Kimihiko Hirao

List of Publications by Citations

375 papers	18,879 citations	64 h-index	123 g-index
387 ext. papers	19,785 ext. citations	3.9 avg, IF	6.76 L-index

#	Paper	IF	Citations
375	A long-range correction scheme for generalized-gradient-approximation exchange functionals. *Journal of Chemical Physics*, **2001**, 115, 3540-3544	3.9	1881
374	A long-range-corrected time-dependent density functional theory. *Journal of Chemical Physics*, **2004**, 120, 8425-33	3.9	1512
373	Multireference Møller-Plesset method. *Chemical Physics Letters*, **1992**, 190, 374-380	2.5	626
372	Cluster expansion of the wavefunction. Symmetry-adapted-cluster expansion, its variational determination, and extension of open-shell orbital theory. *Journal of Chemical Physics*, **1978**, 68, 2053-2065	3.9	593
371	Multireference Møller-Plesset perturbation theory for high-spin open-shell systems. *Chemical Physics Letters*, **1992**, 196, 397-403	2.5	308
370	State-specific multireference Møller-Plesset perturbation treatment for singlet and triplet excited states, ionized states and electron attached states of H2O. *Chemical Physics Letters*, **1993**, 201, 59-66	2.5	263
369	Nonlinear optical property calculations by the long-range-corrected coupled-perturbed Kohn-Sham method. *Journal of Chemical Physics*, **2005**, 122, 234111	3.9	261
368	A new one-parameter progressive Colle-Salvetti-type correlation functional. *Journal of Chemical Physics*, **1999**, 110, 10664-10678	3.9	259
367	On Koopmans' theorem in density functional theory. *Journal of Chemical Physics*, **2010**, 133, 174101	3.9	258
366	Long-range corrected density functional calculations of chemical reactions: redetermination of parameter. *Journal of Chemical Physics*, **2007**, 126, 154105	3.9	258
365	A density functional study of van der Waals interactions. *Journal of Chemical Physics*, **2002**, 117, 6010-6015	3.9	245
364	The higher-order Douglas-Kroll transformation. *Journal of Chemical Physics*, **2000**, 113, 7786-7789	3.9	243
363	On non-negativity of Fukui function indices. *Journal of Chemical Physics*, **1999**, 110, 8236-8245	3.9	204
362	An investigation of density functionals: The first-row transition metal dimer calculations. *Journal of Chemical Physics*, **2000**, 112, 545-553	3.9	197
361	Excited state geometry optimizations by analytical energy gradient of long-range corrected time-dependent density functional theory. *Journal of Chemical Physics*, **2006**, 124, 144106	3.9	188
360	Polarizability and second hyperpolarizability evaluation of long molecules by the density functional theory with long-range correction. *Journal of Chemical Physics*, **2007**, 126, 014107	3.9	176
359	Intruder state avoidance multireference Møller-Plesset perturbation theory. *Journal of Computational Chemistry*, **2002**, 23, 957-65	3.5	172

