Henry F Schaefer

List of Publications by Citations

1,004 papers	50,170 citations	103 h-index	188 g-index
1,026 ext. papers	52,901 ext. citations	4.6 avg, IF	7.41 L-index

#	Paper	IF	Citations
1004	Advances in methods and algorithms in a modern quantum chemistry program package. *Physical Chemistry Chemical Physics*, **2006**, 8, 3172-91	3.6	2371
1003	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics*, **2015**, 113, 184-215	1.7	2068
1002	An efficient reformulation of the closed-shell coupled cluster single and double excitation (CCSD) equations. *Journal of Chemical Physics*, **1988**, 89, 7382-7387	3.9	1382
1001	Atomic and molecular electron affinities: photoelectron experiments and theoretical computations. *Chemical Reviews*, **2002**, 102, 231-82	68.1	1063
1000	Is coupled cluster singles and doubles (CCSD) more computationally intensive than quadratic configuration interaction (QCISD)?. *Journal of Chemical Physics*, **1989**, 90, 3700-3703	3.9	956
999	On the evaluation of analytic energy derivatives for correlated wave functions. *Journal of Chemical Physics*, **1984**, 81, 5031-5033	3.9	752
998	Psi4 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability. *Journal of Chemical Theory and Computation*, **2017**, 13, 3185-3197	6.4	733
997	Psi4: an open-source ab initio electronic structure program. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 556-565	7.9	678
996	A stable silicon(0) compound with a Si=Si double bond. *Science*, **2008**, 321, 1069-71	33.3	622
995	Extensive theoretical studies of the hydrogen-bonded complexes (H2O)2, (H2O)2H+, (HF)2, (HF)2H+, F2H□and (NH3)2. *Journal of Chemical Physics*, **1986**, 84, 2279-2289	3.9	621
994	In pursuit of the ab initio limit for conformational energy prototypes. *Journal of Chemical Physics*, **1998**, 108, 9751-9764	3.9	606
993	A new implementation of the full CCSDT model for molecular electronic structure. *Chemical Physics Letters*, **1988**, 152, 382-386	2.5	525
992	A systematic study of molecular vibrational anharmonicity and vibration□otation interaction by self-consistent-field higher-derivative methods. Asymmetric top molecules. *Chemical Physics*, **1988**, 123, 187-239	2.3	443
991	The C2H5 + O2 Reaction Mechanism: High-Level ab Initio Characterizations. *Journal of Physical Chemistry A*, **2000**, 104, 9823-9840	2.8	436
990	A stable, neutral diborene containing a B=B double bond. *Journal of the American Chemical Society*, **2007**, 129, 12412-3	16.4	434
989	The diagonal correction to the Born□Oppenheimer approximation: Its effect on the singlet□triplet splitting of CH2 and other molecular effects. *Journal of Chemical Physics*, **1986**, 84, 4481-4484	3.9	366
988	An Introduction to Coupled Cluster Theory for Computational Chemists. *Reviews in Computational Chemistry*, **2007**, 33-136		364

987	Analytic evaluation of energy gradients for the single and double excitation coupled cluster (CCSD) wave function: Theory and application. *Journal of Chemical Physics*, **1987**, 87, 5361-5373	3.9	358
986	The graphical unitary group approach to the electron correlation problem. Methods and preliminary applications. *Journal of Chemical Physics*, **1979**, 70, 5092-5106	3.9	332
985	Systematic study of molecular anions within the self-consistent-field approximation: OH□CN□ C2H□NH2, and CH3. *Journal of Chemical Physics*, **1985**, 83, 1784-1794	3.9	305
984	Electronic structure of homoleptic transition metal hydrides: TiH4, VH4, CrH4, MnH4, FeH4, CoH4, and NiH4. *Journal of Chemical Physics*, **1979**, 71, 705-712	3.9	304
983	Localized and Delocalized 1s Hole States of the O 2 + Molecular Ion. *Journal of Chemical Physics*, **1972**, 56, 224-226	3.9	299
982	The closed-shell coupled cluster single and double excitation (CCSD) model for the description of electron correlation. A comparison with configuration interaction (CISD) results. *Journal of Chemical Physics*, **1987**, 86, 2881-2890	3.9	291
981	Analytic Raman intensities from molecular electronic wave functions. *Journal of Chemical Physics*, **1986**, 84, 531-532	3.9	291
980	Toward subchemical accuracy in computational thermochemistry: focal point analysis of the heat of formation of NCO and [H,N,C,O] isomers. *Journal of Chemical Physics*, **2004**, 120, 11586-99	3.9	285
979	Analytic evaluation and basis set dependence of intensities of infrared spectra. *Journal of Chemical Physics*, **1986**, 84, 2262-2278	3.9	267
978	Analytic gradients from correlated wave functions via the two-particle density matrix and the unitary group approach. *Journal of Chemical Physics*, **1980**, 72, 4652-4653	3.9	263
977	Concerning zero-point vibrational energy corrections to electronic energies. *Journal of Chemical Physics*, **1991**, 95, 5128-5132	3.9	260
976	A systematic study of molecular vibrational anharmonicity and vibration-rotation interaction by self-consistent-field higher-derivative methods. Linear polyatomic molecules. *Chemical Physics*, **1990**, 145, 427-466	2.3	250
975	The Configuration Interaction Method: Advances in Highly Correlated Approaches. *Advances in Quantum Chemistry*, **1999**, 143-269	1.4	244
974	Coupling term derivation and general implementation of state-specific multireference coupled cluster theories. *Journal of Chemical Physics*, **2007**, 127, 024102	3.9	242
973	Anchoring the water dimer potential energy surface with explicitly correlated computations and focal point analyses. *Journal of Chemical Physics*, **2002**, 116, 690-701	3.9	239
972	Homonuclear 3d transition-metal diatomics: A systematic density functional theory study. *Journal of Chemical Physics*, **2000**, 113, 690-700	3.9	232
971	The analytic configuration interaction gradient method: Application to the cyclic and open isomers of the S3 molecule. *Journal of Chemical Physics*, **1986**, 85, 963-968	3.9	228
970	Electron affinities of the DNA and RNA bases. *Journal of the American Chemical Society*, **2001**, 123, 4023-8	6.4	221

