Ajit J Thakkar

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/5559451/publications.pdf

Version: 2024-02-01

272	7,624	47006	88630
papers	citations	47 h-index	70 g-index

286	286	286	2625
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Dipole oscillator strength distributions, sum rules, mean excitation energies, and isotropic van der Waals coefficients for benzene, pyridazine, pyrimidine, pyrazine, s-triazine, toluene, hexafluorobenzene, and nitrobenzene. Journal of Chemical Physics, 2020, 153, 124307.	3.0	3
2	Structure prediction of nanoclusters from global optimization techniques: Computational strategies and connection to experiments. Computational and Theoretical Chemistry, 2017, 1107, 1.	2.5	0
3	Constrained dipole oscillator strength distributions, sum rules, and dispersion coefficients for Br 2 and BrCN. Chemical Physics Letters, 2017, 672, 31-33.	2.6	1
4	How Can One Locate the Global Energy Minimum for Hydrogen-Bonded Clusters?. , 2016, , 25-55.		1
5	Constrained Dipole Oscillator Strength Distributions for CF₄, CClF₃, CCl₂F₂, CCl₃F, CHF₃, CH₃F, CH₃Cl, CH₃Br, CH₃I, C₂F₆, and CCl₃CF₃. Zeitschrift Fur Physikalische Chemie, 2016, 230, 1473-1486.	2.8	2
6	Construction of Constrained Dipole Oscillator Strength Distributions. Zeitschrift Fur Physikalische Chemie, 2016, 230, 633-650.	2.8	5
7	Ab initio calculations of static dipole polarizabilities and Cauchy moments for the halomethanes, CH Cl F4â^'â^'. Chemical Physics Letters, 2016, 644, 20-24.	2.6	3
8	Dipole properties of PH3, PF3, PF5, PCl3, SiCl4, GeCl4, and SnCl4. Molecular Physics, 2016, 114, 1657-1663.	1.7	4
9	How well do static electronic dipole polarizabilities from gas-phase experiments compare with density functional and MP2 computations?. Journal of Chemical Physics, 2015, 143, 144302.	3.0	26
10	The life and work of JiÅ™Ã-ÄŒÃÅ¾ek. AIP Conference Proceedings, 2015, , .	0.4	1
11	Clusters: From trimers to nanoparticles. AIP Conference Proceedings, 2015, , .	0.4	0
12	Preface of the â€œSymposium on methods in quantum chemistryâ€• A symposium in honor of JiÅ™Ã-ÄŒÃÅ¾ek and Josef Paldus. , 2015, , .		0
13	The life and work of Josef Paldus. AIP Conference Proceedings, 2015, , .	0.4	1
14	On the dipole polarisability and dipole sum rules of ozone. Molecular Physics, 2015, 113, 2939-2942.	1.7	6
15	Choosing a density functional for static molecular polarizabilities. Chemical Physics Letters, 2015, 635, 257-261.	2.6	39
16	Electric properties of stannous and stannic halides: How good are the experimental values?. Chemical Physics Letters, 2015, 626, 69-72.	2.6	6
17	Relating polarizability to volume, ionization energy, electronegativity, hardness, moments of momentum, and other molecular properties. Journal of Chemical Physics, 2014, 141, 074306.	3.0	57
18	Molecular size from moments of the momentum density. Chemical Physics Letters, 2014, 609, 113-116.	2.6	7

#	Article	IF	Citations
19	Additive models for the molecular polarizability and volume. Chemical Physics Letters, 2014, 610-611, 163-166.	2.6	20
20	TABS: A database of molecular structures. Computational and Theoretical Chemistry, 2014, 1043, 13-16.	2.5	21
21	A dispersion-corrected density functional theory study of hexamers of formic acid. Canadian Journal of Chemistry, 2013, 91, 527-528.	1.1	3
22	Electron and Electron-Pair Number and Momentum Densities for Low-Lying States of He, Hâ€“, and Li+. Advances in Quantum Chemistry, 2013, 67, 19-54.	0.8	2
23	Small clusters of formic acid: Tests and applications of density functional theory with dispersion-correcting potentials. Chemical Physics Letters, 2013, 560, 71-74.	2.6	14
24	How often is the minimum polarizability principle violated?. Chemical Physics Letters, 2013, 556, 346-349.	2.6	45
25	Methanol clusters (CH3OH)n: Putative global minimum-energy structures from model potentials and dispersion-corrected density functional theory. Journal of Chemical Physics, 2013, 138, 224303.	3.0	42
26	Clusters: From dimers to nanoparticles. Computational and Theoretical Chemistry, 2013, 1021, 1.	2.5	2
27	Water nanodroplets: Predictions of five model potentials. Journal of Chemical Physics, 2013, 138, 194302.	3.0	45
28	Forward for Special Issue. Computational and Theoretical Chemistry, 2013, 1003, 1.	2.5	0
29	When does the non-variational nature of second-order MÃ¸ller-Plesset energies manifest itself? All-electron correlation energies for open-shell atoms from K to Br. Journal of Chemical Physics, 2012, 136, 054107.	3.0	10
30	A hierarchy for additive models of polarizability. AIP Conference Proceedings, 2012, , .	0.4	23
31	New Relationships Connecting the Dipole Polarizability, Radius, and Second Ionization Potential for Atoms. Journal of Physical Chemistry A, 2012, 116, 697-703.	2.5	30
32	Accurate all-electron correlation energies for the closed-shell atoms from Ar to Rn and their relationship to the corresponding MP2 correlation energies. Journal of Chemical Physics, 2011, 134, 044102.	3.0	32
33	Interelectronic angles: Rounding out a geometric picture of the helium atom. Chemical Physics Letters, 2011, 512, 287-289.	2.6	14
34	Dipole polarizability, sum rules, mean excitation energies, and long-range dispersion coefficients for buckminsterfullerene C60. Chemical Physics Letters, 2011, 516, 208-211.	2.6	18
35	Electronâ€pair extracule densities for lowâ€lying excited states of He and Li⁺. International Journal of Quantum Chemistry, 2011, 111, 753-759.	2.0	5
36	Ozone: Unresolved discrepancies for dipole oscillator strength distributions, dipole sums, and van der Waals coefficients. Journal of Chemical Physics, 2011, 135, 074303.	3.0	9