358	A generalization of the Davidson method to large nonsymmetric eigenvalue problems. *Journal of Computational Physics*, **1982**, 45, 246-254	4.1	171
357	A density-functional study on pi-aromatic interaction: benzene dimer and naphthalene dimer. *Journal of Chemical Physics*, **2005**, 123, 104307	3.9	167
356	Ab initio vibrational state calculations with a quartic force field: applications to H2CO, C2H4, CH3OH, CH3CCH, and C6H6. *Journal of Chemical Physics*, **2004**, 121, 1383-9	3.9	156
355	Theoretical investigation of the excited states of coumarin dyes for dye-sensitized solar cells. *Journal of Physical Chemistry A*, **2007**, 111, 5544-8	2.8	152
354	Accurate relativistic Gaussian basis sets for H through Lr determined by atomic self-consistent field calculations with the third-order Douglas-Kroll approximation. *Journal of Chemical Physics*, **2001**, 115, 4463-4472	3.9	148
353	Direct vibrational self-consistent field method: Applications to H2O and H2CO. *Journal of Chemical Physics*, **2000**, 113, 1005-1017	3.9	142
352	The Douglas-Kroll-Hess approach. *Chemical Reviews*, **2012**, 112, 385-402	68.1	141
351	The calculation of higher-order energies in the many-body perturbation theory series. *Chemical Physics Letters*, **1985**, 113, 8-12	2.5	140
350	General SCF operator satisfying correct variational condition. *Journal of Chemical Physics*, **1973**, 59, 1457-1462	3.9	139
349	Theoretical Study of the Q and B Bands of Free-Base, Magnesium, and Zinc Porphyrins, and Their Derivatives. *Journal of Physical Chemistry A*, **1999**, 103, 1894-1904	2.8	138
348	Theoretical study of the π→π* excited states of linear polyenes: The energy gap between 11Bu+ and 21Ag− states and their character. *International Journal of Quantum Chemistry*, **1998**, 66, 157-175	2.1	135
347	Long-range corrected density functional study on weakly bound systems: balanced descriptions of various types of molecular interactions. *Journal of Chemical Physics*, **2007**, 126, 234114	3.9	133
346	Mechanism of ferromagnetic coupling in copper(II)-gadolinium(III) complexes. *Journal of the American Chemical Society*, **2004**, 126, 3321-31	16.4	126
345	A density functional study on the adsorption of methanethiolate on the (111) surfaces of noble metals. *Journal of Chemical Physics*, **2001**, 114, 8555-8564	3.9	126
344	A new relativistic theory: a relativistic scheme by eliminating small components (RESC). *Chemical Physics Letters*, **1999**, 302, 383-391	2.5	126
343	Theoretical study of the valence π→π* excited states of polyacenes: Benzene and naphthalene. *Journal of Chemical Physics*, **1996**, 104, 6244-6258	3.9	126
342	Van der Waals interactions studied by density functional theory. *Molecular Physics*, **2005**, 103, 1151-1164	1.7	105
341	On non-negativity of Fukui function indices. II. *Journal of Chemical Physics*, **2000**, 113, 1372-1379	3.9	105

340	An improved long-range corrected hybrid exchange-correlation functional including a short-range Gaussian attenuation (LCgau-BOP). *Journal of Chemical Physics*, **2007**, 127, 154109	3.9	102
339	Vibrational quasi-degenerate perturbation theory: applications to fermi resonance in CO2, H2CO, and C6H6. *Physical Chemistry Chemical Physics*, **2008**, 10, 1781-8	3.6	99
338	Long-range correction for density functional theory. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 375-390	7.9	98
337	Cluster expansion of the wavefunction. Pseduo-orbital theory applied to spin correlation. *Chemical Physics Letters*, **1977**, 47, 569-571	2.5	97
336	Quasi-degenerate perturbation theory with general multiconfiguration self-consistent field reference functions. *Journal of Computational Chemistry*, **2002**, 23, 1166-75	3.5	96
335	A New Mechanism for the First Carbon□Carbon Bond Formation in the MTG Process: A Theoretical Study. *Journal of the American Chemical Society*, **1998**, 120, 8222-8229	16.4	93
334	Multiresolution potential energy surfaces for vibrational state calculations. *Theoretical Chemistry Accounts*, **2007**, 118, 681-691	1.9	91
333	Generation of full-dimensional potential energy surface of intramolecular hydrogen atom transfer in malonaldehyde and tunneling dynamics. *Journal of Chemical Physics*, **2001**, 115, 10647-10655	3.9	90
332	A complete active space valence bond (CASVB) method. *Journal of Chemical Physics*, **1996**, 105, 9227-9239	3.9	86
331	Mulliken population analysis based evaluation of condensed Fukui function indices using fractional molecular charge. *Journal of Chemical Physics*, **2001**, 115, 2901-2907	3.9	82
330	A new computational scheme for the Dirac□Hartree□Fock method employing an efficient integral algorithm. *Journal of Chemical Physics*, **2001**, 114, 6526-6538	3.9	78
329	On the coupling operator method. *Journal of Chemical Physics*, **1974**, 60, 3215-3222	3.9	77
328	Blind test of density-functional-based methods on intermolecular interaction energies. *Journal of Chemical Physics*, **2016**, 145, 124105	3.9	76
327	Tunneling splitting in polyatomic molecules: Application to malonaldehyde. *Journal of Chemical Physics*, **2003**, 119, 10-13	3.9	75
326	Theoretical study of the excitation spectra of five-membered ring compounds: Cyclopentadiene, furan, and pyrrole. *Journal of Chemical Physics*, **1996**, 104, 2312-2320	3.9	75
325	A Theoretical study of ammonia polymers and cluster ions. *Chemical Physics Letters*, **1984**, 104, 184-190	2.5	75
324	Transition state barrier height for the reaction H2CO->H2+CO studied by multireference Mo/ller□Plesset perturbation theory. *Journal of Chemical Physics*, **1997**, 106, 4912-4917	3.9	74
323	Extended Douglas□Kroll transformations applied to the relativistic many-electron Hamiltonian. *Journal of Chemical Physics*, **2003**, 119, 4105-4111	3.9	74

