# Vladimir KellÃ¶

List of Publications by Year
in descending order

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| 103 | 2,830 | 147801 | 214800 |
|---|---|---|---|
| papers | citations | 31 h-index | 47 g-index |

| 103 | 103 | 103 | 1455 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | <scp>AuSi</scp> molecule revisited: <scp>IOTC</scp>/<scp>CASSCF</scp>/<scp>CASPT2</scp> calculations. International Journal of Quantum Chemistry, 2021, 121, e26502. | 2.0 | 1 |
| 2 | Improved Mechanistic Model of the Atmospheric Redox Chemistry of Mercury. Environmental Science & Technology, 2021, 55, 14445-14456. | 10.0 | 65 |
| 3 | Relativistic calculations of AuSi + and AuSi â^'. International Journal of Quantum Chemistry, 2019, 119, e25951. | 2.0 | 1 |
| 4 | Quadrupole moments of Cd and Zn nuclei: When solid-state, molecular, atomic, and nuclear theory meet. Europhysics Letters, 2017, 117, 62001. | 2.0 | 21 |
| 5 | 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 |
| 6 | Determination of nuclear quadrupole moments â€“ An example of the synergy of ab initio calculations and microwave spectroscopy. , 2015, , . | | 0 |
| 7 | 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 |
| 8 | 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 |
| 9 | Ab initio calculations of molecular properties of lowâ€“lying electronic states of 2â€“cyclopentenâ€“1â€“one â€“ link with biological activity. Journal of Molecular Modeling, 2012, 18, 4751-4759. | 1.8 | 7 |
| 10 | Relativistic effects in low-lying electronic states of iron. Theoretical Chemistry Accounts, 2011, 129, 561-566. | 1.4 | 4 |
| 11 | 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 |
| 12 | Relativistic effects in atomic and molecular properties. Acta Physica Slovaca, 2010, 60, . | 1.4 | 58 |
| 13 | Linear and nonlinear optical properties of a series of Ni-dithiolene derivatives. Journal of Chemical Physics, 2009, 131, 134312. | 3.0 | 50 |
| 14 | The (hyper)polarizabilities of AuXeF and XeAuF. Chemical Physics Letters, 2009, 472, 185-189. | 2.6 | 17 |
| 15 | Theoretical study of molecular properties of low-lying electronic excited states of H<sub>2</sub>O and H<sub>2</sub>S. Molecular Physics, 2008, 106, 2333-2344. | 1.7 | 30 |
| 16 | The Nuclear Quadrupole Moment of 14N from Accurate Electric Field Gradient Calculations and Microwave Spectra of NP Molecule. Collection of Czechoslovak Chemical Communications, 2007, 72, 64-82. | 1.0 | 8 |
| 17 | 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 |
| 18 | Optimized virtual orbitals for relativistic calculations: an alternative approach to the basis set construction for correlation calculations. Molecular Physics, 2006, 104, 2277-2292. | 1.7 | 34 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | 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 |
| 20 | Theoretical study of PbO and the PbO anion. Chemical Physics Letters, 2005, 408, 210-215. | 2.6 | 86 |
| 21 | 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 |
| 22 | Polarizabilities of confined two-electron systems: the 2-electron quantum dot, the hydrogen anion, the helium atom and the lithium cation. Molecular Physics, 2005, 103, 2747-2761. | 1.7 | 36 |
| 23 | The quadrupole moment of the 3âˆ•2+ nuclear ground state of Au197 from electric field gradient relativistic coupled cluster and density-functional theory of small molecules and the solid state. Journal of Chemical Physics, 2005, 122, 124317. | 3.0 | 37 |
| 24 | 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 |
| 25 | Electric field gradients from shifted-nucleus calculations:â€,An alternative to the point charge nuclear quadrupole moment model. Journal of Chemical Physics, 2004, 120, 9424-9426. | 3.0 | 13 |
| 26 | Electric properties of hydrogen iodide: Reexamination of correlation and relativistic effects. Theoretical Chemistry Accounts, 2003, 110, 176-184. | 1.4 | 7 |
| 27 | 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 |
| 28 | Dipole moments calculations of transition metal mononitrides: ScN, TiN, VN, and CrN: Limits of the CCSD(T) method. International Journal of Quantum Chemistry, 2002, 90, 1240-1248. | 2.0 | 9 |
| 29 | Inclusion of mean-field spinâ€“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 |
| 30 | Nuclear quadrupole moments of Kr and Xe from molecular data. Chemical Physics Letters, 2001, 346, 155-159. | 2.6 | 25 |
| 31 | The change of picture of the Hellmannâ€“Feynman force operator in approximate relativistic methods. Computational and Theoretical Chemistry, 2001, 547, 35-53. | 1.5 | 21 |
| 32 | Accuracy assessment of the ROHF â€” CCSD(T) calculations of static dipole polarizabilities of diatomic radicals: O2, CN, and NO. Computational and Theoretical Chemistry, 2001, 547, 219-232. | 1.5 | 31 |
| 33 | Nuclear quadrupole moments of bromine and iodine from combined atomic and molecular data. Physical Review A, 2001, 64, . | 2.5 | 46 |
| 34 | An ab initio Investigation of the dipole moment of the CO2â€¦CO complex. Chemical Physics Letters, 2000, 319, 231-237. | 2.6 | 7 |
| 35 | The nuclear quadrupole moment of 45Sc. Chemical Physics Letters, 2000, 329, 112-118. | 2.6 | 25 |
| 36 | The nuclear quadrupole moment of from molecular data for ZrO and ZrS. Chemical Physics Letters, 2000, 318, 222-231. | 2.6 | 27 |

