# Ernest Davidson

List of Publications by Year
in descending order

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|---|---|---|---|
| 399 papers | 35,042 citations | 7251 80 h-index | 4853 174 g-index |
| 462 all docs | 462 docs citations | 462 times ranked | 12929 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Atomic isotropic hyperfine properties for first row elements (Bâ€“F) revisited. Journal of Chemical Physics, 2022, 156, 034304. | 1.2 | 3 |
| 2 | A viewpoint on population analyses. International Journal of Quantum Chemistry, 2022, 122, . | 1.0 | 5 |
| 3 | Complete-active-space extended Koopmans theorem method. Journal of Chemical Physics, 2021, 155, 051102. | 1.2 | 7 |
| 4 | The Right Answer for the Right Reason: My Personal Goal for Quantum Chemistry. Annual Review of Physical Chemistry, 2019, 70, 1-20. | 4.8 | 11 |
| 5 | A theoretical study of the adiabatic and vertical ionization potentials of water. Journal of Chemical Physics, 2018, 148, 234308. | 1.2 | 5 |
| 6 | Nature of ground and electronic excited states of higher acenes. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E5098-107. | 3.3 | 147 |
| 7 | Approximate singly excited states from a two-component Hartree-Fock reference. Journal of Chemical Physics, 2015, 143, 144106. | 1.2 | 10 |
| 8 | The benzene radical anion: A computationally demanding prototype for aromatic anions. Journal of Chemical Physics, 2015, 142, 204304. | 1.2 | 24 |
| 9 | Singletâ€“Triplet Energy Gaps for Diradicals from Particleâ€“Particle Random Phase Approximation. Journal of Physical Chemistry A, 2015, 119, 4923-4932. | 1.1 | 34 |
| 10 | A systematic approach to vertically excited states of ethylene using configuration interaction and coupled cluster techniques. Journal of Chemical Physics, 2014, 141, 104302. | 1.2 | 41 |
| 11 | Canonical form of the Hartree-Fock orbitals in open-shell systems. Journal of Chemical Physics, 2014, 140, 014102. | 1.2 | 21 |
| 12 | Linear inequalities for density matrices: IV Factorizations. Computational and Theoretical Chemistry, 2013, 1003, 28-31. | 1.1 | 3 |
| 13 | Variational definitions of orbital energies. , 2012, , . | | 1 |
| 14 | Koopmansâ€™s theorem in the restricted open-shell Hartreeâ€“Fock method. II. The second canonical set for orbitals and orbital energies. Journal of Chemical Physics, 2010, 132, . | 1.2 | 22 |
| 15 | Spin-state splittings, highest-occupied-molecular-orbital and lowest-unoccupied-molecular-orbital energies, and chemical hardness. Journal of Chemical Physics, 2010, 133, 164107. | 1.2 | 14 |
| 16 | Comment on â€œCombined open shell Hartreeâ€“Fock theory of atomic-molecular and nuclear systemsâ€•[J. Math. Chem. 42 (2007) 177]. Journal of Mathematical Chemistry, 2009, 45, 859-866. | 0.7 | 2 |
| 17 | Qualitatively significant effects of electron correlation. International Journal of Quantum Chemistry, 2009, 20, 65-68. | 1.0 | 0 |
| 18 | Theoretical and Spectroscopic Investigations of the Bonding and Reactivity of (RO)<sub>3</sub>Mâ‰¡N Molecules, where M = Cr, Mo, and W. Inorganic Chemistry, 2009, 48, 828-837. | 1.9 | 8 |

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| 19 | Koopmansâ€™ Theorem in the Restricted Open-Shell Hartreeâ^'Fock Method. 1. A Variational Approach. Journal of Physical Chemistry A, 2009, 113, 12386-12395. | 1.1 | 47 |
| 20 | Size extensivity of the direct optimized effective potential method. Journal of Chemical Physics, 2008, 128, 114702. | 1.2 | 5 |
| 21 | The effective local potential method: Implementation for molecules and relation to approximate optimized effective potential techniques. Journal of Chemical Physics, 2007, 126, 084107. | 1.2 | 35 |
| 22 | Self-consistent effective local potentials. Journal of Chemical Physics, 2007, 127, 084113. | 1.2 | 20 |