322	Theoretical study of the valence □-> □* excited states of polyacenes: anthracene and naphthacene. *Theoretical Chemistry Accounts*, **1999**, 102, 49-64	1.9	74
321	Cluster expansion of the wavefunction. Pseudo-orbital theory based on the SAC expansion and its application to the spin density of open-shell systems. *Journal of Chemical Physics*, **1978**, 68, 4279-4291	3.9	74
320	Third-order Douglas-Kroll relativistic coupled-cluster theory through connected single, double, triple, and quadruple substitutions: applications to diatomic and triatomic hydrides. *Journal of Chemical Physics*, **2004**, 120, 3297-310	3.9	73
319	Study of low-lying electronic states of ozone by multireference Mo/llerPlesset perturbation method. *Journal of Chemical Physics*, **1995**, 103, 6520-6528	3.9	73
318	Numerical illustration of third-order DouglasKroll method: atomic and molecular properties of superheavy element 112. *Chemical Physics Letters*, **2000**, 329, 511-516	2.5	72
317	Theoretical study of the electronic ground state of iron(II) porphine. II. *Journal of Chemical Physics*, **1999**, 111, 3837-3845	3.9	72
316	Accurate relativistic Gaussian basis sets determined by the third-order DouglasKroll approximation with a finite-nucleus model. *Journal of Chemical Physics*, **2002**, 116, 8270	3.9	68
315	Cluster expansion of the wave function. Electron correlations in the ground state, valence and Rydberg excited states, ionized states, and electron attached states of formaldehyde by SAC and SACCI theories. *Journal of Chemical Physics*, **1981**, 75, 2952-2958	3.9	68
314	An ab initio molecular orbital study of the nuclear volume effects in uranium isotope fractionations. *Journal of Chemical Physics*, **2008**, 129, 164309	3.9	66
313	Cluster expansion of the wave function. Electron correlations in singlet and triplet excited states, ionized states, and electron attached states by SAC and SACCI theories. *International Journal of Quantum Chemistry*, **1981**, 20, 1301-1313	2.1	65
312	Stability and structure of cluster ions in the gas phase: Carbon dioxide with Cl□H3O+, HCO+2, and HCO+. *Journal of Chemical Physics*, **1986**, 84, 2091-2096	3.9	64
311	A new spin-polarized Colle-Salvetti-type correlation energy functional. *Chemical Physics Letters*, **1997**, 268, 510-520	2.5	63
310	Core-excitation energy calculations with a long-range corrected hybrid exchange-correlation functional including a short-range Gaussian attenuation (LCgau-BOP). *Journal of Chemical Physics*, **2008**, 129, 184113	3.9	62
309	Theoretical study of the reactions of pentacoordinated trigonal bipyramidal phosphorus compounds: PH5, PF5, PF4H, PF3H2, PF4CH3, PF3(CH3)2, P(O2C2H4)H3, P(OC3H6)H3, and PO5H4-. *Journal of the American Chemical Society*, **1992**, 114, 16-27	16.4	62
308	An arbitrary order Douglas-Kroll method with polynomial cost. *Journal of Chemical Physics*, **2009**, 130, 044102	3.9	61
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306	Nonlinear optical property calculations of polyynes with long-range corrected hybrid exchange-correlation functionals. *Journal of Chemical Physics*, **2008**, 129, 024117	3.9	59
305	A new implementation of four-component relativistic density functional method for heavy-atom polyatomic systems. *Journal of Chemical Physics*, **2001**, 115, 8267-8273	3.9	59

