

Vladimir KellÄ

List of Publications by Year in descending order

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103
papers

2,830
citations

147801

31
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214800

47
g-index

103
all docs

103
docs citations

103
times ranked

1455
citing authors

#	ARTICLE	IF	CITATIONS
1	Electron Correlation in Molecules. , 1987, , 117-250.		165
2	Picture change and calculations of expectation values in approximate relativistic theories. International Journal of Quantum Chemistry, 1998, 68, 159-174.	2.0	132
3	Estimates of relativistic contributions to molecular properties. Journal of Chemical Physics, 1990, 93, 8122-8132.	3.0	99
4	The fourth order diagrammatic MBPT calculations of the correlation energy of ten electron systems. Journal of Chemical Physics, 1980, 72, 3378-3385.	3.0	95
5	Ionization potentials and electron affinities of Cu, Ag, and Au: Electron correlation and relativistic effects. International Journal of Quantum Chemistry, 1997, 63, 557-565.	2.0	94
6	Relativistic effects on electric properties of many-electron systems in spin-averaged Douglas-Kroll and Pauli approximations. Journal of Chemical Physics, 1996, 105, 1995-2003.	3.0	88
7	Theoretical study of PbO and the PbO anion. Chemical Physics Letters, 2005, 408, 210-215.	2.6	86
8	Electric quadrupole moment of the ²⁷ Al nucleus: Converging results from the AlF and AlCl molecules and the Al atom. Chemical Physics Letters, 1999, 304, 414-422.	2.6	73
9	Improved Mechanistic Model of the Atmospheric Redox Chemistry of Mercury. Environmental Science & Technology, 2021, 55, 14445-14456.	10.0	65
10	Perturbation theory of the electron correlation effects for atomic and molecular properties. VII. Complete fourth-order MBPT study of the dipole moment and dipole polarizability of H ₂ O. Journal of Chemical Physics, 1983, 79, 2918-2923.	3.0	63
11	Polarized basis sets for high-level-correlated calculations of molecular electric properties. Theoretica Chimica Acta, 1995, 91, 353-371.	0.8	62
12	Standardized Medium-Size Basis Sets for Calculations of Molecular Electric Properties: Group IIIA. Collection of Czechoslovak Chemical Communications, 2003, 68, 211-239.	1.0	61
13	Relativistic effects in atomic and molecular properties. Acta Physica Slovaca, 2010, 60, .	1.4	58
14	Medium-size polarized basis sets for high-level-correlated calculations of molecular electric properties. Theoretica Chimica Acta, 1992, 83, 351-366.	0.8	53
15	Standardized basis sets for high-level-correlated relativistic calculations of atomic and molecular electric properties in the spin-averaged Douglas-Kroll (no-pair) approximation. Theoretica Chimica Acta, 1996, 94, 93.	0.8	51
16	Linear and nonlinear optical properties of a series of Ni-dithiolene derivatives. Journal of Chemical Physics, 2009, 131, 134312.	3.0	50
17	Inclusion of mean-field spin-orbit effects based on all-electron two-component spinors: Pilot calculations on atomic and molecular properties. Journal of Chemical Physics, 2001, 115, 9667-9674.	3.0	48
18	Polarization functions for gaussian basis sets for the first row atoms. Theoretica Chimica Acta, 1977, 45, 205-213.	0.8	47