#	ARTICLE	IF	CITATIONS
37	Simple models for electron correlation energies in atoms. Chemical Physics Letters, 2010, 494, 312-314.	2.6	10
38	How many intramolecular hydrogen bonds does the oxalic acid dimer have?. Chemical Physics Letters, 2010, 495, 198-202.	2.6	12
39	Dipole oscillator strength distributions with improved high-energy behavior: Dipole sum rules and dispersion coefficients for Ne, Ar, Kr, and Xe revisited. Journal of Chemical Physics, 2010, 132, 074301.	3.0	32
40	Are there any magic numbers for water nanodroplets, (H₂O)_n, in the range 36 â‰¤nâ‰¤ 50?. Molecular Physics, 2010, 108, 2187-2193.	1.7	10
41	Microsolvation of the formic acid dimer â€" (HCOOH)2(H2O)n clusters with n = 1, . . ., 5. Canadian Journal of Chemistry, 2010, 88, 736-743.	1.1	8
42	Toward improved density functionals for the correlation energy. Journal of Chemical Physics, 2009, 131, 134109.	3.0	46
43	A simple model of hydrogen bonding with particular application to trends in hydrogen-bonded dimers. International Journal of Quantum Chemistry, 2009, 110, NA-NA.	2.0	0
44	A simple additive model for polarizabilities: Application to amino acids. Chemical Physics Letters, 2009, 472, 232-236.	2.6	20
45	Improved minima-hopping. TIP4P water clusters, <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si3.gif" display="inline" overflow="scroll"><mml:mrow><mml:mo stretchy="false">(</mml:mo><mml:msub><mml:mrow><mml:mi) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 417 Td (mathvariant="r	2.6	60
46	Can periodane accommodate neon?. Computational and Theoretical Chemistry, 2009, 900, 55-58.	1.5	2
47	New Algorithms for Locating Global Minima of Molecular Clusters: A Progress Report and Test Applications to Water Clusters (H[sub 2]O)[sub n], nâ‰34. , 2009, , .		7
48	Structural characteristics of formic acid dodecamers, <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si19.gif" display="inline" overflow="scroll"><mml:mrow><mml:mo stretchy="false">(</mml:mo><mml:mtext>HCOOH</mml:mtext><mml:msub><mml:mrow><mml:mo) Tj ETQq0 0 0 rgBT /Overlock 10 T	2.6	14
49	Chemical Physics Letters, 2008, 450, 258-262. Nonlocal Wigner-like correlation energy density functional: Parametrization and tests on two-electron systems. Journal of Chemical Physics, 2007, 127, 024101.	3.0	11
50	The Rodney Bartlett Honor Symposium. AIP Conference Proceedings, 2007, , .	0.4	0
51	Clusters of glycolic acid and 16 water molecules. Chemical Physics Letters, 2007, 434, 176-181.	2.6	19
52	Is combining meta-GGA correlation functionals with the OPTX exchange functional useful?. International Journal of Quantum Chemistry, 2006, 106, 436-446.	2.0	11
53	Molecular quantum mechanics to biodynamics: Essential connections. Computational and Theoretical Chemistry, 2006, 764, 1-8.	1.5	9
54	Polarizabilities of the alkali anions: Liâ^' to Frâ^'. Journal of Chemical Physics, 2006, 125, 194317.	3.0	9

#	Article	IF	Citations
55	Does the most stable formic acid tetramer have Ï€ stacking or Câ€“Hâ‹¯O interactions?. Journal of Chemical Physics, 2006, 124, 224313.	3.0	20
56	ATOMIC POLARIZABILITIES AND HYPERPOLARIZABILITIES: A CRITICAL COMPILATION. , 2006, , 505-529.		18
57	Pentamers of formic acid. Chemical Physics, 2005, 312, 119-126.	1.9	26
58	Nitric acid dimers. Computational and Theoretical Chemistry, 2005, 714, 217-220.	1.5	9
59	The polarizability of sodium: theory and experiment reconciled. Chemical Physics Letters, 2005, 402, 270-273.	2.6	23
60	Moments of the electron momentum density: Requirements for ab initio and density functional theory calculations. International Journal of Quantum Chemistry, 2005, 102, 673-683.	2.0	33
61	Electronic structure. , 2005, , 483-505.		6
62	Low-lying states of two-dimensional double-well potentials. Journal of Physics A, 2005, 38, 2189-2199.	1.6	10
63	Clusters of glycolic acid with three to six water molecules. Journal of Chemical Physics, 2005, 122, 074313.	3.0	14
64	Polarizabilities and hyperpolarizabilities for the atoms Al, Si, P, S, Cl, and Ar: Coupled cluster calculations. Journal of Chemical Physics, 2005, 122, 044301.	3.0	54
65	Are polarizabilities useful as aromaticity indices? Tests on azines, azoles, oxazoles and thiazoles. Journal of Computational Methods in Sciences and Engineering, 2004, 4, 427-438.	0.2	3
66	Are quasi-relativistic kinetic energies useful?. Computational and Theoretical Chemistry, 2004, 711, 209-211.	1.5	1
67	Structures of the formic acid trimer. Chemical Physics Letters, 2004, 386, 162-168.	2.6	40
68	Hydrogen-bonded complexes of glycolic acid with one and two water molecules. Chemical Physics Letters, 2004, 387, 142-148.	2.6	19
69	Formic acid tetramers: a structural study. Chemical Physics Letters, 2004, 393, 347-354.	2.6	27
70	The Momentum Density Perspective of the Electronic Structure of Atoms and Molecules. Advances in Chemical Physics, 2004, , 303-352.	0.3	33
71	Variational calculations for helium-like ions using generalized Kinoshita-type expansions. Theoretical Chemistry Accounts, 2003, 109, 36-39.	1.4	13
72	Accurate electron-pair, momentum-space properties for the helium atom. Chemical Physics Letters, 2003, 381, 80-85.	2.6	9

