Uzi Kaldor

List of Publications by Citations

152 papers	5,673 citations	49 h-index	69 g-index
153 ext. papers	5,883 ext. citations	3 avg, IF	5.58 L-index

#	Paper	IF	Citations
152	The Fock space coupled cluster method: theory and application. *Theoretica Chimica Acta*, **1991**, 80, 427-439		211
151	Open-shell relativistic coupled-cluster method with Dirac-Fock-Breit wave functions: Energies of the gold atom and its cation. *Physical Review A*, **1994**, 49, 1724-1729	2.6	177
150	Formulation and implementation of the relativistic Fock-space coupled cluster method for molecules. *Journal of Chemical Physics*, **2001**, 115, 9720-9726	3.9	174
149	Open-shell coupled-cluster theory applied to atomic and molecular systems. *Chemical Physics Letters*, **1985**, 117, 347-351	2.5	131
148	Ionization potentials and excitation energies of the alkali-metal atoms by the relativistic coupled-cluster method. *Physical Review A*, **1994**, 50, 1121-1128	2.6	113
147	The open-shell coupled-cluster method: Excitation energies and ionization potentials of H2O. *Journal of Chemical Physics*, **1987**, 87, 467-471	3.9	113
146	Transition energies of ytterbium, lutetium, and lawrencium by the relativistic coupled-cluster method. *Physical Review A*, **1995**, 52, 291-296	2.6	110
145	Transition energies of mercury and ekamercury (element 112) by the relativistic coupled-cluster method. *Physical Review A*, **1995**, 52, 2765-2769	2.6	109
144	Ground state electron configuration of element 111. *Physical Review Letters*, **1994**, 73, 3203-3206	7.4	105
143	Intermediate Hamiltonian Fock-space coupled-cluster method: Excitation energies of barium and radium. *Journal of Chemical Physics*, **2000**, 113, 9905-9910	3.9	104
142	Intermediate Hamiltonian Fock-space coupled-cluster method. *Chemical Physics Letters*, **1999**, 313, 399-403	2.5	103
141	A General-Model-Space Diagrammatic Perturbation Theory. *Physica Scripta*, **1980**, 21, 357-361	2.6	102
140	Three-electron excitation in open-shell coupled-cluster theory. *Chemical Physics Letters*, **1985**, 120, 261-265	2.5	101
139	Calculated energy levels of thallium and eka-thallium (element 113). *Physical Review A*, **1996**, 53, 3926-3933	2.6	100
138	Ground state electron configuration of Rutherfordium: Role of dynamic correlation. *Physical Review Letters*, **1995**, 74, 1079-1082	7.4	93
137	Element 118: The First Rare Gas with an Electron Affinity. *Physical Review Letters*, **1996**, 77, 5350-5352	7.4	93
136	Relativistic coupled-cluster method: Intrashell excitations in the f2 shells of Pr+3 and U+4. *Physical Review A*, **1995**, 51, 225-230	2.6	88

