Jack Simons

List of Publications by Citations

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	Ab initio electronic structure of anions. *Chemical Reviews*, **1987**, 87, 535-555	68.1	317
187	Molecular anions. *Journal of Physical Chemistry A*, **2008**, 112, 6401-511	2.8	315
186	How do low-energy (0.1-2 eV) electrons cause DNA-strand breaks?. *Accounts of Chemical Research*, **2006**, 39, 772-9	24.3	303
185	Mechanism for Damage to DNA by Low-Energy Electrons *Journal of Physical Chemistry B*, **2002**, 106, 7991-7994	3.4	247
184	Theory of electron affinities of small molecules. *Journal of Chemical Physics*, **1973**, 58, 4899-4907	3.9	245
183	First experimental photoelectron spectra of superhalogens and their theoretical interpretations. *Journal of Chemical Physics*, **1999**, 110, 4763-4771	3.9	243
182	The Only Stable State of O2- Is the X 2 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
181	The coupled-cluster method with a multiconfiguration reference state. *International Journal of Quantum Chemistry*, **1981**, 19, 207-216	2.1	159
180	Small Multiply Charged Anions as Building Blocks in Chemistry. *Accounts of Chemical Research*, **1996**, 29, 497-502	24.3	156
179	Contribution of electron correlation to the stability of dipole-bound anionic states. *Physical Review A*, **1996**, 54, 1906-1909	2.6	156
178	Comparison of the convergence characteristics of some iterative wave function optimization methods. *Journal of Chemical Physics*, **1982**, 76, 543-557	3.9	147
177	Ab initio analytical molecular gradients and Hessians. *Journal of Chemical Physics*, **1983**, 79, 334-357	3.9	145
176	Tetracoordinated Planar Carbon in Pentaatomic Molecules. *Journal of the American Chemical Society*, **1998**, 120, 7967-7972	16.4	134
175	A unitary multiconfigurational coupled-cluster method: Theory and applications. *Journal of Chemical Physics*, **1988**, 88, 993-1002	3.9	132
174	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
173	Resonance state lifetimes from stabilization graphs. *Journal of Chemical Physics*, **1981**, 75, 2465-2467	3.9	122
172	Propensity rules for vibration-induced electron detachment of anions. *Journal of the American Chemical Society*, **1981**, 103, 3971-3976	16.4	115

171	Adiabatic electron affinities of small superhalogens: LiF2, LiCl2, NaF2, and NaCl2. *Journal of Chemical Physics*, **1997**, 107, 3867-3875	3.9	112
170	Applications of multiconfigurational coupled-cluster theory. *Journal of Chemical Physics*, **1982**, 76, 4548-4559	3.9	102
169	Walking on potential energy surfaces. *Journal of Chemical Physics*, **1990**, 92, 340-346	3.9	97
168	Damage to Model DNA Fragments by 0.25−1.0 eV Electrons Attached to a Thymine π* Orbital. *Journal of Physical Chemistry B*, **2004**, 108, 5800-5805	3.4	96
167	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
166	Theoretical study of negative molecular ions. *Annual Review of Physical Chemistry*, **2011**, 62, 107-28	15.7	93
165	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
164	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
163	Energies of dipole-bound anionic states. *International Journal of Quantum Chemistry*, **1997**, 64, 183-191	2.1	82
162	Mechanisms for S−S and N−C bond cleavage in peptide ECD and ETD mass spectrometry. *Chemical Physics Letters*, **2010**, 484, 81-95	2.5	79
161	A complete treatment of the electron propagator through third order. *Journal of Chemical Physics*, **1975**, 63, 5302-5304	3.9	72
160	Direct Calculation of First- and Second-Order Density Matrices. The Higher RPA Method. *Journal of Chemical Physics*, **1971**, 55, 1218-1230	3.9	72
159	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
158	Complex coordinate rotation of the electron propagator. *Journal of Chemical Physics*, **1980**, 73, 2858-2866	3.9	68
157	Double-Rydberg anions: Ground-state electronic and geometric stabilities. *Journal of Chemical Physics*, **1990**, 93, 3874-3880	3.9	66
156	Effects of Base π-Stacking on Damage to DNA by Low-Energy Electrons. *Journal of Physical Chemistry A*, **2004**, 108, 11381-11387	2.8	60
155	Repulsive Coulomb Barriers in Compact Stable and Metastable Multiply Charged Anions. *Journal of the American Chemical Society*, **2000**, 122, 11893-11899	16.4	59
154	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

153	Energy-Shift Theory of Low-Lying Excited Electronic States of Molecules. *Journal of Chemical Physics*, **1972**, 57, 3787-3792	3.9	52
152	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
151	Ab Initio Study of the Stabilization of Multiply Charged Anions in Water. *Journal of Physical Chemistry B*, **1998**, 102, 4205-4208	3.4	48
150	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
149	Negative electron affinities from conventional electronic structure methods. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	46
148	Stabilization calculation of the energy and lifetime of metastable SO42□*Journal of Chemical Physics*, **2002**, 116, 2848-2851	3.9	46
147	Is TeF2□ the MX2□ dianion with the largest electron detachment energy (5 eV). *Journal of Chemical Physics*, **1992**, 97, 2826-2827	3.9	46
146	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
145	Theoretical studies of molecular ions. Ionization potentials of CN□and BO□*Journal of Chemical Physics*, **1976**, 64, 3610-3614	3.9	46
144	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
143	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
142	General-Order Many-Body Green's Function Method. *Journal of Chemical Theory and Computation*, **2015**, 11, 1595-606	6.4	43
141	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
140	Direct atomic-orbital-based time-dependent Hartree□Fock calculations of frequency-dependent polarizabilities. *Journal of Chemical Physics*, **1992**, 96, 2978-2987	3.9	42
139	The electron propagator and superoperator resolvent. *Journal of Chemical Physics*, **1976**, 64, 4541-4543	3.9	42
138	Modified rotationally adiabatic model for rotational autoionization of dipole-bound molecular anions. *Journal of Chemical Physics*, **1989**, 91, 6858-6865	3.9	40
137	Theoretical studies of molecular ions. Vertical ionization potentials of hydrogen fluoride. *Journal of Chemical Physics*, **1974**, 61, 2670-2674	3.9	39
136	Theoretical study of the dipole-bound anion (HPPH3)□*Journal of Chemical Physics*, **1999**, 110, 274-280	3.9	38

