
39	Propensity rules for vibration-induced electron detachment of anions. *Journal of the American Chemical Society*, **1981**, 103, 3971-3976	16.4	115
38	The coupled-cluster method with a multiconfiguration reference state. *International Journal of Quantum Chemistry*, **1981**, 19, 207-216	2.1	159
37	The Siegert methods in resonance scattering: Relation to L2 methods. *International Journal of Quantum Chemistry*, **1981**, 20, 779-780	2.1	5
36	Resonance state lifetimes from stabilization graphs. *Journal of Chemical Physics*, **1981**, 75, 2465-2467	3.9	122
35	Comment on the electronic structure of small beryllium and magnesium clusters and their anions. *Journal of Chemical Physics*, **1980**, 72, 2889-2890	3.9	23
34	Monte Carlo simulation of small hydrate clusters of NO□. *Journal of Chemical Physics*, **1980**, 73, 1814-1826	3.9	25
33	Analysis of the □harge resonance□transition in anthracene dimer anion. *Journal of Chemical Physics*, **1980**, 72, 425-428	3.9	19
32	Should one use complex basis functions in coordinate rotation calculations on molecules?. *Journal of Chemical Physics*, **1980**, 73, 992-993	3.9	2
31	Complex coordinate rotation of the electron propagator. *Journal of Chemical Physics*, **1980**, 73, 2858-2866	3.9	68
30	Polarization Green's function with multiconfiguration self-consistent-field reference states. *International Journal of Quantum Chemistry*, **1979**, 16, 1209-1237	2.1	18
29	An experimental and theoretical determination of the electron affinity of the ethynyl radical, HC2?. *Journal of Chemical Physics*, **1979**, 71, 2057	3.9	35
28	Line shapes of charge-transfer spectra. *Journal of Chemical Physics*, **1979**, 70, 4974-4981	3.9	5

27	Electronic spectroscopy in condensed media: The lowest n-π* transition of the solvated nitrite anion. *Journal of Chemical Physics*, **1979**, 71, 60-67	3.9	6
26	Dynamics of molecules in contact with an external medium at equilibrium. *International Journal of Quantum Chemistry*, **1978**, 13, 553-562	2.1	9
25	Nature of the autodetaching sub 2P□ threshold states of the alkali anions. *International Journal of Quantum Chemistry*, **1978**, 14, 333-336	2.1	6
24	Excess electrons in condensed media: Theory of optical absorption spectrum in molecular solutions. *Journal of Chemical Physics*, **1978**, 68, 415-432	3.9	35
23	Electronic spectrocopy in condensed media: Spectra of styrene and cyclo-octatetraene anions. *Journal of Chemical Physics*, **1978**, 69, 5538-5544	3.9	3
22	Diffusion of excess electrons in one- and two-component molecular solutions. A theoretical model. *Journal of Chemical Physics*, **1978**, 68, 1695-1700	3.9	1
21	Spectroscopy of binary solutions. The benzene□odine charge-transfer spectrum. *Journal of Chemical Physics*, **1978**, 69, 1406-1417	3.9	11
20	Electronic structure of small metal clusters. II. Anions of Li2, LiNa, and Na2. *Journal of Chemical Physics*, **1978**, 69, 1788-1789	3.9	17
19	A calculation of the electron detachment energy of NO2□*Journal of Chemical Physics*, **1977**, 66, 2427-2430	3.9	34
18	An analysis of the natural orbital theory of ionization potentials. *Journal of Chemical Physics*, **1977**, 66, 1067-1069	3.9	11
17	Excess electrons in condensed media. A model for migration in dilute molecular solutions. *Journal of Chemical Physics*, **1977**, 67, 389-398	3.9	14
16	A survey of some theoretical studies of negative ions. *International Journal of Quantum Chemistry*, **1977**, 11, 971-978	2.1	4
15	A Note on Differences Between Operator-Level and Function-Level Equations of Motion. *International Journal of Quantum Chemistry*, **1977**, 12, 227-229	2.1	7
14	A calculation of the electron affinity of the lithium molecule. *Journal of Chemical Physics*, **1976**, 64, 4548-4550	3.9	28
13	The electron propagator and superoperator resolvent. *Journal of Chemical Physics*, **1976**, 64, 4541-4543	3.9	42
12	Analysis of the equation-of-motion theory of electron affinities and ionization potentials. *Chemical Physics*, **1976**, 14, 145-158	2.3	24
11	Theoretical studies of molecular ions. Ionization potentials of CN□and BO□*Journal of Chemical Physics*, **1976**, 64, 3610-3614	3.9	46
10	Theoretical studies of molecular ions: Be□. *Journal of Chemical Physics*, **1976**, 65, 1601-1602	3.9	24

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