304	Multireference Mller-Plesset method with a complete active space configuration interaction reference function. *Journal of Chemical Physics*, **2001**, 115, 621-629	3.9	58
303	Relativistic and correlated calculations on the ground and excited states of ThO. *Journal of Chemical Physics*, **2003**, 119, 798-805	3.9	57
302	Calculations of alkane energies using long-range corrected DFT combined with intramolecular van der Waals correlation. *Organic Letters*, **2010**, 12, 1440-3	6.2	56
301	The excited states of long linear polyenes studied by the CASCI-MRMP method. *Chemical Physics Letters*, **2004**, 400, 425-429	2.5	56
300	Identifying and removing intruder states in multireference Mo/ller-Plesset perturbation theory. *Journal of Chemical Physics*, **2001**, 114, 3913-3918	3.9	56
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298	Simple and accurate method to evaluate tunneling splitting in polyatomic molecules. *Journal of Chemical Physics*, **2004**, 120, 5036-45	3.9	54
297	Second-order quasi-degenerate perturbation theory with quasi-complete active space self-consistent field reference functions. *Journal of Chemical Physics*, **2001**, 114, 1133-1141	3.9	53
296	Self-interaction corrections in density functional theory. *Journal of Chemical Physics*, **2014**, 140, 18A513	3.9	52
295	Efficient configuration selection scheme for vibrational second-order perturbation theory. *Journal of Chemical Physics*, **2007**, 127, 034111	3.9	52
294	Density functional studies of UO22+ and AnF6 (An=U, Np, and Pu) using scalar-relativistic effective core potentials. *Journal of Chemical Physics*, **2000**, 113, 7345-7350	3.9	52
293	Approaches to bifurcating reaction path. *Journal of Chemical Physics*, **1996**, 105, 1933-1939	3.9	52
292	A quasi-complete active space self-consistent field method. *Chemical Physics Letters*, **2000**, 317, 90-96	2.5	50
291	Theoretical study of electronic and geometric structures of a series of lanthanide trihalides LnX3 (Ln=La-Lu; X=Cl, F). *Computational and Theoretical Chemistry*, **1999**, 461-462, 203-222		50
290	Theoretical study of bifurcating reaction paths. *Journal of Chemical Physics*, **1997**, 107, 1137-1146	3.9	49
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287	Ab initio calculation of hyperfine splitting constants of molecules. *Journal of Chemical Physics*, **1980**, 73, 1770-1776	3.9	47

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285	Long-range corrected functionals satisfy KoopmansM theorem: calculation of correlation and relaxation energies. *Journal of Computational Chemistry*, **2013**, 34, 958-64	3.5	46
284	Ab initio potential energy surface by modified Shepard interpolation: Application to the CH3+H2->CH4+H reaction. *Journal of Chemical Physics*, **1998**, 109, 4281-4289	3.9	46
283	Direct cluster expansion method. Application to glyoxal. *Journal of Chemical Physics*, **1983**, 79, 5000-5010	3.9	46
282	Theoretical study on the structure and stability of hydrogen-ion clusters Hn+ and Hn (n = 3, 5, 7, 9, 11, 13). *Chemical Physics*, **1983**, 80, 237-243	2.3	45
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267	Communication: a new hybrid exchange correlation functional for band-gap calculations using a short-range Gaussian attenuation (Gaussian-Perdue-Burke-Ernzerhof). *Journal of Chemical Physics*, **2011**, 135, 071103	3.9	40
266	An improved long-range corrected hybrid functional with vanishing Hartree-Fock exchange at zero interelectronic distance (LC2gau-BOP). *Journal of Chemical Physics*, **2009**, 131, 144108	3.9	40
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263	A theoretical study of transition metal hydroxides: CuOH, AgOH and AuOH. *Molecular Physics*, **2003**, 101, 105-110	1.7	40
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248	Cluster expansion of the wavefunction. *Chemical Physics Letters*, **1981**, 79, 292-298	2.5	37
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246	The relativistic complete active-space second-order perturbation theory with the four-component Dirac Hamiltonian. *Journal of Chemical Physics*, **2006**, 125, 234110	3.9	36
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244	Multireference perturbation theory with optimized partitioning. I. Theoretical and computational aspects. *Journal of Chemical Physics*, **2003**, 118, 8197-8206	3.9	36
243	Investigation of the use of density functionals in second- and third-row transition metal dimer calculations. *Journal of Computational Chemistry*, **2001**, 22, 1995-2009	3.5	36
242	A polarizable mixed Hamiltonian model of electronic structure for micro-solvated excited states. I. Energy and gradients formulation and application to formaldehyde (1A2). *Journal of Chemical Physics*, **2002**, 117, 1242-1255	3.9	35
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226	Theoretical study of CH4 photodissociation on the Pt(111) surface. *Journal of Chemical Physics*, **1997**, 107, 415-424	3.9	30
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218	A dual-level approach to density-functional theory. *Journal of Chemical Physics*, **2006**, 124, 184108	3.9	28
217	Theoretical study of valence photoelectron spectrum of OsO4: A spin-orbit RESC-CASPT2 study. *Journal of Chemical Physics*, **2000**, 112, 10142-10148	3.9	28
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