Ephraim Eliav

List of Publications by Year
in descending order

92	4,312	76294	114418
papers	citations	40 h-index	63 g-index

95	95	95	1584
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Formulation and implementation of the relativistic Fock-space coupled cluster method for molecules. Journal of Chemical Physics, 2001, 115, 9720-9726.	1.2	207
2	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.	1.0	195
3	The DIRAC code for relativistic molecular calculations. Journal of Chemical Physics, 2020, 152, 204104.	1.2	191
4	Measurement of the first ionization potential of lawrencium, element 103. Nature, 2015, 520, 209-211.	13.7	129
5	Ionization potentials and excitation energies of the alkali-metal atoms by the relativistic coupled-cluster method. Physical Review A, 1994, 50, 1121-1128.	1.0	117
6	Transition energies of ytterbium, lutetium, and lawrencium by the relativistic coupled-cluster method. Physical Review A, 1995, 52, 291-296.	1.0	117
7	Ground State Electron Configuration of Element 111. Physical Review Letters, 1994, 73, 3203-3206.	2.9	116
8	Transition energies of mercury and ekamercury (element 112) by the relativistic coupled-cluster method. Physical Review A, 1995, 52, 2765-2769.	1.0	114
9	Intermediate Hamiltonian Fock-space coupled-cluster method. Chemical Physics Letters, 1999, 313, 399-403.	1.2	111
10	Intermediate Hamiltonian Fock-space coupled-cluster method: Excitation energies of barium and radium. Journal of Chemical Physics, 2000, 113, 9905-9910.	1.2	111
11	Calculated energy levels of thallium and eka-thallium (element 113). Physical Review A, 1996, 53, 3926-3933.	1.0	109
12	Element 118: The First Rare Gas with an Electron Affinity. Physical Review Letters, 1996, 77, 5350-5352.	2.9	105
13	Ground State Electron Configuration of Rutherfordium: Role of Dynamic Correlation. Physical Review Letters, 1995, 74, 1079-1082.	2.9	101
14	Relativistic coupled-cluster method: Intrashell excitations in thef2shells ofPr+3andU+4. Physical Review A, 1995, 51, 225-230.	1.0	89
15	A Fock space coupled cluster study on the electronic structure of the UO2, UO2+, U4+, and U5+ species. Journal of Chemical Physics, 2007, 127, 124308.	1.2	88
16	Electronic structure of eka-lead (element 114) compared with lead. Journal of Chemical Physics, 2001, 114, 2977-2980.	1.2	79
17	High-Accuracy Calculations for Heavy and Super-Heavy Elements. Advances in Quantum Chemistry, 1998, 31, 313-336.	0.4	77
18	Relativistic Coupled Cluster Calculations with Variational Quantum Electrodynamics Resolve the Discrepancy between Experiment and Theory Concerning the Electron Affinity and Ionization Potential of Gold. Physical Review Letters, 2017, 118, 023002.	2.9	73