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19	Nuclear quadrupole moments of bromine and iodine from combined atomic and molecular data. <i>Physical Review A</i> , 2001, 64, .	2.5	46
20	Polarized basis sets for high-level-correlated calculations of molecular electric properties. <i>Theoretica Chimica Acta</i> , 1996, 93, 101-129.	0.8	41
21	Electron-correlation and relativistic contributions to atomic dipole polarizabilities: Alkali-metal atoms. <i>Physical Review A</i> , 1993, 47, 1715-1725.	2.5	40
22	Standardized basis sets for high-level-correlated relativistic calculations of atomic and molecular electric properties in the spin-averaged Douglas-Kroll approximation. <i>Theoretical Chemistry Accounts</i> , 1997, 96, 166-175.	1.4	40
23	Determination of the quadrupole moment of the halogen nuclei (Cl,Br,I) from molecular data. <i>Molecular Physics</i> , 1996, 89, 127-137.	1.7	38
24	The ground state potential energy. Curve of Be ₂ : Is the MBPT approach capable of predicting it?. <i>Chemical Physics</i> , 1985, 96, 59-79.	1.9	37
25	The quadrupole moment of the 3s ² nuclear ground state of Au ¹⁹⁷ from electric field gradient relativistic coupled cluster and density-functional theory of small molecules and the solid state. <i>Journal of Chemical Physics</i> , 2005, 122, 124317.	3.0	37
26	Relativistic contributions to molecular electric-field gradients in hydrogen halides. <i>Chemical Physics Letters</i> , 1990, 174, 641-648.	2.6	36
27	Polarizabilities of confined two-electron systems: the 2-electron quantum dot, the hydrogen anion, the helium atom and the lithium cation. <i>Molecular Physics</i> , 2005, 103, 2747-2761.	1.7	36
28	Nuclear quadrupole moments from molecular microwave data: The quadrupole moment of ⁸⁵ Rb and ⁸⁷ Rb nuclei and survey of molecular data for alkali-metal nuclei. <i>Physical Review A</i> , 1999, 60, 3575-3585.	2.5	34
29	Optimized virtual orbitals for relativistic calculations: an alternative approach to the basis set construction for correlation calculations. <i>Molecular Physics</i> , 2006, 104, 2277-2292.	1.7	34
30	Fourth-order MB-RSPT calculations of the spectroscopic constants and potential energy curve of F ₂ . <i>Theoretica Chimica Acta</i> , 1983, 62, 549-562.	0.8	32
31	Quadrupole moments of CuH, AgH, and AuH. A study of the electron correlation and relativistic effects. <i>Journal of Chemical Physics</i> , 1991, 95, 8248-8253.	3.0	32
32	Accuracy assessment of the ROHF + CCSD(T) calculations of static dipole polarizabilities of diatomic radicals: O ₂ , CN, and NO. <i>Computational and Theoretical Chemistry</i> , 2001, 547, 219-232.	1.5	31
33	MBPT studies of van der Waals molecules. III. The reliability of apparently accurate calculations for the magnesium dimer. <i>Chemical Physics</i> , 1986, 103, 55-74.	1.9	30
34	A theoretical study of the $\text{A}^{\infty} \text{I}^{\dagger} \text{X}^{\infty} \text{I}^{\dagger} \text{S}$ -system of SiH ⁺ . <i>Journal of Chemical Physics</i> , 1988, 89, 423-432.	3.0	30
35	The quadrupole moment of the K and K nuclei from microwave data for KF and KCl. <i>Chemical Physics Letters</i> , 1998, 292, 403-410.	2.6	30
36	Theoretical study of molecular properties of low-lying electronic excited states of H ₂ and H ₂ S. <i>Molecular Physics</i> , 2008, 106, 2333-2344.	1.7	30