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| 37 | The point charge model of nuclear quadrupoles: How and why does it work. Journal of Chemical Physics, 2000, 112, 522-526. | 3.0 | 24 |
| 38 | Nuclear quadrupole moments from molecular microwave data: The quadrupole moment of85Rband87Rbnuclei and survey of molecular data for alkali-metal nuclei. Physical Review A, 1999, 60, 3575-3585. | 2.5 | 34 |
| 39 | Electric quadrupole moment of the 27Al nucleus: Converging results from the AlF and AlCl molecules and the Al atom. Chemical Physics Letters, 1999, 304, 414-422. | 2.6 | 73 |
| 40 | The nuclear quadrupole moment of <sup>73</sup>Ge from molecular microwave data. Molecular Physics, 1999, 96, 275-281. | 1.7 | 7 |
| 41 | Electron correlation and relativistic effects in electric properties of the alkali metal fluorides. Molecular Physics, 1999, 96, 179-187. | 1.7 | 12 |
| 42 | The nuclear quadrupole moment of data 73Ge from molecular microwave. Molecular Physics, 1999, 96, 275-281. | 1.7 | 14 |
| 43 | Electron correlation and relativistic effects in electric properties of the alkali metal fluorides. Molecular Physics, 1999, 96, 179-187. | 1.7 | 0 |
| 44 | Static dipole polarizabilities and hyperpolarizabilities of dicyanopolyacetylenes. Chemical Physics Letters, 1998, 287, 509-514. | 2.6 | 4 |
| 45 | The quadrupole moment of the K and K nuclei from microwave data for KF and KCl. Chemical Physics Letters, 1998, 292, 403-410. | 2.6 | 30 |
| 46 | Picture change and calculations of expectation values in approximate relativistic theories. International Journal of Quantum Chemistry, 1998, 68, 159-174. | 2.0 | 132 |
| 47 | Electron correlation and relativistic contributions to dipole moments of heavy oxides and sulfides: SnO, PbO, SnS, and PbS. Journal of Chemical Physics, 1998, 108, 2056-2066. | 3.0 | 20 |
| 48 | Standardized basis sets for high-level-correlated relativistic calculations of atomic and molecular electric properties in the spin-averaged Douglas-Kroll approximation. Theoretical Chemistry Accounts, 1997, 96, 166-175. | 1.4 | 40 |
| 49 | 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 |
| 50 | Ionization potentials and electron affinities of Cu, Ag, and Au: Electron correlation and relativistic effects. , 1997, 63, 557. | | 3 |
| 51 | Relativistic effects on electric properties of manyâ€electron systems in spinâ€averaged Douglasâ€“Kroll and Pauli approximations. Journal of Chemical Physics, 1996, 105, 1995-2003. | 3.0 | 88 |
| 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. Theoretica Chimica Acta, 1996, 94, 93-104. | 0.8 | 21 |
| 53 | Polarized basis sets for high-level-correlated calculations of molecular electric properties. Theoretica Chimica Acta, 1996, 93, 101-129. | 0.8 | 41 |
| 54 | Electric dipole polarizabilities of negative ions of the coinage metal atoms. Chemical Physics Letters, 1996, 253, 383-389. | 2.6 | 25 |