#	Article	IF	Citations
73	Interelectronic counter-balance and coalescence densities for the (n<7) states of the helium isoelectronic sequence. Computational and Theoretical Chemistry, 2003, 633, 257-262.	1.5	6
74	Generalized oscillator strengths for electronic excitation from the 21S and 23S metastable states of the helium atom. Journal of Electron Spectroscopy and Related Phenomena, 2003, 129, 9-26.	1.7	1
75	DENSITY FUNCTIONALS FOR MOMENTS OF THE ELECTRON MOMENTUM DISTRIBUTION. , 2003, , .		0
76	Analytical Hartree-Fock Wave Functions for Atoms and Ions. , 2003, , 587-599.		3
77	ELECTRON MOMENTUM DISTRIBUTIONS AT THE ZERO MOMENTUM CRITICAL POINT. , 2002, , 85-107.		7
78	Hydrogen bonding in the glycolic acid dimer. Computational and Theoretical Chemistry, 2002, 591, 189-197.	1.5	14
79	First Born differential cross-sections for electronic excitation in the helium atom. Journal of Electron Spectroscopy and Related Phenomena, 2002, 123, 143-159.	1.7	55
80	Bond orders in heteroaromatic rings. International Journal of Quantum Chemistry, 2002, 90, 534-540.	2.0	25
81	MacLaurin expansions of electron momentum densities for 78 diatomic molecules: a numerical Hartreeâ€“Fock study. Chemical Physics Letters, 2002, 362, 428-434.	2.6	8
82	Compact Hylleraas-type wavefunctions for the lithium isoelectronic sequence. Chemical Physics Letters, 2002, 366, 95-99.	2.6	14
83	Quadrupole oscillator strengths for the helium isoelectronic sequence:n1S-m1D,n3S-m3D,n1P-m1P, andn3P-m3P transitions withn<7 andm<7. Journal of Physics B: Atomic, Molecular and Optical Physics, 2002, 35, 421-435.	1.5	23
84	A fresh look at the computation of spherically averaged electron momentum densities for wave functions built from Gaussian-type functions. International Journal of Quantum Chemistry, 2001, 85, 258-262.	2.0	11
85	Anisotropic polarizabilities and hyperpolarizabilities of second-period cations. Computational and Theoretical Chemistry, 2001, 547, 233-238.	1.5	10
86	Electron momentum densities near zero-momentum. Computational and Theoretical Chemistry, 2000, 527, 221-227.	1.5	10
87	Analytical Hartree-Fock wave functions for the atoms Cs to Lr. Theoretical Chemistry Accounts, 2000, 104, 411-413.	1.4	96
88	Electron-momentum densities of singly charged ions. Physical Review A, 1999, 59, 4805-4808.	2.5	12
89	Electron-pair densities of group 14, 15, and 16 atoms in their low-lying multiplet states. Journal of Chemical Physics, 1999, 110, 5763-5771.	3.0	23
90	Expansion coefficients and moments of electron momentum densities for singly charged ions. Theoretical Chemistry Accounts, 1999, 103, 70-76.	1.4	12

#	Article	IF	Citations
91	Geometries and multipole moments of AlH4â^', SiH4, PH3, H2S and HCl. Computational and Theoretical Chemistry, 1999, 488, 217-221.	1.5	10
92	Analytical Hartree-Fock wave functions subject to cusp and asymptotic constraints: He to Xe, Li+ to Cs+, H? to I?. International Journal of Quantum Chemistry, 1999, 71, 491-497.	2.0	117
93	Structures, Vibrational Frequencies and Polarizabilities of Diazaborinines, Triazadiborinines, Azaboroles, and Oxazaboroles. Journal of Physical Chemistry A, 1999, 103, 2141-2151.	2.5	33
94	Quadrupole and Octopole Moments of Heteroaromatic Rings. Journal of Physical Chemistry A, 1999, 103, 10009-10014.	2.5	64
95	Analytical Hartreeâ€"Fock wave functions subject to cusp and asymptotic constraints: He to Xe, Li+ to Cs+, Hâ^' to Iâ^'. , 1999, 71, 491.		3
96	Azaborinines:Â Structures, Vibrational Frequencies, and Polarizabilities. Journal of Physical Chemistry A, 1998, 102, 4679-4686.	2.5	23
97	Static response properties of second-period atoms: coupled cluster calculations. Journal of Physics B: Atomic, Molecular and Optical Physics, 1998, 31, 2215-2223.	1.5	50
98	Cross sections for x-ray and high-energy electron scattering by small molecules. Journal of Physics B: Atomic, Molecular and Optical Physics, 1998, 31, 3675-3692.	1.5	15
99	Electron momentum densities of atoms. Journal of Chemical Physics, 1998, 109, 1601-1606.	3.0	27
100	Interaction potentials for Heâ€"Fâ^' and Neâ€"Fâ^'. Journal of Chemical Physics, 1998, 109, 3072-3076.	3.0	10
101	Vibrational deactivation of N2(v=1) by inelastic collisions with He3 and He4: An experimental and a theoretical study. Journal of Chemical Physics, 1997, 107, 2329-2339.	3.0	19
102	Reliable anisotropic dipole properties and dispersion energy coefficients for NO, evaluated using constrained dipole oscillator strength techniques. Molecular Physics, 1997, 90, 721-728.	1.7	15
103	Benchmark ab initio calculations of small molecules. Computational and Theoretical Chemistry, 1997, 400, 1-5.	1.5	3
104	Noninteger principal quantum numbers increase the efficiency of Slater-type basis sets. International Journal of Quantum Chemistry, 1997, 62, 1-11.	2.0	35
105	Radial limit of lithium revisited. International Journal of Quantum Chemistry, 1997, 63, 287-290.	2.0	1
106	Reliable anisotropic dipole properties and dispersion energy coefficients for NO, evaluated using constrained dipole oscillator strength techniques. Molecular Physics, 1997, 90, 721-728.	1.7	3
107	Reliable anisotropic dipole properties, and dispersion energy coefficients, for O2evaluated using constrained dipole oscillator strength techniques. Journal of Chemical Physics, 1996, 105, 4927-4937.	3.0	48
108	Potential energy surface for interactions between N2 and He: Ab initio calculations, analytic fits, and second virial coefficients. Journal of Chemical Physics, 1996, 104, 2541-2547.	3.0	29