969	Coupled cluster energy derivatives. Analytic Hessian for the closed-shell coupled cluster singles and doubles wave function: Theory and applications. *Journal of Chemical Physics*, **1990**, 92, 4924-4940	3.9	214
968	The shape-driven graphical unitary group approach to the electron correlation problem. Application to the ethylene molecule. *Journal of Chemical Physics*, **1982**, 77, 5584-5592	3.9	213
967	Transition structures for the interchange of hydrogen atoms within the water dimer. *Journal of Chemical Physics*, **1990**, 92, 1240-1247	3.9	208
966	High-order excitations in state-universal and state-specific multireference coupled cluster theories: model systems. *Journal of Chemical Physics*, **2006**, 125, 154113	3.9	199
965	The balance between theoretical method and basis set quality: A systematic study of equilibrium geometries, dipole moments, harmonic vibrational frequencies, and infrared intensities. *Journal of Chemical Physics*, **1993**, 99, 403-416	3.9	196
964	Concerning the precision of standard density functional programs: Gaussian, Molpro, NWChem, Q-Chem, and Gamess. *Computational and Theoretical Chemistry*, **2006**, 768, 175-181		192
963	Gradient techniques for open-shell restricted Hartree□Fock and multiconfiguration self-consistent-field methods. *Journal of Chemical Physics*, **1979**, 71, 1525-1530	3.9	189
962	Concerning the applicability of density functional methods to atomic and molecular negative ions. *Journal of Chemical Physics*, **1996**, 105, 862-864	3.9	186
961	Definitive ab initio studies of model SN2 reactions CH(3)X+F- (X=F, Cl, CN, OH, SH, NH(2), PH(2)). *Chemistry - A European Journal*, **2003**, 9, 2173-92	4.8	185
960	Remarkable aspects of unsaturation in trinuclear metal carbonyl clusters: the triiron species Fe3(CO)n (n = 12, 11, 10, 9). *Journal of the American Chemical Society*, **2006**, 128, 11376-84	16.4	178
959	A viable anionic N-heterocyclic dicarbene. *Journal of the American Chemical Society*, **2010**, 132, 14370-2	16.4	177
958	Potential energy surface for the model unimolecular reaction HNC -□HCN. *Journal of Chemical Physics*, **1975**, 62, 350	3.9	176
957	The photodissociation of formaldehyde: Potential energy surface features. *Journal of Chemical Physics*, **1979**, 70, 5117-5134	3.9	175
956	Interfacing Q-Chem and CHARMM to perform QM/MM reaction path calculations. *Journal of Computational Chemistry*, **2007**, 28, 1485-1502	3.5	170
955	A systematic theoretical study of harmonic vibrational frequencies: The ammonium ion NH4+ and other simple molecules. *Journal of Chemical Physics*, **1980**, 73, 2310-2318	3.9	168
954	Structures and stability of hydrated clusters of hydrogen chloride, HCl(H2O)n, n=1□5. *Journal of Chemical Physics*, **1998**, 109, 973-977	3.9	165
953	The protonated water dimer: Extensive theoretical studies of H5O+2. *Journal of Chemical Physics*, **1994**, 101, 4878-4884	3.9	164
952	Vinylidene: Potential energy surface and unimolecular reaction dynamics. *Journal of Chemical Physics*, **1984**, 80, 4347-4354	3.9	161

