Ernest Davidson

List of Publications by Citations

399 papers	32,044 citations	78 h-index	167 g-index
462 ext. papers	33,366 ext. citations	6 avg, IF	7.01 L-index

#	Paper	IF	Citations
399	Coherent X-Ray Scattering for the Hydrogen Atom in the Hydrogen Molecule. *Journal of Chemical Physics*, **1965**, 42, 3175-3187	3.9	5158
398	Configuration interaction calculations on the nitrogen molecule. *International Journal of Quantum Chemistry*, **1974**, 8, 61-72	2.1	2517
397	The iterative calculation of a few of the lowest eigenvalues and corresponding eigenvectors of large real-symmetric matrices. *Journal of Computational Physics*, **1975**, 17, 87-94	4.1	1976
396	Ligand spin polarization and antiferromagnetic coupling in transition metal dimers. *Chemical Physics*, **1986**, 109, 131-143	2.3	815
395	Basis set selection for molecular calculations. *Chemical Reviews*, **1986**, 86, 681-696	68.1	680
394	Effects of electron repulsion in conjugated hydrocarbon diradicals. *Journal of the American Chemical Society*, **1977**, 99, 4587-4594	16.4	549
393	Size consistency in the dilute helium gas electronic structure. *Chemical Physics Letters*, **1977**, 52, 403-406	2.5	537
392	One- and two-electron integrals over cartesian gaussian functions. *Journal of Computational Physics* , **1978**, 26, 218-231	4.1	510
391	Ground-state correlation energies for atomic ions with 3 to 18 electrons. *Physical Review A*, **1993**, 47, 3649-3670	2.6	457
390	Ground-state correlation energies for two- to ten-electron atomic ions. *Physical Review A*, **1991**, 44, 7071-7083	2.6	337
389	Studies in Configuration Interaction: The First-Row Diatomic Hydrides. *Physical Review*, **1969**, 183, 23-30		336
388	Comment on Comment on Dunning's correlation-consistent basis sets *Chemical Physics Letters*, **1996**, 260, 514-518	2.5	325
387	A Natural Orbital Based Energy Calculation for Helium Hydride and Lithium Hydride. *The Journal of Physical Chemistry*, **1966**, 70, 2675-2685		315
386	Electronic Population Analysis of Molecular Wavefunctions. *Journal of Chemical Physics*, **1967**, 46, 3320-3324	3.9	312
385	Porphyrins XXVIII. Extended Hückel calculations on metal phthalocyanines and tetrazaporphins. *Theoretica Chimica Acta*, **1973**, 30, 9-30		254
384	Symmetry breaking in polyatomic molecules: real and artifactual. *The Journal of Physical Chemistry*, **1983**, 87, 4783-4790		253
383	Asymptotic behavior of atomic and molecular wave functions. *Proceedings of the National Academy of Sciences of the United States of America*, **1980**, 77, 4403-6	11.5	250

382	A test of the Hirshfeld definition of atomic charges and moments. *Theoretica Chimica Acta*, **1992**, 83, 319-330		249
381	The Importance of Including Dynamic Electron Correlation in ab Initio Calculations. *Accounts of Chemical Research*, **1996**, 29, 67-75	24.3	221
380	One-electron properties of several small molecules using near Hartree□Fock limit basis sets. *Journal of Chemical Physics*, **1987**, 86, 3424-3440	3.9	221
379	The two lowest energy 2A? states of NO2. *Journal of Chemical Physics*, **1976**, 64, 2908-2917	3.9	192
378	An approximation to frozen natural orbitals through the use of the Hartree□Fock exchange potential. *Journal of Chemical Physics*, **1981**, 74, 3977-3979	3.9	184
377	Properties and Uses of Natural Orbitals. *Reviews of Modern Physics*, **1972**, 44, 451-464	40.5	174
376	Distribution of effectively unpaired electrons. *Chemical Physics Letters*, **2000**, 330, 161-168	2.5	171
375	Electron momentum spectroscopy of the valence orbitals of H2O and D2O: Quantitative comparisons using Hartree□Fock limit and correlated wavefunctions. *Chemical Physics*, **1987**, 113, 19-42	2.3	169
374	Considerations in constructing a multireference second-order perturbation theory. *Journal of Chemical Physics*, **1994**, 100, 3672-3682	3.9	164
373	Optimized effective potentials yielding Hartree-Fock energies and densities. *Journal of Chemical Physics*, **2006**, 124, 141103	3.9	162
372	Is the Hydrogen Bond in Water Dimer and Ice Covalent?. *Journal of the American Chemical Society*, **2000**, 122, 1210-1214	16.4	161
371	Ab initio configuration interaction calculations of the hyperfine structure in small radicals. *Journal of Chemical Physics*, **1984**, 80, 1006-1017	3.9	158
370	Local spin. *Journal of Chemical Physics*, **2001**, 115, 7382-7392	3.9	156
369	An analysis of the hydrogen bond in ice. *Journal of Chemical Physics*, **1990**, 93, 8029-8035	3.9	149
368	Nature of the Configuration-Interaction Method in Ab Initio Calculations. I. Ne Ground State. *Physical Review A*, **1970**, 1, 644-658	2.6	147
367	Single-molecule magnets: two-electron reduced version of a Mn12 complex and environmental influences on the magnetization relaxation of (PPh4)(2)[Mn(12)O(12)(O(2)CCHCl2)(16)(H2O)4]. *Journal of the American Chemical Society*, **2003**, 125, 3576-88	16.4	144
366	An ab initio potential-energy surface study of several electronic states of NO2. *Journal of Chemical Physics*, **1976**, 65, 2941-2957	3.9	137
365	Theoretical studies of diradicals containing four .pi. electrons. *Accounts of Chemical Research*, **1981**, 14, 69-76	24.3	136