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37	Finite-field many-body perturbation theory. <i>Molecular Physics</i> , 1983, 49, 711-725.	1.7	28
38	Calculation of the correlation energy of molecules by many-body rayleigh-schrödinger perturbation theory up to third order. <i>Chemical Physics Letters</i> , 1977, 51, 170-174.	2.6	27
39	Perturbation theory of the electron correlation effects for atomic and molecular properties VI. Complete active space (CAS) SCF and MBPT calculations of electric properties of the FH molecule. <i>Chemical Physics</i> , 1983, 77, 93-101.	1.9	27
40	The nuclear quadrupole moment of from molecular data for ZrO and ZrS. <i>Chemical Physics Letters</i> , 2000, 318, 222-231.	2.6	27
41	A study of the performance of high-level correlated methods: The energy, dipole moment, and polarizability functions of CO. <i>Chemical Physics Letters</i> , 1988, 152, 387-392.	2.6	26
42	Electric dipole polarizabilities of negative ions of the coinage metal atoms. <i>Chemical Physics Letters</i> , 1996, 253, 383-389.	2.6	25
43	The nuclear quadrupole moment of ⁴⁵ Sc. <i>Chemical Physics Letters</i> , 2000, 329, 112-118.	2.6	25
44	Nuclear quadrupole moments of Kr and Xe from molecular data. <i>Chemical Physics Letters</i> , 2001, 346, 155-159.	2.6	25
45	Complete fourth-order many-body perturbation theory calculations of the dipole moment and dipole polarizability of FH. <i>Chemical Physics Letters</i> , 1983, 95, 226-231.	2.6	24
46	Activation barriers of SN2 reactions: F ⁺ + CH3F and H ⁺ + CH3F. Fourth-order MB RSPT calculations. <i>Chemical Physics Letters</i> , 1984, 105, 625-629.	2.6	24
47	Electric properties of the chloride ion. <i>Theoretica Chimica Acta</i> , 1988, 74, 185-194.	0.8	24
48	Electron correlation and relativistic effects in the coinage metal compounds. II. Heteronuclear dimers: CuAg, CuAu, and AgAu. <i>Journal of Chemical Physics</i> , 1995, 103, 2991-2999.	3.0	24
49	The point charge model of nuclear quadrupoles: How and why does it work. <i>Journal of Chemical Physics</i> , 2000, 112, 522-526.	3.0	24
50	Quasirelativistic studies of molecular electric properties: Dipole moments of the group IVa oxides and sulfides. <i>Journal of Chemical Physics</i> , 1993, 98, 1345-1351.	3.0	23
51	Correlation effects and bond-correlation energies in the series of molecules including C1 to C4 hydrocarbons. Fourth-order MB-RSPT (many-body Rayleigh-Schroedinger perturbation theory) calculations. <i>Journal of the American Chemical Society</i> , 1984, 106, 5864-5871.	13.7	22
52	Standardized basis sets for high-level-correlated relativistic calculations of atomic and molecular electric properties in the spin-averaged Douglas-Kroll (no-pair) approximation I. Groups Ib and IIb. <i>Theoretica Chimica Acta</i> , 1996, 94, 93-104.	0.8	21
53	The change of picture of the Hellmann-Feynman force operator in approximate relativistic methods. <i>Computational and Theoretical Chemistry</i> , 2001, 547, 35-53.	1.5	21
54	Quadrupole moments of Cd and Zn nuclei: When solid-state, molecular, atomic, and nuclear theory meet. <i>Europhysics Letters</i> , 2017, 117, 62001.	2.0	21