#	Article	IF	Citations
19	The relativistic Fock-space coupled-cluster method for molecules: CdH and its ions. Journal of Chemical Physics, 1998, 108, 3409-3415.	1.2	72
20	Prediction of the adsorption behavior of elements 112 and 114 on inert surfaces from ab initio Dirac-Coulomb atomic calculations. Journal of Chemical Physics, 2008, 128, 024707.	1.2	72
21	Electronic structure theory of the superheavy elements. Nuclear Physics A, 2015, 944, 518-550.	0.6	69
22	Extrapolated intermediate Hamiltonian coupled-cluster approach: Theory and pilot application to electron affinities of alkali atoms. Journal of Chemical Physics, 2005, 122, 224113.	1.2	67
23	Identification of the Predicted<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>5</mml:mn><mml:mi>s</mml:mi><mml:mtext>â^'</mml:mtext><mml:mn>4</mml:mn><mml: Crossing Optical Lines with Applications to Metrology and Searches for the Variation of Fundamental Constants. Physical Review Letters, 2015, 114, 150801.	2.9	67
24	Transition energies of lanthanum, actinium, and eka-actinium (element 121). Journal of Chemical Physics, 1998, 109, 3954-3958.	1.2	63
25	Probing Sizes and Shapes of Nobelium Isotopes by Laser Spectroscopy. Physical Review Letters, 2018, 120, 232503.	2.9	63
26	Benchmarking Electronic Structure Calculations on the Bare UO₂²⁺ Ion: How Different are Single and Multireference Electron Correlation Methods?. Journal of Physical Chemistry A, 2009, 113, 12504-12511.	1.1	62
27	Laser-coolable polyatomic molecules with heavy nuclei. Journal of Physics B: Atomic, Molecular and Optical Physics, 2017, 50, 225101.	0.6	62
28	Transition energies of barium and radium by the relativistic coupled-cluster method. Physical Review A, 1996, 53, 3050-3056.	1.0	58
29	Mixed-sector intermediate Hamiltonian Fock-space coupled cluster approach. Journal of Chemical Physics, 2004, 121, 6634-6639.	1.2	58
30	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.	1.2	56
31	Benchmark calculations of electron affinities of the alkali atoms sodium to eka-francium (element) Tj ETQq1 1 0.784314 rgBT /Overlo	1.2	53
32	QED corrections to the binding energy of the eka-radon(Z=118)negative ion. Physical Review A, 2003, 67, .	1.0	50
33	Enhancement factor for the electric dipole moment of the electron in the BaOH and YbOH molecules. Physical Review A, 2019, 99, .	1.0	50
34	Intermediate Hamiltonian Fock-space coupled-cluster method. Advances in Quantum Chemistry, 2001, 39, 171-188.	0.4	49
35	Transition energies of atomic lawrencium. European Physical Journal D, 2007, 45, 115-119.	0.6	48
36	Adsorption of inert gases including element 118 on noble metal and inert surfaces from ab initio Diracâ€“Coulomb atomic calculations. Journal of Chemical Physics, 2008, 129, 144106.	1.2	48

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37	Comparison of relativistic effective core potential and all-electron Dirac-Coulomb calculations of mercury transition energies by the relativistic coupled-cluster method. Journal of Physics B: Atomic, Molecular and Optical Physics, 2000, 33, 667-676.	0.6	46
38	Ionization potentials and electron affinities of the superheavy elements 115â€“117 and their sixth-row homologues Bi, Po, and At. Physical Review A, 2015, 91, .	1.0	45
39	Relativistic coupled cluster method based on Diracâ€”Coulombâ€”Breit wavefunctions. Ground state energies of atoms with two to five electrons. Chemical Physics Letters, 1994, 222, 82-87.	1.2	43
40	The electron affinity of astatine. Nature Communications, 2020, 11, 3824.	5.8	42
41	Electronic structure of eka-thorium (element 122) compared with thorium. Journal of Physics B: Atomic, Molecular and Optical Physics, 2002, 35, 1693-1700.	0.6	41
42	Analysis of the fine structure of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mrow><mml:mi>Sn</mml:mi></mml:mrow><mml:mrow><m by optical spectroscopy in an electron-beam ion trap. Physical Review A, 2016, 94, .	1.0	41
43	Electron affinities of boron, aluminum, gallium, indium, and thallium. Physical Review A, 1997, 56, 4532-4536.	1.0	37
44	Atomic Properties of Element 113 and Its Adsorption on Inert Surfaces from ab Initio Diracâ^'Coulomb Calculations. Journal of Physical Chemistry A, 2008, 112, 13712-13716.	1.1	36
45	The relativistic four-component coupled cluster method for molecules: spectroscopic constants of SnH4. Chemical Physics Letters, 1996, 248, 405-408.	1.2	33
46	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.	1.2	33
47	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.	6.6	33
48	Ionization potentials of alkali atoms: towards meV accuracy. Chemical Physics, 2005, 311, 163-168.	0.9	32
49	Bonding in the homologous series CsAu, CsAg, and CsCu studied at the 4-component density functional theory and coupled cluster levels. Journal of Chemical Physics, 2003, 119, 9355-9363.	1.2	30
50	The electronic structure of the triiodide ion from relativistic correlated calculations: A comparison of different methodologies. Journal of Chemical Physics, 2010, 133, 064305.	1.2	29
51	Approximate relativistic coupled-cluster calculations on heavy alkali-metal diatomics: Application to the spin-orbit-coupled <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msup><mml:mi>A</mml:mi><mml:mn>1</mml:mn></mml:msup></mml:mrow></mml:math mathvariant="normal">Î£</mml:mi><mml:mo>+</mml:mo></mml:msup></mml:mrow></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msup><mml:mi>b</mml:mi><mml:mn>3</mml:mn></mml:msup>	1.0	28
52	Relativistic coupled cluster theory based on the no-pair dirac-coulomb-breit hamiltonian: Relativistic pair correlation energies of the xe atom. International Journal of Quantum Chemistry, 1994, 52, 205-214.	1.0	27
53	Intermediate Hamiltonian Hilbert space coupled cluster method: Theory and pilot application. International Journal of Quantum Chemistry, 2009, 109, 2909-2915.	1.0	27
54	Large Shape Staggering in Neutron-Deficient Bi Isotopes. Physical Review Letters, 2021, 127, 192501.	2.9	27