| 23 | Understanding Electron Correlation: Recent Progress in Molecular Synchrotron Photoelectron Spectroscopy. Advances in Chemical Physics, 2007, , 215-266. | 0.3 | 22 |
| 24 | Linear Inequalities for Diagonal Elements of Density Matrices. Advances in Chemical Physics, 2007, , 443-483. | 0.3 | 23 |
| 25 | Analysis of wave functions for open-shell molecules. Physical Chemistry Chemical Physics, 2007, 9, 1881. | 1.3 | 52 |
| 26 | Large Ground-State Entropy Changes for Hydrogen Atom Transfer Reactions of Iron Complexes. Journal of the American Chemical Society, 2007, 129, 5153-5166. | 6.6 | 134 |
| 27 | Basis Sets for Ab Initio Molecular Orbital Calculations and Intermolecular Interactions. Reviews in Computational Chemistry, 2007, , 1-43. | 1.5 | 36 |
| 28 | Ab Initio Diradical/Zwitterionic Polarizabilities and Hyperpolarizabilities in Twisted Double Bonds. Journal of Physical Chemistry A, 2006, 110, 7189-7196. | 1.1 | 30 |
| 29 | Optimized effective potentials yielding Hartreeâ€“Fock energies and densities. Journal of Chemical Physics, 2006, 124, 141103. | 1.2 | 175 |
| 30 | Necessary conditions for theN-representability of pair distribution functions. International Journal of Quantum Chemistry, 2006, 106, 1487-1498. | 1.0 | 49 |
| 31 | LÃ¶wdin population analysis with and without rotational invariance. International Journal of Quantum Chemistry, 2006, 106, 2065-2072. | 1.0 | 65 |
| 32 | Stoichiometric oxidations of Ïƒ-bonds: Radical and possible non-radical pathways. Journal of Molecular Catalysis A, 2006, 251, 24-33. | 4.8 | 30 |
| 33 | Effective local potentials for orbital-dependent density functionals. Journal of Chemical Physics, 2006, 125, 081104. | 1.2 | 81 |
| 34 | High-density limit of the Perdew-Burke-Ernzerhof generalized gradient approximation and related density functionals. Physical Review A, 2006, 74, . | 1.0 | 52 |
| 35 | Charge and Spin Distributions. , 2006, , 1001-1001. | | 0 |
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| 37 | Computational Studies of the Thermal Fragmentation of P-Arylphosphiranes:â€‰ Have Arylphosphinidenes Been Generated by This Method?. Journal of the American Chemical Society, 2005, 127, 9886-9894. | 6.6 | 20 |
| 38 | Ligand-Assisted Reduction of Osmium Tetroxide with Molecular Hydrogen via a [3+2] Mechanism. Journal of the American Chemical Society, 2005, 127, 3423-3432. | 6.6 | 37 |
| 39 | Energies of isoelectronic atomic ions from a successful metageneralized gradient approximation and other density functionals. Physical Review A, 2004, 70, . | 1.0 | 33 |
| 40 | Bonding in FHF?, (HF)2, and FHF. International Journal of Quantum Chemistry, 2004, 98, 317-324. | 1.0 | 22 |
| 41 | Large Spin Differences in Structurally Related Fe6Molecular Clusters and Their Magnetostructural Explanation. Inorganic Chemistry, 2004, 43, 5505-5521. | 1.9 | 140 |
| 42 | Polynuclear Manganese Complexes with the Dicarboxylate Ligand m-Phenylenedipropionate:â€‰ A Hexanuclear Mixed-Valence (3MnIII, 3MnIV) Complex. Inorganic Chemistry, 2004, 43, 101-115. | 1.9 | 53 |
| 43 | p-Benzyne Derivatives that Have Exceptionally Small Singletâ€”Triplet Gaps and Even a Triplet Ground State.. ChemInform, 2003, 34, no. | 0.1 | 0 |
| 44 | An investigation into the relative influence of alkoxide and thiolate ligands on the metalâ€“carbon triple bond in X3Mî˜†CH compounds, where M=Cr, Mo and W and X=OH, SH, OCH3, SCH3, OCF3 and SCF3 from electronic structure calculations. Polyhedron, 2003, 22, 145-152. | 1.0 | 3 |
| 45 | Linear inequalities for density matrices: III. International Journal of Quantum Chemistry, 2003, 91, 1-4. | 1.0 | 23 |