135	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
134	Theoretical study of C2 and C2 : X 1g , a 3 , X 2g , and B 2u potentials. *Journal of Chemical Physics*, **1987**, 86, 6972-6981	3.9	36
133	An experimental and theoretical determination of the electron affinity of the ethynyl radical, HC2?. *Journal of Chemical Physics*, **1979**, 71, 2057	3.9	35
132	Excess electrons in condensed media: Theory of optical absorption spectrum in molecular solutions. *Journal of Chemical Physics*, **1978**, 68, 415-432	3.9	35
131	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
130	A calculation of the electron detachment energy of NO2. *Journal of Chemical Physics*, **1977**, 66, 2427-2430	3.9	34
129	Strategies for walking on potential energy surfaces using local quadratic approximations. *International Journal of Quantum Chemistry*, **1990**, 38, 263-276	2.1	32
128	Resonance state energies and lifetimes via analytic continuation of stabilization graphs. *Journal of Chemical Physics*, **1986**, 84, 4462-4469	3.9	32
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118	Anionic states of LiFLi. *Journal of Chemical Physics*, **1994**, 100, 1308-1311	3.9	27

117	Geometrical derivatives of dipole moments and polarizabilities. *International Journal of Quantum Chemistry*, **1984**, 25, 1135-1150	2.1	27
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115	Why Are (MgO)n Clusters and Crystalline MgO So Reactive?. *The Journal of Physical Chemistry*, **1996**, 100, 8023-8030		25
114	Monte Carlo simulation of small hydrate clusters of NO2. *Journal of Chemical Physics*, **1980**, 73, 1814-1826	3.9	25
113	An excess electron bound to urea. I. Canonical and zwitterionic tautomers. *Journal of Chemical Physics*, **2001**, 115, 8373-8380	3.9	24
112	Dissociative Recombination of H3O+. *Journal of Physical Chemistry A*, **1999**, 103, 6552-6563	2.8	24
111	Analysis of the equation-of-motion theory of electron affinities and ionization potentials. *Chemical Physics*, **1976**, 14, 145-158	2.3	24
110	Theoretical studies of molecular ions: Be2. *Journal of Chemical Physics*, **1976**, 65, 1601-1602	3.9	24
109	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
108	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
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106	Ab initio study of geometrically metastable multiprotonated species: MHk+n. *Journal of Chemical Physics*, **1992**, 97, 4272-4281	3.9	21
105	Theoretical study of electron capture dissociation of [Mg(H2O)n]2+ clusters. *International Journal of Mass Spectrometry*, **2008**, 277, 166-174	1.9	20
104	Two-photon ionization spectroscopy and all-electron ab initio study of LiCa. *Journal of Chemical Physics*, **1998**, 109, 6655-6665	3.9	20
103	Rydberg bonding in ammonium dimer ((NH4)2). *The Journal of Physical Chemistry*, **1992**, 96, 8840-8843		19
102	Analysis of the charge resonance transition in anthracene dimer anion. *Journal of Chemical Physics*, **1980**, 72, 425-428	3.9	19
101	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
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94	Is 9-acridinamine anion a dispersion-bound anion?. *Journal of Chemical Physics*, **2001**, 115, 11193-11199	3.9	16
93	Calculation of hyperfine coupling constants of the ground state X 3□ of NH and B2. *Journal of Chemical Physics*, **1993**, 99, 5995-6003	3.9	16
92	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
91	A multiconfiguration self-consistent-field group function method for problems with repeating potentials. *Journal of Chemical Physics*, **1983**, 79, 6104-6111	3.9	15
90	Associative electron detachment: O□H-□OH+e□*Journal of Chemical Physics*, **1985**, 83, 3888-3893	3.9	15
89	Mixed valence/dipole-bound dianions. *Journal of Chemical Physics*, **1999**, 111, 9469-9474	3.9	14
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80	Singlet-to-triplet energy transfer via 1□/3□1 curve crossings in group 2 and 12 metal□tom/rare-gas systems. *Journal of Chemical Physics*, **1993**, 99, 3815-3822	3.9	12
79	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
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76	Dissociation of vibronic states of C□A? DCN: Quantum treatment. *Journal of Chemical Physics*, **1984**, 80, 176-185	3.9	11
75	An analysis of the natural orbital theory of ionization potentials. *Journal of Chemical Physics*, **1977**, 66, 1067-1069	3.9	11
74	Spectroscopy of binary solutions. The benzene□odine charge-transfer spectrum. *Journal of Chemical Physics*, **1978**, 69, 1406-1417	3.9	11
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59	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
58	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
57	Resolvent operator approach to many-body perturbation theory. III. Applications. *Journal of Chemical Physics*, **1982**, 76, 1995-2002	3.9	8
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53	Characterization of the Rydberg Bonding in (NH4)2-. *Journal of Physical Chemistry A*, **2000**, 104, 10855-10858	2.8	7
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41	Nature of the autodetaching sub 2P□ threshold states of the alkali anions. *International Journal of Quantum Chemistry*, **1978**, 14, 333-336	2.1	6
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