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| 55 | Determination of the quadrupole moment of the halogen nuclei (Cl,Br,I) from molecular data. Molecular Physics, 1996, 89, 127-137. | 1.7 | 38 |
| 56 | Polarized basis sets for high-level-correlated calculations of molecular electric properties. Theoretica Chimica Acta, 1996, 93, 101. | 0.8 | 2 |
| 57 | Standardized basis sets for high-level-correlated relativistic calculations of atomic and molecular electric properties in the spin-averaged Douglasâ€“Kroll (no-pair) approximation. Theoretica Chimica Acta, 1996, 94, 93. | 0.8 | 51 |
| 58 | Simple sparse matrix multiplication algorithm. Computer Physics Communications, 1995, 85, 213-216. | 7.5 | 3 |
| 59 | Electron correlation and relativistic effects in the coinage metal compounds. II. Heteronuclear dimers: CuAg, CuAu, and AgAu. Journal of Chemical Physics, 1995, 103, 2991-2999. | 3.0 | 24 |
| 60 | Electron correlation and relativistic effects in the coinage metal compounds. Theoretica Chimica Acta, 1995, 92, 253-267. | 0.8 | 1 |
| 61 | Polarized basis sets for high-level-correlated calculations of molecular electric properties. Theoretica Chimica Acta, 1995, 91, 353-371. | 0.8 | 62 |
| 62 | Polarized basis sets for high-level-correlated calculations of molecular electric properties. Theoretica Chimica Acta, 1995, 91, 353. | 0.8 | 15 |
| 63 | Electron correlation and relativistic effects in the coinage metal compounds.. Theoretica Chimica Acta, 1995, 92, 253. | 0.8 | 14 |
| 64 | Electron-correlation and relativistic contributions to atomic dipole polarizabilities: Alkali-metal atoms. Physical Review A, 1993, 47, 1715-1725. | 2.5 | 40 |
| 65 | Quasirelativistic studies of molecular electric properties: Dipole moments of the group IVa oxides and sulfides. Journal of Chemical Physics, 1993, 98, 1345-1351. | 3.0 | 23 |
| 66 | Electron correlation and relativistic contributions to molecular electric properties: dipole and quadrupole moments of cyanogen halides. Molecular Physics, 1992, 75, 209-220. | 1.7 | 18 |
| 67 | Medium-size polarized basis sets for high-level-correlated calculations of molecular electric properties. Theoretica Chimica Acta, 1992, 83, 351-366. | 0.8 | 53 |
| 68 | A CAS SCF study of reactive interactions between Be(3 P) and H2(1? g + ). Theoretica Chimica Acta, 1992, 81, 417-424. | 0.8 | 3 |
| 69 | Interaction potentials in rare gas-halide ion systems. Chemical Physics, 1991, 157, 123-133. | 1.9 | 17 |
| 70 | Quadrupole moments of CuH, AgH, and AuH. A study of the electron correlation and relativistic effects. Journal of Chemical Physics, 1991, 95, 8248-8253. | 3.0 | 32 |
| 71 | The beryllium atomâ€”water molecule interaction A many-body perturbation theory study. Chemical Physics Letters, 1990, 174, 19-24. | 2.6 | 8 |
| 72 | Relativistic contributions to molecular electric-field gradients in hydrogen halides. Chemical Physics Letters, 1990, 174, 641-648. | 2.6 | 36 |