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55	Many-Body Rayleigh-Schrödinger Perturbation calculations of the correlation energy of open shell molecules in the restricted Roothaan-Hartree-Fock formalism. Application to heats of reaction and energies of activation. <i>Theoretica Chimica Acta</i> , 1980, 56, 315-328.	0.8	20
56	Electron correlation and relativistic contributions to dipole moments of heavy oxides and sulfides: SnO, PbO, SnS, and PbS. <i>Journal of Chemical Physics</i> , 1998, 108, 2056-2066.	3.0	20
57	Fourth-order diagrammatic MB-RSPT calculations of the correlation energy: N ₂ , CO, F ₂ and the reaction energy of the process $\frac{1}{2}F_2 + \frac{1}{2}H_2 = HF$. <i>International Journal of Quantum Chemistry</i> , 1980, 18, 1431-1448.	2.0	19
58	Electron correlation and relativistic contributions to molecular electric properties: dipole and quadrupole moments of cyanogen halides. <i>Molecular Physics</i> , 1992, 75, 209-220.	1.7	18
59	Interaction potentials in rare gas-halide ion systems. <i>Chemical Physics</i> , 1991, 157, 123-133.	1.9	17
60	The (hyper)polarizabilities of AuXeF and XeAuF. <i>Chemical Physics Letters</i> , 2009, 472, 185-189.	2.6	17
61	Polarized basis sets for high-level-correlated calculations of molecular electric properties. <i>Theoretica Chimica Acta</i> , 1995, 91, 353.	0.8	15
62	Electron correlation and relativistic effects in the coinage metal compounds. <i>Theoretica Chimica Acta</i> , 1995, 92, 253.	0.8	14
63	The nuclear quadrupole moment of data ⁷³ Ge from molecular microwave. <i>Molecular Physics</i> , 1999, 96, 275-281.	1.7	14
64	Electric field gradients from shifted-nucleus calculations: An alternative to the point charge nuclear quadrupole moment model. <i>Journal of Chemical Physics</i> , 2004, 120, 9424-9426.	3.0	13
65	Applications of perturbation theory to the chemical problems potential energy curves of BH, F ₂ and N ₂ . <i>Molecular Physics</i> , 1979, 38, 1621-1633.	1.7	12
66	Accuracy in ab initio reaction-energy computations. 1. Compounds of first-row elements. <i>The Journal of Physical Chemistry</i> , 1990, 94, 5694-5710.	2.9	12
67	Electron correlation and relativistic effects in electric properties of the alkali metal fluorides. <i>Molecular Physics</i> , 1999, 96, 179-187.	1.7	12
68	Ab initio MB RSPT calculations of barriers of non-rigid rearrangements of complex hydrides LiBH ₄ and Li ₂ BeH ₄ . <i>Chemical Physics Letters</i> , 1984, 106, 455-459.	2.6	11
69	Can the coupled cluster method improve many-body perturbation theory reaction energies significantly? the H ₂ CO → H ₂ + CO reaction. <i>Chemical Physics Letters</i> , 1987, 135, 346-351.	2.6	11
70	The effect of disconnected wavefunction clusters of double excitations on the correlation energy of molecules. <i>Chemical Physics Letters</i> , 1979, 62, 584-588.	2.6	10
71	Dipole moments calculations of transition metal mononitrides: ScN, TiN, VN, and CrN: Limits of the CCSD(T) method. <i>International Journal of Quantum Chemistry</i> , 2002, 90, 1240-1248.	2.0	9
72	The beryllium atom-water molecule interaction A many-body perturbation theory study. <i>Chemical Physics Letters</i> , 1990, 174, 19-24.	2.6	8