#	Article	IF	Citations
109	Kinetic energy analysis of atomic multiplets. Theoretica Chimica Acta, 1996, 93, 157-163.	0.8	2
110	Polarizabilities of Oxazoles:Â Ab Initio Calculations and Simple Models. The Journal of Physical Chemistry, 1996, 100, 8752-8757.	2.9	38
111	Kinetic energy analysis of atomic multiplets. II. smdn configurations. Canadian Journal of Chemistry, 1996, 74, 775-780.	1.1	2
112	Polarizabilities of purine, allopurinol, hypoxanthine, xanthine and alloxanthine. Computational and Theoretical Chemistry, 1996, 366, 185-193.	1.5	22
113	Moments of the quadrupole oscillator strength distribution for O2, N2, CO, HF, HCl, N2O, CO2, OCS, CS2 and C2H2: ab initio sum rule calculations. Chemical Physics Letters, 1996, 261, 625-632.	2.6	2
114	High energy electron and X-ray scattering from atoms using Monte Carlo methods. Computational and Theoretical Chemistry, 1996, 388, 7-17.	1.5	7
115	Kinetic energy analysis of atomic multiplets. International Journal of Quantum Chemistry, 1996, 57, 89-94.	2.0	4
116	Polarizabilities of heteroaromatic molecules: Azines revisited. International Journal of Quantum Chemistry, 1996, 60, 1633-1642.	2.0	21
117	Moments and expansion coefficients of atomic electron momentum densities: numerical Hartree - Fock calculations for hydrogen to lawrencium. Journal of Physics B: Atomic, Molecular and Optical Physics, 1996, 29, 2973-2983.	1.5	53
118	High energy electron and X-ray scattering from atoms using Monte Carlo methods. Computational and Theoretical Chemistry, 1996, 388, 7-17.	1.5	2
119	Numerical Hartree-Fock results for atoms Cs through Lr. International Journal of Quantum Chemistry, 1995, 54, 261-263.	2.0	29
120	High-energy electron and X-ray scattering from H2 using Monte Carlo techniques. International Journal of Quantum Chemistry, 1995, 56, 627-630.	2.0	9
121	Dipole and quadrupole moments of small molecules. An ab initio study using perturbatively corrected, multi-reference, configuration interaction wave functions. Computational and Theoretical Chemistry, 1995, 334, 7-13.	1.5	50
122	Accurate Heitler-London interaction energy for He2. Computational and Theoretical Chemistry, 1995, 343, 43-48.	1.5	16
123	Improved Roothaan-Hartree-Fock wavefunctions for isoelectronic series of the atoms He to Ne. Journal of Physics B: Atomic, Molecular and Optical Physics, 1995, 28, 3113-3121.	1.5	29
124	Polarizabilities of Aromatic Five-Membered Rings: Azoles. The Journal of Physical Chemistry, 1995, 99, 12790-12796.	2.9	55
125	Improved Roothaanâ€“Hartreeâ€“Fock wave functions for atoms and ions with Nâ‰54. Journal of Chemical Physics, 1995, 103, 3000-3005.	3.0	130
126	Roothaan-Hartree-Fock wave functions for cations and anions in Slater-type basis sets with doubly even tempered exponents. Theoretica Chimica Acta, 1995, 91, 47-66.	0.8	3