135	Relativistic all-electron coupled-cluster calculations on Au2 in the framework of the Douglas-Kroll transformation. *Journal of Chemical Physics*, **2000**, 112, 1809-1813	3.9	83
134	A Fock space coupled cluster study on the electronic structure of the UO(2), UO(2) (+), U(4+), and U(5+) species. *Journal of Chemical Physics*, **2007**, 127, 124308	3.9	82
133	Relativistic all-electron coupled-cluster calculations on the gold atom and gold hydride in the framework of the douglas-kroll transformation. *Chemical Physics Letters*, **1994**, 230, 1-7	2.5	76
132	Electronic structure of eka-lead (element 114) compared with lead. *Journal of Chemical Physics*, **2001**, 114, 2977-2980	3.9	74
131	High-Accuracy Calculations for Heavy and Super-Heavy Elements. *Advances in Quantum Chemistry*, **1998**, 31, 313-336	1.4	73
130	Spin-Optimized Self-Consistent Field Wave Functions. *Physical Review*, **1969**, 183, 1-7		73
129	N2 excitations below 15 eV by the multireference coupled-cluster method. *Journal of Chemical Physics*, **1990**, 92, 3680-3682	3.9	72
128	Quasidegenerate perturbation theory. *The Journal of Physical Chemistry*, **1982**, 86, 2133-2140		71
127	Symmetry breaking in radicals: NO2, NS2 and NO3. *Chemical Physics Letters*, **1991**, 185, 131-135	2.5	70
126	Intruder states and incomplete model spaces in multireference coupled-cluster theory: The 2p2 states of Be. *Physical Review A*, **1988**, 38, 6013-6016	2.6	70
125	The relativistic Fock-space coupled-cluster method for molecules: CdH and its ions. *Journal of Chemical Physics*, **1998**, 108, 3409-3415	3.9	64
124	Extrapolated intermediate Hamiltonian coupled-cluster approach: theory and pilot application to electron affinities of alkali atoms. *Journal of Chemical Physics*, **2005**, 122, 224113	3.9	63
123	Direct calculation of excitation energies by the coupled-cluster method: Mg and Ar atoms. *International Journal of Quantum Chemistry*, **1986**, 30, 445-453	2.1	62
122	Electronic structure theory of the superheavy elements. *Nuclear Physics A*, **2015**, 944, 518-550	1.3	61
121	Open-shell coupled-cluster method: Direct calculation of excitation energies. *Chemical Physics Letters*, **1986**, 128, 45-48	2.5	60
120	The open-shell coupled-cluster method in general model space: Five states of LiH. *Journal of Chemical Physics*, **1988**, 89, 956-958	3.9	60
119	Many-Body Perturbation-Theory Calculations with Finite, Bound Basis Sets. *Physical Review A*, **1973**, 7, 427-434	2.6	60
118	Large relativistic effects in molecular properties of the hydride of superheavy element 111. *Chemical Physics Letters*, **1996**, 250, 461-465	2.5	59

117	Open-Shell coupled-cluster method: Variational and nonvariational calculation of ionization potentials. *International Journal of Quantum Chemistry*, **1986**, 29, 425-433	2.1	58
116	Degenerate many-body perturbation theory: Excited states of H2 . *Journal of Chemical Physics*, **1975**, 63, 2199-2205	3.9	58
115	Mixed-sector intermediate Hamiltonian Fock-space coupled cluster approach. *Journal of Chemical Physics*, **2004**, 121, 6634-9	3.9	57
114	Transition energies of lanthanum, actinium, and eka-actinium (element 121). *Journal of Chemical Physics*, **1998**, 109, 3954-3958	3.9	57
113	Transition energies of barium and radium by the relativistic coupled-cluster method. *Physical Review A*, **1996**, 53, 3050-3056	2.6	54
112	Many-body perturbation theory applied to eight states of BH. *Journal of Chemical Physics*, **1976**, 64, 2002-2009	3.9	54
111	Intermediate Hamiltonian Fock-space coupled cluster method in the one-hole one-particle sector: Excitation energies of xenon and radon. *Journal of Chemical Physics*, **2001**, 115, 6862-6865	3.9	53
110	Many-body perturbation theory applied to H2 . *Journal of Chemical Physics*, **1975**, 62, 4634-4638	3.9	52
109	Degeneracy breaking in the Hilbert-space coupled cluster method. *Journal of Chemical Physics*, **1993**, 98, 3090-3094	3.9	51
108	The ground state geometry of the NO3 radical. *Chemical Physics Letters*, **1990**, 166, 599-601	2.5	51
107	The open-shell coupled-cluster method: Ionization potentials and electron affinities of the alkali atoms, Li to Cs. *Journal of Chemical Physics*, **1987**, 87, 4693-4695	3.9	51
106	Calculation of Extended Hartree-Fock Wavefunctions. *Journal of Chemical Physics*, **1968**, 48, 835-837	3.9	51
105	Many-Body Perturbation-Theory Calculations for Excited Molecular States. *Physical Review Letters*, **1973**, 31, 1338-1340	7.4	51
104	General-model-space perturbation theory: Excitation and ionization of N2. *Journal of Chemical Physics*, **1984**, 81, 2406-2410	3.9	50
103	Benchmark calculations of electron affinities of the alkali atoms sodium to eka-francium (element 119). *Journal of Chemical Physics*, **2001**, 115, 2389-2392	3.9	48
102	Li2 ground and excited states by the open-shell coupled-cluster method. *Chemical Physics*, **1990**, 140, 1-6	2.3	47
101	Open-shell coupled-cluster method: Electron affinities of Li and Na. *Journal of Computational Chemistry*, **1987**, 8, 448-453	3.5	47
100	Intermediate Hamiltonian Fock-space coupled-cluster method. *Advances in Quantum Chemistry*, **2001**, 39, 171-188	1.4	42