364	Selection of the Proper Canonical Roothaan-Hartree-Fock Orbitals for Particular Applications. I. Theory. *Journal of Chemical Physics*, **1972**, 57, 1999-2005	3.9	136
363	Global topology of triatomic potential surfaces. *Journal of the American Chemical Society*, **1977**, 99, 397-402	16.4	135
362	Spin-restricted open-shell self-consistent-field theory. *Chemical Physics Letters*, **1973**, 21, 565-567	2.5	132
361	Large spin differences in structurally related Fe6 molecular clusters and their magnetostructural explanation. *Inorganic Chemistry*, **2004**, 43, 5505-21	5.1	130
360	Natural Expansion of Exact Wavefunctions. II. The Hydrogen-Molecule Ground State. *Journal of Chemical Physics*, **1962**, 37, 2966-2971	3.9	130
359	Extended x-ray-absorption fine-structure amplitudes□Wave-function relaxation and chemical effects. *Physical Review B*, **1978**, 17, 560-565	3.3	129
358	Perturbation theory for open shell systems. *Chemical Physics Letters*, **1991**, 187, 451-454	2.5	124
357	An SCF method for hole states. *Journal of Chemical Physics*, **1976**, 65, 609-613	3.9	118
356	Large ground-state entropy changes for hydrogen atom transfer reactions of iron complexes. *Journal of the American Chemical Society*, **2007**, 129, 5153-66	16.4	116
355	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	11.5	113
354	Diradical Character of the Cope Rearrangement Transition State. *Journal of the American Chemical Society*, **2000**, 122, 186-187	16.4	111
353	Validity of first-order perturbation theory for relativistic energy corrections. *Chemical Physics Letters*, **1981**, 84, 226-227	2.5	111
352	Improved algorithms for the lowest few eigenvalues and associated eigenvectors of large matrices. *Journal of Computational Physics*, **1992**, 103, 382-389	4.1	110
351	Theoretical Calculation of the Potential Curves of the Be2 Molecule. *Journal of Chemical Physics*, **1967**, 47, 4972-4978	3.9	109
350	Experimental evidence for a C2v (2B1) ground-state structure of the methane cation radical: ESR and ab initio CI investigations of methane cation radicals (CH4+ and CD2H2+) in neon matrixes at 4 K. *Journal of the American Chemical Society*, **1984**, 106, 3700-3701	16.4	108
349	Configuration interaction calculations on the planar 1(□□) state of ethylene. *Journal of Chemical Physics*, **1977**, 66, 2959-2971	3.9	108
348	Single-Configuration Calculations on Excited States of Helium. II. *Journal of Chemical Physics*, **1965**, 42, 4199-4200	3.9	108
347	Refinement of the Asymptotic Z Expansion for the Ground-State Correlation Energies of Atomic Ions. *The Journal of Physical Chemistry*, **1996**, 100, 6167-6172		105