#	Article	IF	Citations
127	Roothaanâ€“Hartreeâ€“Fock wave functions for cations and anions in Slater-type basis sets with doubly even tempered exponents. Theoretica Chimica Acta, 1995, 91, 47.	0.8	6
128	Small-angle elastic scattering of high-energy electrons byH2, HD, andD2. Physical Review A, 1994, 49, 965-968.	2.5	6
129	Static hyperpolarizability of N2. Journal of Chemical Physics, 1994, 100, 7471-7475.	3.0	18
130	Double even tempering of orbital exponents: Application to Roothaan-Hartree-Fock calculations for He through Xe in Slater-type basis sets. Theoretica Chimica Acta, 1994, 88, 273-283.	0.8	15
131	An improved potential energy curve for the C1Îu state of H2. Chemical Physics Letters, 1994, 222, 65-68.	2.6	22
132	Pump-probe studies of the effects of permanent dipoles in one- and two-colour molecular excitations. Chemical Physics, 1994, 186, 375-394.	1.9	39
133	Contracted gaussian basis sets for sodium through to argon. Computational and Theoretical Chemistry, 1994, 306, 249-260.	1.5	25
134	Numerical Hartreeâ€“Fock energies of lowâ€lying excited states of neutral atoms with Zâ‰18. Journal of Chemical Physics, 1994, 101, 4945-4948.	3.0	53
135	Ground-state energies for the helium isoelectronic series. Physical Review A, 1994, 50, 854-856.	2.5	89
136	Numerical Hartreeâ€“Fock energies of singly charged cations and anions with Nâ‰54. Journal of Chemical Physics, 1994, 100, 8140-8144.	3.0	44
137	Static hyperpolarizability of atomic lithium. Physical Review A, 1994, 50, 2948-2952.	2.5	31
138	Polarizabilities of aromatic six-membered rings: azines and â€˜inorganic benzenesâ€™. Molecular Physics, 1994, 81, 557-567.	1.7	56
139	Static polarizabilities and hyperpolarizabilities, and multipole moments for Cl2 and Br2. Electron correlation and molecular vibration effects. Chemical Physics Letters, 1993, 201, 485-492.	2.6	36
140	Vibrational effects on cross sections for elastic scattering of X-rays and fast electrons by H2O molecules. Chemical Physics Letters, 1993, 207, 407-413.	2.6	4
141	Accurate algebraic densities and intracules for heliumlike ions. International Journal of Quantum Chemistry, 1993, 46, 689-699.	2.0	51
142	Electron correlation effects in the Rydberg-like 33D and 31D states of helium-like ions. International Journal of Quantum Chemistry, 1993, 48, 1-14.	2.0	10
143	Statistical electron correlation coefficients for 29 states of the heliumlike ions. International Journal of Quantum Chemistry, 1993, 48, 33-42.	2.0	22
144	Double and quadruple zeta contracted Gaussian basis sets for hydrogen through neon. International Journal of Quantum Chemistry, 1993, 48, 343-354.	2.0	100

#	Article	IF	Citations
145	Optimal single-zeta description for the atoms Al through Xe. Theoretica Chimica Acta, 1993, 85, 363-370.	0.8	13
146	Medium-size Gaussian basis sets for hydrogen through argon. Theoretica Chimica Acta, 1993, 85, 391-394.	0.8	30
147	Even-tempered Roothaan-Hartree-Fock wave functions for the third- and fourth-row atoms. Theoretica Chimica Acta, 1993, 86, 477-485.	0.8	5
148	Intramolecular bond length dependence of the anisotropic dispersion coefficients for interactions of rare gas atoms with N2, CO, Cl2, HCl and HBr. Molecular Physics, 1993, 80, 533-548.	1.7	68
149	Electronic energies, dipole moment matrix elements, and static polarizabilities and hyperpolarizabilities for some diphenyl molecules. Canadian Journal of Chemistry, 1993, 71, 1663-1671.	1.1	10
150	Roothaan-Hartree-Fock wavefunctions for ions with N<or=54. Journal of Physics B: Atomic, Molecular and Optical Physics, 1993, 26, 2529-2532.	1.5	20
151	Accurate multipole moments for H2 and D2 including the effects of electron correlation and molecular vibration and rotation. Molecular Physics, 1993, 78, 1039-1046.	1.7	51
152	Elastic scattering of high energy electrons by N2: discrepancy between theory and experiment. Journal of Physics B: Atomic, Molecular and Optical Physics, 1993, 26, L185-L190.	1.5	4
153	Leading corrections to atomic impulse-approximation Compton profiles: A density-functional approach. Physical Review A, 1993, 48, 2946-2951.	2.5	7
154	Charge and intracule densities in singly excited heliumlike ions. Journal of Chemical Physics, 1993, 98, 7132-7139.	3.0	29
155	Intramolecular bond length dependence of the anisotropic dispersion coefficients for H2â€“rare gas interactions. Journal of Chemical Physics, 1993, 98, 7140-7144.	3.0	32
156	Chain length dependence of static longitudinal polarizabilities and hyperpolarizabilities in linear polyynes. Journal of Chemical Physics, 1993, 98, 8324-8329.	3.0	47
157	Roothaan-Hartree-Fock wave functions for atoms withZâ‰54. Physical Review A, 1993, 47, 4510-4512.	2.5	76
158	Roothaan-Hartree-Fock wave functions for atoms from Cs through U. Physical Review A, 1993, 48, 4775-4777.	2.5	10
159	Improved Double-Zeta Description for the Atoms Li through Xe. Bulletin of the Chemical Society of Japan, 1993, 66, 3135-3141.	3.2	20
160	Oscillator strengths forS-PandP-Dtransitions in heliumlike ions. Physical Review A, 1992, 46, 5397-5405.	2.5	95
161	Weakly bound ground states in three-body Coulomb systems with unit charges. Physical Review A, 1992, 46, 4418-4420.	2.5	24
162	Abinitiodispersion coefficients for interactions involving rareâ€gas atoms. Journal of Chemical Physics, 1992, 97, 3252-3257.	3.0	132