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55	Relativistic Fock Space Coupled Cluster Method for Many-Electron Systems: Non-Perturbative Account for Connected Triple Excitations. Symmetry, 2020, 12, 1101.	1.1	26
56	Enhanced P,T-violating nuclear magnetic quadrupole moment effects in laser-coolable molecules. Journal of Chemical Physics, 2020, 152, 084303.	1.2	26
57	Accuracy of RCC-SD and PT2/CI methods in all-electron and RECP calculations on Pb and Pb2+. Journal of Physics B: Atomic, Molecular and Optical Physics, 2000, 33, 5139-5149.	0.6	25
58	Ab initio studies of atomic properties and experimental behavior of element 119 and its lighter homologs. Journal of Chemical Physics, 2013, 138, 124302.	1.2	25
59	Electron affinity of element 114, with comparison to Sn and Pb. Chemical Physics Letters, 2009, 480, 49-51.	1.2	23
60	High-accuracy calculation of nuclear quadrupole moments of atomic halogens. Journal of Chemical Physics, 2007, 126, 054301.	1.2	22
61	Nuclear quadrupole moment of Au197 from high-accuracy atomic calculations. Journal of Chemical Physics, 2007, 126, 184305.	1.2	20
62	Electronic Transition Dipole Moments in Relativistic Coupled-Cluster Theory: the Finite-Field Method. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2018, 124, 451-456.	0.2	18
63	Hyperfine Structure Constants on the Relativistic Coupled Cluster Level with Associated Uncertainties. Journal of Physical Chemistry A, 2020, 124, 3157-3169.	1.1	18
64	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.	0.6	17
65	Transition energies of Rn- and Fr-like actinide ions by relativistic intermediate Hamiltonian Fock-space coupled-cluster methods. Chemical Physics, 2012, 392, 78-82.	0.9	16
66	Nuclear anapole moment interaction in BaF from relativistic coupled-cluster theory. Physical Review A, 2018, 98, .	1.0	16
67	Relativistic Four-Component Multireference Coupled Cluster Methods: Towards A Covariant Approach. Challenges and Advances in Computational Chemistry and Physics, 2010, , 113-144.	0.6	15
68	PadÃ© extrapolated effective Hamiltonians in the Fock space relativistic coupled cluster method. International Journal of Quantum Chemistry, 2018, 118, e25772.	1.0	15
69	High-precision ab initio calculations of the spectrum of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mrow><mml:mi>Lr</mml:mi></mml:mrow><mml:mo>+</mml:mo></m Physical Review A, 2019, 100, .	1.0	15
70	Electron affinity of oganesson. Physical Review A, 2021, 104, .	1.0	15
71	Relativistic coupled cluster study of diatomic compounds of Hg, Cn, and Fl. Journal of Chemical Physics, 2014, 141, 084301.	1.2	13
72	Diagonal and off-diagonal hyperfine structure matrix elements in KCs within the relativistic Fock space coupled cluster theory. Chemical Physics Letters, 2020, 756, 137825.	1.2	13