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73	The Nuclear Quadrupole Moment of ¹⁴ N from Accurate Electric Field Gradient Calculations and Microwave Spectra of NP Molecule. Collection of Czechoslovak Chemical Communications, 2007, 72, 64-82.	1.0	8
74	The nuclear quadrupole moment of ⁷³ Ge from molecular microwave data. Molecular Physics, 1999, 96, 275-281.	1.7	7
75	An ab initio Investigation of the dipole moment of the CO ₂ ⋯CO complex. Chemical Physics Letters, 2000, 319, 231-237.	2.6	7
76	Electric properties of hydrogen iodide: Reexamination of correlation and relativistic effects. Theoretical Chemistry Accounts, 2003, 110, 176-184.	1.4	7
77	The quadrupole moment of the Sb nucleus from molecular microwave data and calculated relativistic electric-field gradients. Journal of Chemical Physics, 2006, 124, 184308.	3.0	7
78	The quadrupole moment of the As nucleus from molecular microwave data and calculated relativistic electric field gradients. Chemical Physics Letters, 2010, 498, 10-13.	2.6	7
79	Ab initio calculations of molecular properties of low-lying electronic states of 2-cyclopentenone – link with biological activity. Journal of Molecular Modeling, 2012, 18, 4751-4759.	1.8	7
80	Off-Center Gaussian Functions, an Alternative Atomic Orbital Basis Set for Accurate Noncovalent Interaction Calculations of Large Systems. Journal of Chemical Theory and Computation, 2013, 9, 5296-5304.	5.3	7
81	Scaling in second order electron correlation calculations of potential energy curves and spectroscopic constants. Molecular Physics, 1983, 50, 1323-1333.	1.7	6
82	Ab initio studies of chemical equilibria. Application of many-body rayleigh-schrödinger perturbation theory up to third order to the proton affinity of water. Chemical Physics Letters, 1978, 58, 83-86.	2.6	5
83	Ab initio studies of chemical equilibria. Equilibria containing first row hydrides AH ₂ , AH ₃ , and AH ₄ and their positive ions. Chemical Physics Letters, 1978, 53, 555-559.	2.6	5
84	Some Trends in Relativistic and Electron Correlation Effects in Electric Properties of Small Molecules. Advances in Quantum Chemistry, 2005, 50, 249-269.	0.8	5
85	Ab initio studies of chemical equilibria. A refined approach to the reaction NH ₂ ⁺ + H ₂ ⇌ NH ₃ + H ⁺ . Chemical Physics Letters, 1979, 61, 85-87.	2.6	4
86	Static dipole polarizabilities and hyperpolarizabilities of dicyanopolyacetylenes. Chemical Physics Letters, 1998, 287, 509-514.	2.6	4
87	Relativistic effects in low-lying electronic states of iron. Theoretical Chemistry Accounts, 2011, 129, 561-566.	1.4	4
88	A CAS SCF study of reactive interactions between Be(3 P) and H ₂ (1 ^g +). Theoretica Chimica Acta, 1992, 81, 417-424.	0.8	3
89	Simple sparse matrix multiplication algorithm. Computer Physics Communications, 1995, 85, 213-216.	7.5	3
90	Ionization potentials and electron affinities of Cu, Ag, and Au: Electron correlation and relativistic effects. , 1997, 63, 557.		3

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91	Interactions of ions. Ab initio SCF-MO-LCAO calculations of Li+H ₂ O-OH- with a minimal Gaussian basis set. Collection of Czechoslovak Chemical Communications, 1975, 40, 587-596.	1.0	3
92	Fourth-order diagrammatic MB-RSPT calculations of the interaction energy between two helium atoms. Theoretica Chimica Acta, 1981, 59, 309-317.	0.8	2
93	Quasi-relativistic coupled cluster calculations of electric dipole moments and dipole polarizabilities of GeO, SnO, and PbO. Journal of Computational Methods in Sciences and Engineering, 2004, 4, 753-764.	0.2	2
94	Role of relativity in energy pattern of low-lying terms of Fe, Ru and Os. Computational and Theoretical Chemistry, 2016, 1084, 157-161.	2.5	2
95	Polarized basis sets for high-level-correlated calculations of molecular electric properties. Theoretica Chimica Acta, 1996, 93, 101.	0.8	2
96	Electron correlation and relativistic effects in the coinage metal compounds. Theoretica Chimica Acta, 1995, 92, 253-267.	0.8	1
97	Relativistic and Electron Correlation Effects as a Tool for Explaining Some Trends in Molecular Properties and Interactions. Computing Letters, 2006, 1, 259-265.	0.5	1
98	Relativistic calculations of low-lying electronic states of ruthenium and osmium. Journal of Physics B: Atomic, Molecular and Optical Physics, 2014, 47, 025001.	1.5	1
99	Relativistic calculations of AuSi + and AuSi $\hat{\sigma}$. International Journal of Quantum Chemistry, 2019, 119, e25951.	2.0	1
100	<sc>AuSi</sc> molecule revisited: <sc>IOTC</sc>/<sc>CASSCF</sc>/<sc>CASPT2</sc> calculations. International Journal of Quantum Chemistry, 2021, 121, e26502.	2.0	1
101	Picture change and calculations of expectation values in approximate relativistic theories. , 0, .		1
102	Determination of nuclear quadrupole moments $\hat{\sigma}$ “ An example of the synergy of ab initio calculations and microwave spectroscopy. , 2015, , .		0
103	Electron correlation and relativistic effects in electric properties of the alkali metal fluorides. Molecular Physics, 1999, 96, 179-187.	1.7	0