99	Relativistic coupled-cluster calculations for open-shell atoms. *Physical Review A*, **1993**, 47, 137-142	2.6	42
98	High sectors in the Fock space coupled-cluster method. *Chemical Physics Letters*, **1992**, 194, 99-104	2.5	42
97	Predicted spectrum of atomic nobelium. *Physical Review A*, **2007**, 75,	2.6	41
96	QED corrections to the binding energy of the eka-radon (Z=118) negative ion. *Physical Review A*, **2003**, 67,	2.6	41
95	Can nondegenerate many-body perturbation theory Be applied to quasidegenerate electronic states?. *International Journal of Quantum Chemistry*, **1985**, 28, 103-108	2.1	40
94	Relativistic coupled-cluster calculations for closed-shell atoms. *Chemical Physics Letters*, **1992**, 194, 95-98	2.5	38
93	Harmonic vibrational frequencies and geometry of NO2 and NO2□ by the multireference coupled-cluster method. *Chemical Physics Letters*, **1990**, 170, 17-20	2.5	38
92	Relativistic coupled cluster method based on Dirac□Coulomb□Breit wavefunctions. Ground state energies of atoms with two to five electrons. *Chemical Physics Letters*, **1994**, 222, 82-87	2.5	37
91	Electronic structure of eka-thorium (element 122) compared with thorium. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2002**, 35, 1693-1700	1.3	36
90	Hilbert space coupled-cluster method in an incomplete model space. *Chemical Physics Letters*, **1992**, 199, 42-46	2.5	36
89	Electron affinities of boron, aluminum, gallium, indium, and thallium. *Physical Review A*, **1997**, 56, 4532-4536	2.6	35
88	The relativistic open shell coupled cluster method: Direct calculation of excitation energies in the Ne atom. *Journal of Chemical Physics*, **1992**, 97, 8455-8458	3.9	35
87	Ground and excited states of K2 and K2+ by the open-shell coupled cluster method. *Journal of Chemical Physics*, **1993**, 98, 7126-7131	3.9	32
86	General-model-space many-body perturbation theory: The (2s3p)P1,3 states in the Be isoelectronic sequence. *Physical Review A*, **1984**, 30, 2932-2935	2.6	32
85	AB initio calculations of electron-molecule scattering cross sections including polarization. *Chemical Physics Letters*, **1977**, 51, 321-324	2.5	32
84	Ionization potentials of alkali atoms: towards meV accuracy. *Chemical Physics*, **2005**, 311, 163-168	2.3	31
83	The shifted scheme in the general-model-space diagrammatic perturbation theory. *Chemical Physics* , **1981**, 62, 469-479	2.3	31
82	Generalized relativistic effective core potential and relativistic coupled cluster calculation of the spectroscopic constants for the HgH molecule and its cation. *Journal of Chemical Physics*, **2001**, 115, 2007-2013	3.9	29