| 46 | Semiempirical local spin: Theory and implementation of the ZILSH method for predicting Heisenberg exchange constants of polynuclear transition metal complexes. International Journal of Quantum Chemistry, 2003, 92, 294-325. | 1.0 | 47 |
| 47 | Population analyses that utilize projection operators. International Journal of Quantum Chemistry, 2003, 93, 384-394. | 1.0 | 70 |
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| 49 | Methanolysis and Phenolysis Routes to Fe6, Fe8, and Fe10Complexes and Their Magnetic Properties:Â A New Type of Fe8Ferric Wheel. Inorganic Chemistry, 2003, 42, 7819-7829. | 1.9 | 59 |
| 50 | 34S Isotope Effect on Sulfate Ester Hydrolysis:Â Mechanistic Implications. Journal of the American Chemical Society, 2003, 125, 13036-13037. | 6.6 | 25 |
| 51 | p-Benzyne Derivatives That Have Exceptionally Small Singletâ€™Triplet Gaps and Even a Triplet Ground State. Journal of Organic Chemistry, 2003, 68, 3387-3396. | 1.7 | 27 |
| 52 | Non-Sternâ€™Volmer Quenching of S1pDFB Fluorescence by O2and the Charge Transfer Complexâ€. Journal of Physical Chemistry A, 2003, 107, 3552-3558. | 1.1 | 7 |
| 53 | A TDDFT description of the low-energy excited states of copper and zinc metalloenediynesElectronic supplementary information (ESI) available: Cartesian coordinates of optimized structures and tables of the TDDFT configurations for each excited state. See http://www.rsc.org/suppdata/cc/b3/b308633j/. Chemical Communications, 2003, , 2876. | 2.2 | 5 |
| 54 | Exactness of the General Two-Body Cluster Expansion in Many-Body Quantum Theory. Physical Review Letters, 2003, 91, 123001. | 2.9 | 22 |

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| 55 | Local spin II. Molecular Physics, 2002, 100, 373-383. | 0.8 | 76 |
| 56 | Local Spin III:Â Wave Function Analysis along a Reaction Coordinate, H Atom Abstraction, and Addition Processes of Benzyne. Journal of Physical Chemistry A, 2002, 106, 6890-6896. | 1.1 | 52 |
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| 60 | Comparison of Î± CH and CF activation in alkyl transition metal complexes: a DFT and CASSCF study. Molecular Physics, 2002, 100, 533-540. | 0.8 | 21 |
| 61 | Two new hexanuclear iron(iii) complexes with SÂ= 5 ground states. Dalton Transactions RSC, 2002, , 4005-4010. | 2.3 | 36 |
| 62 | Insights into the Schrock â€˜chop-chopâ€™ reaction gained from density functional theory and preparation and structure of W2(Î¼-PhCCPh)(SC6H4-2-Me)6. Chemical Communications, 2002, , 2770-2771. | 2.2 | 7 |
| 63 | New time-independent perturbation theory for the multireference problem. International Journal of Quantum Chemistry, 2002, 86, 256-264. | 1.0 | 24 |
| 64 | The effect of the basis set superposition error on the geometry optimization of the p-DFBâ€“N2 complex. Chemical Physics Letters, 2002, 360, 99-103. | 1.2 | 14 |
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| 67 | Structure of the exact wave function. II. Iterative configuration interaction method. Journal of Chemical Physics, 2001, 115, 2000-2006. | 1.2 | 59 |
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| 74 | Use of the dicarboxylate ligand m-phenylenedipropionate for the synthesis of new Mn/O clusters. Synthesis, characterization and magnetic properties. Polyhedron, 2001, 20, 1375-1380. | 1.0 | 23 |
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| 85 | Dimolybdenum Bis((S,S,S)-triisopropanolaminate(3â^')):â€‰ A Blue Compound with an Unusual Moâ^'Mo Triple Bond. Inorganic Chemistry, 2000, 39, 3544-3550. | 1.9 | 9 |
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| 89 | Fate of CH2CHE (E = H, OMe) in the Presence of Unsaturated Ru(X)(H)L2q+(X = Cl,q= 0; X = CO,q= 1):Â Highly Sensitive to X and E. Organometallics, 2000, 19, 2291-2298. | 1.1 | 17 |
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| 91 | Is the Hydrogen Bond in Water Dimer and Ice Covalent?. Journal of the American Chemical Society, 2000, 122, 1210-1214. | 6.6 | 174 |