#	ARTICLE	IF	CITATIONS
163	Comparison of kinetic-energy density functionals. Physical Review A, 1992, 46, 6920-6924.	2.5	99
164	Improvement of the long-range behavior of Gaussian basis sets using asymptotic constraints. Canadian Journal of Chemistry, 1992, 70, 362-365.	1.1	7
165	Constrained self-consistent-field wave functions with improved long-range behavior. International Journal of Quantum Chemistry, 1992, 44, 985-995.	2.0	4
166	Analytic approximations to the momentum moments of neutral atoms. International Journal of Quantum Chemistry, 1992, 44, 291-298.	2.0	10
167	Angle and bond-length dependent C6 coefficients for H2 interacting with H, Li, Be and rare gas atoms. Theoretica Chimica Acta, 1992, 82, 57-73.	0.8	19
168	Finite-field many-body-perturbation-theory calculation of the static hyperpolarizabilities and polarizabilities of Mg,Al+, and Ca. Physical Review A, 1991, 44, 5478-5484.	2.5	44
169	Static hyperpolarizabilities and polarizabilities of linear polyynes. Journal of Chemical Physics, 1991, 95, 9060-9064.	3.0	45
170	Momentum-space properties of the neutral atoms from H through U. Atomic Data and Nuclear Data Tables, 1991, 48, 213-229.	2.4	17
171	Position moments linearly averaged over Hartree-Fock orbitals. Physical Review A, 1991, 43, 3299-3304.	2.5	1
172	Ab initiostatic polarizabilities and multipole moments of I2. Molecular Physics, 1991, 73, 1235-1240.	1.7	16
173	Local density functional approximations and conjectured bounds for momentum moments. International Journal of Quantum Chemistry, 1990, 38, 327-338.	2.0	28
174	Hyperpolarizabilities and polarizabilities of Liâˆ’1 and B+: finite-field coupled-cluster calculations. Chemical Physics Letters, 1990, 173, 579-584.	2.6	29
175	A coupled cluster calculation of the quadrupole polarizability of CO. Journal of Chemical Physics, 1990, 92, 812-813.	3.0	28
176	Momentum-space properties ofN2: Improved configuration-interaction calculations. Physical Review A, 1990, 42, 1336-1345.	2.5	16
177	How important is electron correlation for the hyperpolarizability of ethyne?. Journal of Chemical Physics, 1990, 93, 652-656.	3.0	56
178	Polarizabilities and hyperpolarizabilities of carbon dioxide. Journal of Chemical Physics, 1990, 93, 4164-4171.	3.0	90
179	Coupled-cluster calculation of hyperpolarizabilities and polarizabilities for Be. Physical Review A, 1989, 40, 1130-1132.	2.5	45
180	Polarizabilities and hyperpolarizabilities of F2. Journal of Chemical Physics, 1989, 90, 366-370.	3.0	58

#	Article	IF	Citations
181	Static hyperpolarisabilities and polarisabilities of Li. Journal of Physics B: Atomic, Molecular and Optical Physics, 1989, 22, 2439-2446.	1.5	44
182	Hyperpolarizabilities and polarizabilities of neon: Discrepancy between theory and experiment. Chemical Physics Letters, 1989, 156, 87-90.	2.6	74
183	Scattering of fast electrons and X-rays from molecules: CH4 and C2H2. International Journal of Quantum Chemistry, 1989, 35, 869-885.	2.0	9
184	Maclaurin expansions of the electron momentum densities of linear molecules. International Journal of Quantum Chemistry, 1989, 36, 245-253.	2.0	0
185	Linear integrability of wave functions. International Journal of Quantum Chemistry, 1988, 34, 103-106.	2.0	8
186	Higher dispersion coefficients: Accurate values for hydrogen atoms and simple estimates for other systems. Journal of Chemical Physics, 1988, 89, 2092-2098.	3.0	94
187	Multipole moments, polarizabilities, and hyperpolarizabilities for N2from fourthâ€order manyâ€body perturbation theory calculations. Journal of Chemical Physics, 1988, 88, 7623-7632.	3.0	131
188	Quadrupole polarizabilities and hyperpolarizabilities of Kr and Xe from fourthâ€order manyâ€body perturbation theory calculations. Journal of Chemical Physics, 1988, 89, 7320-7323.	3.0	49
189	Modified zero-momentum energy expression: A general criterion for assessing the accuracy of approximate wave functions. Physical Review A, 1988, 37, 1411-1414.	2.5	11
190	Static hyperpolarisabilities and polarisabilities for Be: a fourth-order Moller-Plesset perturbation theory calculation. Journal of Physics B: Atomic, Molecular and Optical Physics, 1988, 21, 3819-3831.	1.5	44
191	Coulomb holes in the 23P and 21P states of helium-like ions. Journal of Physics B: Atomic and Molecular Physics, 1987, 20, 3939-3945.	1.6	9
192	Asymptotic expansions of the electron momentum densities of the atoms from hydrogen through lawrencium. Journal of Chemical Physics, 1987, 87, 1212-1215.	3.0	35
193	Asymptotic behavior of atomic momentals. Journal of Chemical Physics, 1987, 86, 5060-5062.	3.0	38
194	Moments of the Bethe surface and total inelastic x-ray scattering cross sections forH2. Physical Review A, 1987, 36, 5151-5158.	2.5	5
195	Momentum-space properties ofN2. Physical Review A, 1987, 36, 5111-5117.	2.5	13
196	Moments of the generalised oscillator strength distribution and total inelastic x-ray scattering cross sections for He and H-. Journal of Physics B: Atomic and Molecular Physics, 1987, 20, 6171-6172.	1.6	9
197	Very shortâ€range interatomic potentials. Journal of Chemical Physics, 1987, 87, 2186-2190.	3.0	26
198	Quadrupole and hexadecapole moments for molecular nitrogen. Journal of Physics B: Atomic and Molecular Physics, 1987, 20, L551-L554.	1.6	7