81	The relativistic four-component coupled cluster method for molecules: spectroscopic constants of SnH4. *Chemical Physics Letters*, **1996**, 248, 405-408	2.5	29
80	Spin-Extended Wave Functions for First-Row Atoms. *Physical Review*, **1968**, 176, 19-24		29
79	The relativistic coupled-cluster method: transition energies of bismuth and eka-bismuth. *Molecular Physics*, **1998**, 94, 181-187	1.7	28
78	Intermediate Hamiltonian Hilbert space coupled cluster method: Theory and pilot application. *International Journal of Quantum Chemistry*, **2009**, 109, 2909-2915	2.1	27
77	Spin-Extended Hartree□Fock Functions for Atomic Boron. *Journal of Chemical Physics*, **1968**, 49, 6-8	3.9	27
76	Fock-space coupled-cluster method: The (1,2) sector. *Physical Review A*, **1993**, 47, 4705-4712	2.6	25
75	Spin-Optimized Self-Consistent-Field Function. II. Hyperfine Structure of Atomic Nitrogen. *Physical Review A*, **1970**, 1, 1586-1592	2.6	25
74	Charge transfer excitations in the photoelectron spectrum of Cl□NH3: Experiment and calculation. *Journal of Chemical Physics*, **1993**, 99, 6201-6204	3.9	24
73	Hyperfine Pressure Shift of Hydrogen in Helium. *Journal of Chemical Physics*, **1971**, 55, 4127-4131	3.9	24
72	Relaxation of chlorine anions solvated in small water clusters upon electron photodetachment.: The three lowest potential energy surfaces of the neutral Cl??H2O complex. *Chemical Physics Letters*, **1998**, 293, 309-316	2.5	23
71	First Ionization Potentials of Fm, Md, No, and Lr: Verification of Filling-Up of 5f Electrons and Confirmation of the Actinide Series. *Journal of the American Chemical Society*, **2018**, 140, 14609-14613	16.4	23
70	Rydberg states and the observes spectrum ArH. *Chemical Physics*, **1981**, 63, 165-173	2.3	22
69	Electron affinity of element 114, with comparison to Sn and Pb. *Chemical Physics Letters*, **2009**, 480, 49-51	1.5	21
68	High-accuracy calculation of nuclear quadrupole moments of atomic halogens. *Journal of Chemical Physics*, **2007**, 126, 054301	3.9	21
67	The Fock-space coupled-cluster method: Electron affinities of the five halogen elements with consideration of triple excitations. *Journal of Chemical Physics*, **1993**, 99, 6773-6776	3.9	21
66	Relativistic coupled cluster theory based on the no-pair dirac□oulomb□reit hamiltonian: Relativistic pair correlation energies of the xe atom. *International Journal of Quantum Chemistry*, **1994**, 52, 205-214	2.1	21
65	Multireference coupled cluster and multireference configuration interaction studies of the potential surfaces for deprotonation of NH+4. *Journal of Chemical Physics*, **1989**, 90, 6395-6400	3.9	21
64	An algorithm for generating Goldstone and Bloch-Brandow diagrams. *Journal of Computational Physics*, **1976**, 20, 432-441	4.1	21