951	Analytic second derivatives in restricted Hartree–Fock theory. A method for high-spin open-shell molecular wave functions. *Journal of Chemical Physics*, **1982**, 77, 5647-5654	3.9	161
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949	Generalization of analytic configuration interaction (CI) gradient techniques for potential energy hypersurfaces, including a solution to the coupled perturbed Hartree–Fock equations for multiconfiguration SCF molecular wave functions. *Journal of Chemical Physics*, **1982**, 77, 383-390	3.9	160
948	Psi4 1.4: Open-source software for high-throughput quantum chemistry. *Journal of Chemical Physics* , **2020**, 152, 184108	3.9	158
947	Vinylidene: the final chapter?. *Journal of the American Chemical Society*, **1990**, 112, 8714-8719	16.4	158
946	Large-scale symmetry-adapted perturbation theory computations via density fitting and Laplace transformation techniques: investigating the fundamental forces of DNA-intercalator interactions. *Journal of Chemical Physics*, **2011**, 135, 174107	3.9	145
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943	The automated solution of second quantization equations with applications to the coupled cluster approach. *Theoretica Chimica Acta*, **1991**, 79, 1-42		144
942	Design of a Catalytic Active Site for Electrochemical CO2 Reduction with Mn(I)-Tricarbonyl Species. *Inorganic Chemistry*, **2015**, 54, 5285-94	5.1	138
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940	The optimization of molecular orbitals for coupled cluster wavefunctions. *Chemical Physics Letters*, **1987**, 142, 354-358	2.5	137
939	The weakly exothermic rearrangement of methoxy radical (CH3O?) to the hydroxymethyl radical (CH2OH?). *Journal of Chemical Physics*, **1983**, 78, 845-853	3.9	137
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937	Theoretical Treatment of Penning Ionization. He(1s2s 1S, 3S) + H(1s 2S). *Journal of Chemical Physics*, **1970**, 53, 1421-1427	3.9	136
936	Potential energy surface for the Li+HF–LiF+H reaction. *Journal of Chemical Physics*, **1980**, 72, 4376-4393	3.9	130
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933	Hartree–Fock orbital instability envelopes in highly correlated single-reference wave functions. *Journal of Chemical Physics*, **1997**, 107, 10626-10632	3.9	128
932	An energetically low-lying silacyclopropyne isomer of SiC2. *Journal of Chemical Physics*, **1984**, 80, 3552-3555	3.9	126
931	Interaction potential between two rigid HF molecules. *Journal of Chemical Physics*, **1974**, 60, 855-865	3.9	124
930	Binuclear Homoleptic Iron Carbonyls: Incorporation of Formal Iron–Iron Single, Double, Triple, and Quadruple Bonds, Fe2(CO)x (x = 9, 8, 7, 6). *Journal of the American Chemical Society*, **2000**, 122, 8746-8761	16.4	122
929	Triple excitations in state-specific multireference coupled cluster theory: application of Mk-MRCCSDT and Mk-MRCCSDT-n methods to model systems. *Journal of Chemical Physics*, **2008**, 128, 124104	3.9	119
928	Carbene Rearrangements Unsurpassed: Details of the C(7)H(6) Potential Energy Surface Revealed. *Journal of Organic Chemistry*, **1996**, 61, 7030-7039	4.2	119
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926	Is the uniform electron gas limit important for small Ag clusters? Assessment of different density functionals for Ag(n) (n Journal of Chemical Physics, **2006**, 124, 184102	3.9	118
925	Electron affinity of the guanine-cytosine base pair and structural perturbations upon anion formation. *Journal of the American Chemical Society*, **2002**, 124, 10163-70	16.4	118
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920	The remarkable monobridged structure of Si2H2. *Journal of Chemical Physics*, **1992**, 97, 7990-7998	3.9	116
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917	Ab Initio Potential Curve for the X 3Σg− State of O2. *Journal of Chemical Physics*, **1971**, 54, 2207-2211	3.9	113
916	The dichotomy of dimetallocenes: coaxial versus perpendicular dimetal units in sandwich compounds. *Journal of the American Chemical Society*, **2005**, 127, 2818-9	16.4	112

915	Model studies of chemisorption. Interaction between atomic hydrogen and beryllium clusters. *Journal of Chemical Physics*, **1975**, 62, 4815-4825	3.9	112
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912	Characteristics of novel sandwiched beryllium, magnesium, and calcium dimers: C5H5BeBeC5H5, C5H5MgMgC5H5, and C5H5CaCaC5H5. *Chemical Physics Letters*, **2005**, 402, 414-421	2.5	110
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907	Predicting electron affinities with density functional theory: Some positive results for negative ions. *Journal of Chemical Physics*, **1997**, 107, 2529-2541	3.9	106
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898	A systematic theoretical study of harmonic vibrational frequencies: The single and double excitation coupled cluster (CCSD) method. *Journal of Chemical Physics*, **1988**, 89, 360-366	3.9	99

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894	Avoided intersection of potential energy surfaces: The (H+ + H2, H + H2+) system. *Journal of Chemical Physics*, **1973**, 59, 1286-1292	3.9	97
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