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| 73 | Estimates of relativistic contributions to molecular properties. Journal of Chemical Physics, 1990, 93, 8122-8132. | 3.0 | 99 |
| 74 | Accuracy in ab initio reaction-energy computations. 1. Compounds of first-row elements. The Journal of Physical Chemistry, 1990, 94, 5694-5710. | 2.9 | 12 |
| 75 | A study of the performance of high-level correlated methods: The energy, dipole moment, and polarizability functions of CO. Chemical Physics Letters, 1988, 152, 387-392. | 2.6 | 26 |
| 76 | Electric properties of the chloride ion. Theoretica Chimica Acta, 1988, 74, 185-194. | 0.8 | 24 |
| 77 | A theoretical study of theAâ€‰1Îâ†Xâ€‰1Î£+system of SiH+. Journal of Chemical Physics, 1988, 89, 423-432. | 3.0 | 30 |
| 78 | Can the coupled cluster method improve many-body perturbation theory reaction energies significantly? the H2CO â†' H2 + CO reaction. Chemical Physics Letters, 1987, 135, 346-351. | 2.6 | 11 |
| 79 | Electron Correlation in Molecules. , 1987, , 117-250. | | 165 |
| 80 | MBPT studies of van der Waals molecules. III. The reliability of apparently accurate calculations for the magnesium dimer. Chemical Physics, 1986, 103, 55-74. | 1.9 | 30 |
| 81 | The ground state potential energy. Curve of Be2: Is the MBPT approach capable of predicting it?. Chemical Physics, 1985, 96, 59-79. | 1.9 | 37 |
| 82 | Ab initio MB RSPT calculations of barriers of non-rigid rearrangements of complex hydrides LiBH4 and Li2BeH4. Chemical Physics Letters, 1984, 106, 455-459. | 2.6 | 11 |
| 83 | Activation barriers of SN2 reactions: Fâ^' + CH3F and Hâ^' + CH3F. Fourth-order MB RSPT calculations. Chemical Physics Letters, 1984, 105, 625-629. | 2.6 | 24 |
| 84 | 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. Journal of the American Chemical Society, 1984, 106, 5864-5871. | 13.7 | 22 |
| 85 | Fourth-order MB-RSPT calculations of the spectroscopic constants and potential energy curve of F2. Theoretica Chimica Acta, 1983, 62, 549-562. | 0.8 | 32 |
| 86 | Complete fourth-order many-body perturbation theory calculations of the dipole moment and dipole polarizability of FH. Chemical Physics Letters, 1983, 95, 226-231. | 2.6 | 24 |
| 87 | 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. Chemical Physics, 1983, 77, 93-101. | 1.9 | 27 |
| 88 | Scaling in second order electron correlation calculations of potential energy curves and spectroscopic constants. Molecular Physics, 1983, 50, 1323-1333. | 1.7 | 6 |
| 89 | Perturbation theory of the electron correlation effects for atomic and molecular properties. VII. Complete fourthâ€order MBPT study of the dipole moment and dipole polarizability of H2O. Journal of Chemical Physics, 1983, 79, 2918-2923. | 3.0 | 63 |
| 90 | Finite-field many-body perturbation theory. Molecular Physics, 1983, 49, 711-725. | 1.7 | 28 |

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|---|---|---|---|
| 91 | Fourth-order diagrammatic MB-RSPT calculations of the interaction energy between two helium atoms. Theoretica Chimica Acta, 1981, 59, 309-317. | 0.8 | 2 |
| 92 | Many-Body Rayleigh-SchrÃ¶dinger 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. Theoretica Chimica Acta, 1980, 56, 315-328. | 0.8 | 20 |
| 93 | Fourth-order diagrammaticMB-RSPTcalculations of the correlation energy: N2, CO, F2and the reaction energy of the process Â½F2+ Â½H2= HF. International Journal of Quantum Chemistry, 1980, 18, 1431-1448. | 2.0 | 19 |
| 94 | The fourth order diagrammatic MBâ€RSPT calculations of the correlation energy of ten electron systems. Journal of Chemical Physics, 1980, 72, 3378-3385. | 3.0 | 95 |
| 95 | Applications of perturbation theory to the chemical problems potential energy curves of BH, F2and N2. Molecular Physics, 1979, 38, 1621-1633. | 1.7 | 12 |
| 96 | The effect of disconnected wavefunction clusters of double excitations on the correlation energy of molecules. Chemical Physics Letters, 1979, 62, 584-588. | 2.6 | 10 |
| 97 | Ab initio studies of chemical equilibria. A refined approach to the reaction NHâ‚‚ + H2 â‡Œ NH3 + Hâ‚. Chemical Physics Letters, 1979, 61, 85-87. | 2.6 | 4 |
| 98 | AB initio studies of chemical equilibria. Application of many-body rayleigh-schrÃ¶dinger perturbation theory up to third order to the proton affinity of water. Chemical Physics Letters, 1978, 58, 83-86. | 2.6 | 5 |
| 99 | Ab initio studies of chemical equilibria. Equilibria containing first row hydrides AH2, AH3, and AH4 and their positive ions. Chemical Physics Letters, 1978, 53, 555-559. | 2.6 | 5 |
| 100 | Polarization functions for gaussian basis sets for the first row atoms. Theoretica Chimica Acta, 1977, 45, 205-213. | 0.8 | 47 |
| 101 | Calculation of the correlation energy of molecules by many-body rayleigh-schrÃ¶dinger perturbation theory up to third order. Chemical Physics Letters, 1977, 51, 170-174. | 2.6 | 27 |
| 102 | Interactions of ions. Ab initio SCF-MO-LCAO calculations of Li+-H2O-OH- with a minimal Gaussian basis set. Collection of Czechoslovak Chemical Communications, 1975, 40, 587-596. | 1.0 | 3 |
| 103 | Picture change and calculations of expectation values in approximate relativistic theories. , 0, . | | 1 |