#	Article	IF	Citations
199	More on basis set quality tests. International Journal of Quantum Chemistry, 1987, 32, 427-434.	2.0	6
200	Scattering of fast electrons and X-rays from CO2 molecules. International Journal of Quantum Chemistry, 1987, 32, 217-227.	2.0	6
201	Inter-Relationships Between Various Representations of One-Matrices and Related Densities: A Road Map and An Example. , 1987, , 327-337.		7
202	Extracules, Intracules, Correlation Holes, Potentials, Coefficients and All That. , 1987, , 553-581.		56
203	What do kinetic-energy anisotropies tell us about chemical bonding? I. Diatomic hydrides. International Journal of Quantum Chemistry, 1986, 29, 323-332.	2.0	16
204	The quality ofs-orbitals determined by least-squares fitting and constrained variational methods. International Journal of Quantum Chemistry, 1986, 30, 717-735.	2.0	12
205	Moments of the generalised oscillator strength distribution and total inelastic X-ray scattering cross sections for He and H-. Journal of Physics B: Atomic and Molecular Physics, 1986, 19, 1049-1062.	1.6	4
206	Relativistic kinetic energies and massâ€“velocity corrections in diatomic molecules. Journal of Chemical Physics, 1986, 85, 4509-4514.	3.0	11
207	What do kinetic energy anisotropies tell us about chemical bonding? II. Firstâ€row A2, AO, and AF diatomics. Journal of Chemical Physics, 1986, 85, 2845-2849.	3.0	17
208	Approximate relationships between density power integrals, moments of the momentum density, and interelectronic repulsions in diatomic molecules. Journal of Chemical Physics, 1986, 85, 958-962.	3.0	50
209	The higher order electronâ€“electron coalescence condition for the intracule function for states of maximum spin multiplicity. Journal of Chemical Physics, 1986, 84, 6830-6832.	3.0	20
210	Compton profiles and other momentum-space properties ofN2. Physical Review A, 1986, 34, 4695-4703.	2.5	18
211	Gaussian vs. Slater representations ofd orbitals: An information theoretic appraisal based on both position and momentum space properties. International Journal of Quantum Chemistry, 1985, 28, 429-449.	2.0	29
212	Correlation energy generating potentials for molecular hydrogen. Journal of Chemical Physics, 1985, 83, 3577-3583.	3.0	14
213	Sum rules for atomic form factors and total xâ€ray scattering intensities. Journal of Chemical Physics, 1985, 83, 747-749.	3.0	15
214	Momentum space properties of two-electron atoms. Journal of Physics B: Atomic and Molecular Physics, 1985, 18, 3061-3071.	1.6	37
215	Substituent effects in alkynes and cyanides: a momentum density perspective. Canadian Journal of Chemistry, 1985, 63, 1412-1417.	1.1	12
216	A momentum density analysis of strong hydrogen bonding. Computational and Theoretical Chemistry, 1985, 123, 221-229.	1.5	5

#	Article	IF	Citations
217	Charge densities and two-electron intracules for the low-lying excited states of the helium-like ions. Journal of Physics B: Atomic and Molecular Physics, 1984, 17, 3391-3403.	1.6	46
218	Anisotropy of the Coulomb hole in H2. Journal of Physics B: Atomic and Molecular Physics, 1984, 17, 3405-3416.	1.6	34
219	A comparison of the predictions of various model N2â€“He potential energy surfaces with experiment. Journal of Chemical Physics, 1984, 80, 5561-5567.	3.0	30
220	Molecular x-ray- and electron-scattering intensities. Physical Review A, 1984, 29, 1108-1113.	2.5	54
221	Approximate solutions of the momentum-space integral SchrÃ¶dinger equation for two-electron atoms. Physical Review A, 1984, 30, 30-34.	2.5	42
222	Bounding and estimation of van der Waals coefficients. Journal of Chemical Physics, 1984, 81, 1919-1928.	3.0	33
223	Partial wave analysis of the momentum density. Journal of Chemical Physics, 1984, 81, 2953-2961.	3.0	27
224	Anisotropic electronic intracule densities for diatomics. International Journal of Quantum Chemistry, 1984, 26, 157-166.	2.0	59
225	Partial-wave analysis of the momentum densities of 14 electron diatomics. International Journal of Quantum Chemistry, 1984, 26, 385-392.	2.0	15
226	Incoherent scattering factors. Journal of Chemical Physics, 1984, 81, 1943-1946.	3.0	16
227	Interatomic forces and Compton profiles. International Journal of Quantum Chemistry, 1983, 23, 227-234.	2.0	13
228	Discrete and continuum contributions to multipole polarizabilities and shielding factors of hydrogen. International Journal of Quantum Chemistry, 1983, 24, 345-352.	2.0	15
229	Basis set quality. II. Information theoretic appraisal of variouss- orbitals. International Journal of Quantum Chemistry, 1983, 24, 527-550.	2.0	54
230	On separation theorems for van der Waals interactions. Chemical Physics Letters, 1983, 97, 37-40.	2.6	3
231	Approximate energy relationships for molecules. Journal of Chemical Physics, 1983, 79, 523-523.	3.0	6
232	Bonding effects on the momentum densities of alkalineâ€“earth oxides. Journal of Chemical Physics, 1983, 79, 3164-3165.	3.0	8
233	Correlations between average atomic numbers and spectroscopic constants of diatomic molecules. The Journal of Physical Chemistry, 1983, 87, 5361-5367.	2.9	6
234	Intermolecular forces via hybrid Hartreeâ€“Fockâ€“SCF plus damped dispersion (HFD) energy calculations. An improved spherical model. Journal of Chemical Physics, 1982, 76, 3057-3063.	3.0	298