63	Spin-Optimized Self-Consistent-Field Function. III. Ground States of Boron and Carbon Atoms. *Physical Review A*, **1970**, 2, 1267-1274	2.6	21
62	Nuclear quadrupole moment of 197Au from high-accuracy atomic calculations. *Journal of Chemical Physics*, **2007**, 126, 184305	3.9	20
61	The Cl⋯NH3, Cl⋯H2O, F⋯NH3 and F⋯H2O clusters and their photoelectron spectra. *Zeitschrift Für Physik D-Atoms Molecules and Clusters*, **1994**, 31, 279-282		20
60	Ultrafast Dynamics of Chlorine⋯Water and Bromine⋯Water Radical Complexes Following Electron Photodetachment in Their Anionic Precursors. *Journal of Physical Chemistry A*, **2000**, 104, 6523-6531	2.8	19
59	The coupled-cluster method with full inclusion of single, double and triple excitations applied to high sectors of the Fock space. *Chemical Physics Letters*, **1993**, 204, 339-342	2.5	19
58	The coupled-cluster method in high sectors of the Fock space. *International Journal of Quantum Chemistry*, **1995**, 55, 127-132	2.1	17
57	Four-Component Electronic Structure Methods. *Challenges and Advances in Computational Chemistry and Physics*, **2010**, 279-349	0.7	16
56	Relativistic Many-Body Calculations on Atoms and Molecules. *Computational Chemistry - Reviews of Current Trends*, **1996**, 1-52		14
55	Ground State of He2 by the Spin-Optimized Method. *Journal of Chemical Physics*, **1972**, 56, 1741-1745	3.9	14
54	Transition energies of Rn- and Fr-like actinide ions by relativistic intermediate Hamiltonian Fock-space coupled-cluster methods. *Chemical Physics*, **2012**, 392, 78-82	2.3	13
53	On the performance of two-component energy-consistent pseudopotentials in atomic Fock-space coupled cluster calculations. *Journal of Chemical Physics*, **2008**, 128, 024106	3.9	13
52	Ab initiocalculations of the ground-state electron affinities of gallium and indium. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **1999**, 32, 5853-5859	1.3	13
51	Vibrational frequencies and geometry of N3 and N3− by the coupled‐cluster method. *International Journal of Quantum Chemistry*, **1990**, 38, 291-294	2.1	13
50	Distinguishable-Electron Method for Electronic Structure Calculations. III. Contact Spin Densities - The S2 and P2 States of Atomic Li. *Physical Review A*, **1971**, 3, 1295-1304	2.6	11
49	Relativistic Four-Component Multireference Coupled Cluster Methods: Towards A Covariant Approach. *Challenges and Advances in Computational Chemistry and Physics*, **2010**, 113-144	0.7	10
48	Potential of the A 1Σu + state of He2. *Molecular Physics*, **1971**, 22, 1107-1117	1.7	10
47	Calculation of Spin Densities for Light Atoms. *Journal of Chemical Physics*, **1968**, 49, 469-470	3.9	9
46	Atomic and Molecular Applications of the Multireference Coupled-Cluster Method. *Lecture Notes in Quantum Chemistry II*, **1989**, 199-213	0.6	9

45	Precision of calculated static polarizabilities: Ga, In and Tl atoms. *Chemical Physics*, **2012**, 395, 104-107	2.3	8
44	Atomic transition energies and the variation of the fine-structure constant *Physical Review A*, **2006**, 74,	2.6	8
43	The open-shell coupled-cluster method: Effect of single excitations on electronic transition energies. *Journal of Chemical Physics*, **1988**, 88, 5248-5249	3.9	8
42	Electronic structure of three-dimensional isotropic quantum dots by four-component relativistic coupled cluster methods. *Journal of Chemical Physics*, **2011**, 134, 054503	3.9	7
41	Study of Heavy Elements by Relativistic Fock Space and Intermediate Hamiltonian Coupled Cluster Methods **2004**, 365-406		7
40	Na2 Ground and Excited States by the Open-Shell Coupled-Cluster Method. *Israel Journal of Chemistry*, **1991**, 31, 345-349	3.4	7
39	Spin-Extended Wave Function for Atomic Sodium. *Physical Review*, **1968**, 176, 71-73		7
38	Electronic Structure at the Edge of the Periodic Table. *Nuclear Physics News*, **2019**, 29, 16-20	0.7	6
37	RELATIVISTIC COUPLED CLUSTER: METHOD AND APPLICATIONS. *Recent Advances in Computational* , **1997**, 125-153		6
36	Impurity effects on the electronic structure and spectra of spherical quantum dots by the 4-component relativistic coupled cluster method. *Computational and Theoretical Chemistry*, **2014**, 1040-1041, 61-71	2	5
35	Accurate Relativistic Fock-Space Calculations for Many-Electron Atoms. *Theoretical and Computational Chemistry*, **2004**, 14, 81-119		5
34	FOUR-COMPONENT RELATIVISTIC COUPLED CLUSTER METHOD AND APPLICATIONS. *Recent Advances in Computational*, **2004**, 283-327		5
33	Spin-extended and configuration-interaction studies of first-row atoms. *International Journal of Quantum Chemistry*, **2009**, 2, 13-20	2.1	4
32	Intermediate Hamiltonian coupled cluster methods: meV accuracy for alkaline earth transition energies. *Computational and Theoretical Chemistry*, **2006**, 768, 127-132		4
31	INTERMEDIATE HAMILTONIAN FOCK-SPACE COUPLED CLUSTER METHOD AND APPLICATIONS. *International Journal of Modern Physics B*, **2003**, 17, 5335-5345	1.1	4
30	Electron-molecule scattering with polarization using the schwinger variational principle. *Chemical Physics Letters*, **1981**, 79, 489-493	2.5	4
29	Electron affinity of gallium and fine structure of Ga Experiment and theory. *Physical Review A*, **2019**, 100,	2.6	4
28	Relativistic coupled cluster calculation of Mssbauer isomer shifts of iodine compounds. *Molecular Physics*, **2017**, 115, 138-143	1.7	3