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73	Towards High Performance Relativistic Electronic Structure Modelling: The EXP-T Program Package. Communications in Computer and Information Science, 2020, , 375-386.	0.4	12
74	Nuclear spin-dependent parity-violating effects in light polyatomic molecules. Physical Review A, 2020, 102, .	1.0	12
75	Finite-Field Calculations of Transition Properties by the Fock Space Relativistic Coupled Cluster Method: Transitions between Different Fock Space Sectors. Symmetry, 2020, 12, 1845.	1.1	11
76	Ionization potentials and electron affinities of Rg, Cn, Nh, and Fl superheavy elements. Physical Review A, 2022, 105, .	1.0	11
77	Resolving all-order method convergence problems for atomic physics applications. Physical Review A, 2011, 83, .	1.0	10
78	Systematic study and uncertainty evaluation of P, T-odd molecular enhancement factors in BaF. Journal of Chemical Physics, 2021, 155, 034309.	1.2	10
79	Ab initio study and assignment of electronic states in molecular RaCl. Journal of Quantitative Spectroscopy and Radiative Transfer, 2021, 269, 107649.	1.1	10
80	Precision of calculated static polarizabilities: Ga, In and Tl atoms. Chemical Physics, 2012, 395, 104-107.	0.9	9
81	Electronic Structure at the Edge of the Periodic Table. Nuclear Physics News, 2019, 29, 16-20.	0.1	9
82	Ab initio calculations of the spectrum of lawrencium. Physical Review A, 2021, 104, .	1.0	9
83	Accurate Relativistic Fock-Space Calculations for Many-Electron Atoms. Theoretical and Computational Chemistry, 2004, 14, 81-119.	0.2	7
84	Energy-level structure of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mrow><mml:mi>Sn</mml:mi></mml:mrow><mml:mrow><m Physical Review A, 2018, 98, .	1.0	7
85	FOUR-COMPONENT RELATIVISTIC COUPLED CLUSTER â€" METHOD AND APPLICATIONS. Recent Advances in Computational, 2004, , 283-327.	0.8	5
86	INTERMEDIATE HAMILTONIAN FOCK-SPACE COUPLED CLUSTER METHOD AND APPLICATIONS. International Journal of Modern Physics B, 2003, 17, 5335-5345.	1.0	4
87	Intermediate Hamiltonian coupled cluster methods: meV accuracy for alkaline earth transition energies. Computational and Theoretical Chemistry, 2006, 768, 127-132.	1.5	4
88	Relativistic coupled cluster calculation of MÃ¶ssbauer isomer shifts of iodine compounds. Molecular Physics, 2017, 115, 138-143.	0.8	3
89	INTERMEDIATE HAMILTONIAN FOCK-SPACE COUPLED CLUSTER METHOD AND APPLICATIONS. , 2002, , .		3
90	RELATIVISTIC COUPLED CLUSTER CALCULATIONS FOR HEAVY AND SUPER-HEAVY ELEMENTS. , 2002, , 260-292.		2

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91	The nuclear quadrupole moments of 191,193,195,197Pb and 139La. Theoretical Chemistry Accounts, 2011, 129, 409-412.	0.5	2
92	High-accuracy coupled cluster calculations of atomic properties. , 2015, , .		0