| 92 | Charge densities for singlet and triplet electron pairs. , 2000, 77, 651. | | 1 |
| 93 | MULTI-REFERENCE PERTURBATION THEORY. Recent Advances in Computational, 1999, , 31-63. | 0.8 | 16 |
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| 97 | Reassignment of the AlSiâ€" photoelectron spectrum by ab initio configuration interaction calculations. Molecular Physics, 1999, 96, 735-740. | 0.8 | 3 |
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| 103 | [2.2.2]propellane rearrangements. Chemical Physics Letters, 1998, 284, 301-307. | 1.2 | 21 |
| 104 | Zero point corrections to vertical excitation energies. Chemical Physics Letters, 1998, 285, 155-159. | 1.2 | 64 |
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| 106 | How robust is present-day DFT?. International Journal of Quantum Chemistry, 1998, 69, 241-245. | 1.0 | 72 |
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| 111 | Density functional calculations for Mgn+ clusters. Journal of Chemical Physics, 1997, 106, 2331-2341. | 1.2 | 24 |
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| 115 | Calculational Evidence for Lack of Intermediates in the Thermal Unimolecular Vinylcyclopropane to Cyclopentene 1,3-Sigmatropic Shift. Journal of the American Chemical Society, 1997, 119, 10543-10544. | 6.6 | 62 |
| 116 | Could 2.2.2-Propellatriene Exist?. Journal of the American Chemical Society, 1997, 119, 1449-1449. | 6.6 | 7 |
| 117 | The ground state of ethylene. Computational and Theoretical Chemistry, 1997, 400, 169-176. | 1.5 | 6 |
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| 120 | The Importance of Including Dynamic Electron Correlation inab InitioCalculations. Accounts of Chemical Research, 1996, 29, 67-75. | 7.6 | 240 |
| 121 | Electron momentum spectroscopy experiments and calculations for the production of excited states of He<sup>+</sup> and. Canadian Journal of Physics, 1996, 74, 748-756. | 0.4 | 20 |
| 122 | Electron spin resonance matrix isolation and ab initio theoretical investigations of 69,71GaH2, 69,71GaD2, H69,71GaCH3, and D69,71GaCD3. Journal of Chemical Physics, 1996, 105, 6607-6615. | 1.2 | 39 |
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| 124 | Comment on â€œComment on Dunning's correlation-consistent basis setsâ€• Chemical Physics Letters, 1996, 260, 514-518. | 1.2 | 375 |
| 125 | Refinement of the Asymptotic Z Expansion for the Ground-State Correlation Energies of Atomic Ions. The Journal of Physical Chemistry, 1996, 100, 6167-6172. | 2.9 | 110 |
| 126 | An electron spin resonance investigation of vanadium dioxide (51V16O2 and 51V17O2) and 51V17O in neon matrices with preliminary assignments for VO3 and V+2: Comparison with ab initio theoretical calculations. Journal of Chemical Physics, 1996, 105, 10237-10250. | 1.2 | 63 |

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| 133 | ESR observation of the Hâ‹…â‹…â‹…H, Hâ‹…â‹…â‹…D, and Dâ‹…â‹…â‹…D spinâ€pair radicals in rare gas matrices. Journal of Chemical Physics, 1995, 103, 5275-5278. | 1.2 | 13 |
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| 146 | Some Perspectives on Quantum Calculations. Israel Journal of Chemistry, 1993, 33, 243-252. | 1.0 | 10 |
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| 153 | Zero kinetic energy photoelectron spectra of jetâ€cooled aniline. Journal of Chemical Physics, 1993, 99, 3224-3233. | 1.2 | 103 |
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| 159 | Momentum distributions, spin distributions, and bonding in methylamine and its radical cation. Journal of the American Chemical Society, 1992, 114, 6496-6504. | 6.6 | 22 |
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