27	The nuclear quadrupole moment of 69Ga and 115In. *Canadian Journal of Chemistry*, **2009**, 87, 802-805	0.9	3
26	The intrinsic viscosity of a suspension of nonharmonic dumbbells. *Journal of Chemical Physics*, **1977**, 66, 5505-5508	3.9	3
25	INTERMEDIATE HAMILTONIAN FOCK-SPACE COUPLED CLUSTER METHOD AND APPLICATIONS **2002**,		3
24	High-Accuracy Relativistic Coupled Cluster Calculations for the Heaviest Elements **2015**, 1-31		3
23	Applications of the Open-Shell Coupled-Cluster Method. *Lecture Notes in Quantum Chemistry II*, **1989**, 155-164	0.6	3
22	Four-Component Electronic Structure Methods for Atoms. *Progress in Theoretical Chemistry and Physics*, **2003**, 171-210	0.6	3
21	Potential Functions of Al2 by the Relativistic Fock-Space Coupled Cluster Method. *International Journal of Molecular Sciences*, **2002**, 3, 498-507	6.3	2
20	Atomic and molecular applications of the coupled cluster method **1998**, 71-92		2
19	Augmented random phase approximation applied to H2 excitations. *Journal of Chemical Physics*, **1976**, 64, 4812-4814	3.9	2
18	L2-basis-set theory of electron-molecule scattering with vibrational and rotational coupling. *Physical Review A*, **1979**, 19, 105-110	2.6	2
17	Multireference Coupled-Cluster Approach to Spectroscopic Constants: Molecular Geometries and Harmonic Frequencies **1992**, 213-231		2
16	Study of Actinides by Relativistic Coupled Cluster Methods **2015**, 23-54		1
15	High-Accuracy Relativistic Coupled-Cluster Calculations for the Heaviest Elements **2017**, 825-855		1
14	The nuclear quadrupole moments of 191,193,195,197Pb and 139La. *Theoretical Chemistry Accounts*, **2011**, 129, 409-412	1.9	1
13	Bernd A. Hess (ed): Relativistic Effects in Heavy-Element Chemistry and Physics. *Theoretical Chemistry Accounts*, **2003**, 110, 358-358	1.9	1
12	Isaiah Shavitt. *The Journal of Physical Chemistry*, **1996**, 100, 6017-6022		1
11	Ab initio calculation of the He2 A 1□u ++X 1□g + absorption spectrum. *Molecular Physics*, **1973**, 26, 291-295	1.7	1
10	Open-Shell Coupled-Cluster Studies of Atomic and Molecular Systems **1988**, 83-92		1

9	Developments in Multireference Coupled-Cluster Applications to Molecular Systems **1990**, 283-294	1
8	Electronic Structure of the Transactinide Atoms **2018**, 1-16	1
7	Relativistic Coupled Cluster Calculations **1995**, 135-142	1
6	RELATIVISTIC COUPLED CLUSTER CALCULATIONS FOR HEAVY AND SUPER-HEAVY ELEMENTS **2002**, 260-292	0
5	Multireference many-body methods. Perspective on linked-cluster expansions for the nuclear many-body problem *Theoretical Chemistry Accounts*, **2000**, 103, 276-277	1.9
4	Multireference many-body methods. Perspective on linked-cluster expansions for the nuclear many-body problem **2000**, 276-277	
3	Direct Calculation of Molecular Transition Energies by the Open-Shell Coupled-Cluster Method **1988**, 197-208	
2	The Fock-Space Coupled Cluster Method Extended to Higher Sectors **1993**, 385-394	
1	Nonempirical Polarization in Low-Energy Electron-Molecule Scattering Theory **1979**, 123-131	