#	Article	IF	Citations
235	Angular-correlation coefficients for first-row atoms. Physical Review A, 1982, 25, 1820-1825.	2.5	29
236	Comments on inequalities among atomic expectation values. Journal of Chemical Physics, 1982, 76, 747-748.	3.0	26
237	Momentum space properties of various orbital basis sets used in quantum chemical calculations. International Journal of Quantum Chemistry, 1982, 21, 419-429.	2.0	51
238	Internally folded densities. Chemical Physics, 1981, 63, 175-183.	1.9	69
239	Statistical electron correlation coefficients for the five lowest states of the heliumlike ions. Physical Review A, 1981, 23, 473-478.	2.5	70
240	The generator coordinate method applied to variational perturbation theory. Multipole polarizabilities, spectral sums, and dispersion coefficients for helium. Journal of Chemical Physics, 1981, 75, 4496-4501.	3.0	140
241	Electronic extracule densities. International Journal of Quantum Chemistry, 1981, 20, 393-400.	2.0	9
242	Isotropic and directional Compton profiles for N2, CO and BF. Molecular Physics, 1980, 41, 1143-1151.	1.7	26
243	Extraction of momentum expectation values from Compton profiles. Molecular Physics, 1980, 41, 1153-1162.	1.7	42
244	Model studies of the Tamm-like and field-sustained surface states of germanium. Surface Science, 1978, 74, 168-180.	1.9	19
245	Form factors and total scattering intensities for the helium-like ions from explicitly correlated wavefunctions. Journal of Physics B: Atomic and Molecular Physics, 1978, 11, 3803-3820.	1.6	50
246	N-electron zero-momentum energy expression: A criterion for assessing the accuracy of approximate wave functions. Physical Review A, 1978, 18, 841-844.	2.5	20
247	A technique for increasing the utility of the Wigner-Kirkwood expansion for the second virial coefficient. Molecular Physics, 1978, 36, 887-892.	1.7	17
248	Field-sustained states. Journal of Physics C: Solid State Physics, 1977, 10, L659-L662.	1.5	3
249	Accurate Compton profiles for H2 and D2 including the effects of electron correlation and molecular vibration and rotation. Journal of Chemical Physics, 1977, 67, 3676-3682.	3.0	33
250	Compact and accurate integral-transform wave functions. I. The1S1state of the helium-like ions fromHâ^'throughMg10+. Physical Review A, 1977, 15, 1-15.	2.5	269
251	Compact and accurate integral-transform wave functions. II. The2S1,2S3,2P1, and2P3states of the helium-like ions from He throughMg10+. Physical Review A, 1977, 15, 16-22.	2.5	86
252	Comments on explicitly correlated wave functions for the ground state of the helium atom. Physical Review A, 1977, 16, 1740-1742.	2.5	18

#	ARTICLE	IF	CITATIONS
253	Compact and accurate integral-transform wave functions. III. Radially correlated wave functions for the ground state of the lithium atom. Physical Review A, 1977, 15, 2143-2146.	2.5	12
254	A suggestion concerning modification of the n(R)-6 potential model. Molecular Physics, 1977, 34, 597-599.	1.7	4
255	Accurate charge densities and two-electron intracule functions for the heliumlike ions. Journal of Chemical Physics, 1977, 67, 1191.	3.0	64
256	Mixed-pole terms in the anisotrophy of the long-range interaction coefficients for H2î—¸He and H2î—¸H2. Chemical Physics Letters, 1977, 46, 453-456.	2.6	14
257	The electronâ€"electron cusp condition for the spherical average of the intracule matrix. Chemical Physics Letters, 1976, 42, 476-481.	2.6	120
258	Analytic approximations to the vibrational eigenvalues of the ST potential. Molecular Physics, 1975, 29, 1283-1285.	1.7	0
259	An analysis of energy differences in atomic multiplets in connection with the inequality formulation of Hund's rules. Molecular Physics, 1975, 29, 1861-1875.	1.7	39
260	A strategy for the numerical evaluation of Fourier sine and cosine transforms to controlled accuracy. Computer Physics Communications, 1975, 10, 73-79.	7.5	12
261	Ring and other contributions to the higher virial coefficients. Computer Physics Communications, 1975, 10, 80-85.	7.5	0
262	A new generalized expansion for the potential energy curves of diatomic molecules. Journal of Chemical Physics, 1975, 62, 1693-1701.	3.0	138
263	Molecular interactions in nitrogen and oxygen. Molecular Physics, 1975, 29, 731-744.	1.7	11
264	Atomic interactions in the heavy Noble gases. Molecular Physics, 1974, 27, 191-208.	1.7	19
265	Atomic interactions in neon and helium. Molecular Physics, 1974, 27, 593-604.	1.7	22
266	Mist: A New Interatomic Potential Function. Chemical Physics Letters, 1974, 24, 157-161.	2.6	14
267	Comments on the 14-12-8-6 Potential Function. Canadian Journal of Chemistry, 1974, 52, 2444-2448.	1.1	3
268	On a representation of the long-range interatomic interaction potential. Journal of Physics B: Atomic and Molecular Physics, 1974, 7, L321-L325.	1.6	46
269	Fourier transform of the Morse-V DD potential. Journal of Low Temperature Physics, 1973, 13, 331-335.	1.4	3
270	Natural Analysis of theS2andP2States of the Lithiumlike Ions. Physical Review A, 1973, 7, 1192-1195.	2.5	5

#	Article	IF	Citations
271	Examination of a new intermolecular potential function. Chemical Physics Letters, 1972, 17, 274-276.	2.6	29
272	Intermolecular interactions. , 0, , .		3