346	The transition metal-carbonyl bond. *Accounts of Chemical Research*, **1993**, 26, 628-635	24.3	104
345	First Excited 1Σ+ State of the Hydrogen Molecule. *Journal of Chemical Physics*, **1961**, 35, 1189-1202	3.9	104
344	Configuration Interaction Description of Electron Correlation **1974**, 17-30		101
343	A possible definition of basis set superposition error. *Chemical Physics Letters*, **1994**, 217, 48-54	2.5	98
342	The Cope Rearrangement Revisited with Multireference Perturbation Theory. *Journal of the American Chemical Society*, **1995**, 117, 774-778	16.4	97
341	Structure of ice Ih. Ab initio two- and three-body water−water potentials and geometry optimization. *Journal of Chemical Physics*, **1985**, 83, 1223-1231	3.9	96
340	Natural Orbitals for Hydrogen-Molecule Excited States. *Journal of Chemical Physics*, **1966**, 45, 2560-2576	3.9	95
339	Zero kinetic energy photoelectron spectra of jet-cooled aniline. *Journal of Chemical Physics*, **1993**, 99, 3224-3233	3.9	93
338	Potential energy surfaces of CH+4. *Journal of Chemical Physics*, **1988**, 88, 1775-1785	3.9	93
337	A multireference CI determination of the isotropic hyperfine constants for first row atoms B−F. *Journal of Chemical Physics*, **1988**, 88, 7580-7587	3.9	93
336	A theoretical study on the potential surfaces of the lower electronic states of HCO. *Journal of Chemical Physics*, **1979**, 70, 2904-2913	3.9	90
335	A configuration interaction study of the spin dipole-dipole parameters for formaldehyde and methylene. *International Journal of Quantum Chemistry*, **1973**, 7, 999-1019	2.1	90
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333	MCSCF/CI investigation of the low-lying potential energy surfaces of the formyloxyl radical, HCO2.cntdot.. *Journal of the American Chemical Society*, **1983**, 105, 1459-1466	16.4	87
332	A third isolated oxidation state for the Mn12 family of single-molecule magnets. *Chemical Communications*, **2000**, 2417-2418	5.8	86
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330	The potential surfaces for the lowest singlet and triplet states of cyclobutadiene. *Journal of the American Chemical Society*, **1978**, 100, 388-392	16.4	85
329	Theoretical Study of the LiH Molecule. *Journal of Chemical Physics*, **1968**, 49, 4222-4229	3.9	83

328	ESR and ab initio theoretical studies of the cation radicals 14N+4 and 15N+4: The trapping of ion□neutral reaction products in neon matrices at 4 K. *Journal of Chemical Physics*, **1987**, 87, 885-897	3.9	82
327	The water dimer: correlation energy calculations. *The Journal of Physical Chemistry*, **1993**, 97, 6373-6383		81
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323	Correlation Energy and Molecular Properties of Hydrogen Fluoride. *Journal of Chemical Physics*, **1967**, 47, 360-366	3.9	79
322	A theoretical investigation of some low-lying singlet states of 1,3-butadiene. *The Journal of Physical Chemistry*, **1987**, 91, 4481-4490		78
321	Potential surfaces for the planar cyclopentadienyl radical and cation. *Journal of the American Chemical Society*, **1979**, 101, 3771-3775	16.4	78
320	Quasidegenerate variational perturbation theory and the calculation of first-order properties from variational perturbation theory wave functions. *Journal of Chemical Physics*, **1988**, 89, 6798-6814	3.9	76
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317	Some Triplet States of the Hydrogen Molecule. *Journal of Chemical Physics*, **1965**, 43, 834-839	3.9	74
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315	Transition Regions in the Cope Rearrangement of 1,5-Hexadiene and Its Cyano Derivatives. *Journal of the American Chemical Society*, **2000**, 122, 7377-7385	16.4	73
314	Local spin II. *Molecular Physics*, **2002**, 100, 373-383	1.7	70
313	The Cope rearrangement revisited. *Journal of the American Chemical Society*, **1991**, 113, 9756-9759	16.4	70
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308	The electron affinity of oxygen: A systematic configuration interaction approach. *Journal of Chemical Physics*, **1989**, 90, 1024-1030	3.9	65
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298	Ab initio calculation of extended x-ray-absorption fine structure in Br2. *Physical Review B*, **1987**, 35, 2604-2614	3.8	60
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291	Evaluation of a characteristic atomic radius by an ab initio method. *International Journal of Quantum Chemistry*, **1997**, 62, 47-53	2.1	58
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280	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	16.4	54
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259	Allylic resonance - when is it unimportant?. *Journal of the American Chemical Society*, **1984**, 106, 2513-2518	16.4	48
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257	Fluorescence Analysis: A New Approach. *Analytical Letters*, **1975**, 8, 665-681	2.2	48

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255	Local Spin III: Wave Function Analysis along a Reaction Coordinate, H Atom Abstraction, and Addition Processes of Benzyne. *Journal of Physical Chemistry A*, **2002**, 106, 6890-6896	2.8	47
254	Effect of carbon atom pyramidalization on the bonding in ethylene. *Journal of the American Chemical Society*, **1979**, 101, 533-537	16.4	47
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