Martin Head-Gordon

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414 papers	56,032 citations	89 h-index	231 g-index
445 ext. papers	62,697 ext. citations	5.7 avg, IF	8.31 L-index

#	Paper	IF	Citations
414	Long-range corrected hybrid density functionals with damped atom-atom dispersion corrections. *Physical Chemistry Chemical Physics*, **2008**, 10, 6615-20	3.6	7709
413	A fifth-order perturbation comparison of electron correlation theories. *Chemical Physics Letters*, **1989**, 157, 479-483	2.5	6685
412	Advances in methods and algorithms in a modern quantum chemistry program package. *Physical Chemistry Chemical Physics*, **2006**, 8, 3172-91	3.6	2371
411	Systematic optimization of long-range corrected hybrid density functionals. *Journal of Chemical Physics*, **2008**, 128, 084106	3.9	2290
410	Toward a systematic molecular orbital theory for excited states. *The Journal of Physical Chemistry*, **1992**, 96, 135-149		2142
409	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics*, **2015**, 113, 184-215	1.7	2068
408	Single-reference ab initio methods for the calculation of excited states of large molecules. *Chemical Reviews*, **2005**, 105, 4009-37	68.1	2042
407	Failure of time-dependent density functional theory for long-range charge-transfer excited states: the zincbacteriochlorin-bacteriochlorin and bacteriochlorophyll-spheroidene complexes. *Journal of the American Chemical Society*, **2004**, 126, 4007-16	16.4	1425
406	Time-dependent density functional theory within the Tamm□Dancoff approximation. *Chemical Physics Letters*, **1999**, 314, 291-299	2.5	1363
405	Long-range charge-transfer excited states in time-dependent density functional theory require non-local exchange. *Journal of Chemical Physics*, **2003**, 119, 2943-2946	3.9	1316
404	Current status of the AMOEBA polarizable force field. *Journal of Physical Chemistry B*, **2010**, 114, 2549-64	3.4	914
403	Thirty years of density functional theory in computational chemistry: an overview and extensive assessment of 200 density functionals. *Molecular Physics*, **2017**, 115, 2315-2372	1.7	891
402	Q-Chem 2.0: a high-performance ab initio electronic structure program package. *Journal of Computational Chemistry*, **2000**, 21, 1532-1548	3.5	588
401	Simulated quantum computation of molecular energies. *Science*, **2005**, 309, 1704-7	33.3	555
400	A doubles correction to electronic excited states from configuration interaction in the space of single substitutions. *Chemical Physics Letters*, **1994**, 219, 21-29	2.5	553
399	The spin□flip approach within time-dependent density functional theory: Theory and applications to diradicals. *Journal of Chemical Physics*, **2003**, 118, 4807-4818	3.9	489
398	Scaled opposite-spin second order M□ller-Plesset correlation energy: an economical electronic structure method. *Journal of Chemical Physics*, **2004**, 121, 9793-802	3.9	440

397	Size-consistent Brueckner theory limited to double substitutions. *Chemical Physics Letters*, **1989**, 164, 185-192	2.5	440
396	Unravelling the origin of intermolecular interactions using absolutely localized molecular orbitals. *Journal of Physical Chemistry A*, **2007**, 111, 8753-65	2.8	433
395	Highly correlated calculations with a polynomial cost algorithm: A study of the density matrix renormalization group. *Journal of Chemical Physics*, **2002**, 116, 4462-4476	3.9	399
394	B97X-V: a 10-parameter, range-separated hybrid, generalized gradient approximation density functional with nonlocal correlation, designed by a survival-of-the-fittest strategy. *Physical Chemistry Chemical Physics*, **2014**, 16, 9904-24	3.6	384
393	Mechanism of CO2 Reduction at Copper Surfaces: Pathways to C2 Products. *ACS Catalysis*, **2018**, 8, 1490-1499	13.7	377
392	The continuous fast multipole method. *Chemical Physics Letters*, **1994**, 230, 8-16	2.5	342
391	B97M-V: A combinatorially optimized, range-separated hybrid, meta-GGA density functional with VV10 nonlocal correlation. *Journal of Chemical Physics*, **2016**, 144, 214110	3.9	332
390	Identification of Possible Pathways for C-C Bond Formation during Electrochemical Reduction of CO2: New Theoretical Insights from an Improved Electrochemical Model. *Journal of Physical Chemistry Letters*, **2016**, 7, 1471-7	6.4	313
389	Resonance-stabilized hydrocarbon-radical chain reactions may explain soot inception and growth. *Science*, **2018**, 361, 997-1000	33.3	286
388	Linear scaling density functional calculations via the continuous fast multipole method. *Chemical Physics Letters*, **1996**, 253, 268-278	2.5	285
387	Fifth order Moeller-Plesset perturbation theory: comparison of existing correlation methods and implementation of new methods correct to fifth order. *The Journal of Physical Chemistry*, **1990**, 94, 5579-5586		285
386	Linear and sublinear scaling formation of Hartree-Fock-type exchange matrices. *Journal of Chemical Physics*, **1998**, 109, 1663-1669	3.9	277
385	Long-range corrected double-hybrid density functionals. *Journal of Chemical Physics*, **2009**, 131, 174105	3.9	271
384	Analysis of Electronic Transitions as the Difference of Electron Attachment and Detachment Densities. *The Journal of Physical Chemistry*, **1995**, 99, 14261-14270		254
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382	How Accurate Are the Minnesota Density Functionals for Noncovalent Interactions, Isomerization Energies, Thermochemistry, and Barrier Heights Involving Molecules Composed of Main-Group Elements?. *Journal of Chemical Theory and Computation*, **2016**, 12, 4303-25	6.4	248
381	Characterizing unpaired electrons from the one-particle density matrix. *Chemical Physics Letters*, **2003**, 372, 508-511	2.5	238
380	Energies and analytic gradients for a coupled-cluster doubles model using variational Brueckner orbitals: Application to symmetry breaking in O4+. *Journal of Chemical Physics*, **1998**, 109, 4171-4181	3.9	216

379	Mapping the genome of meta-generalized gradient approximation density functionals: the search for B97M-V. *Journal of Chemical Physics*, **2015**, 142, 074111	3.9	213
378	Optimized spin-component scaled second-order Møller-Plesset perturbation theory for intermolecular interaction energies. *Molecular Physics*, **2007**, 105, 1073-1083	1.7	213
377	Size-consistent wave functions for nondynamical correlation energy: The valence active space optimized orbital coupled-cluster doubles model. *Journal of Chemical Physics*, **1998**, 109, 10669-10678	3.9	211
376	Quantum Chemistry and Molecular Processes. *The Journal of Physical Chemistry*, **1996**, 100, 13213-13225		210
375	Time-dependent density functional study on the electronic excitation energies of polycyclic aromatic hydrocarbon radical cations of naphthalene, anthracene, pyrene, and perylene. *Journal of Chemical Physics*, **1999**, 111, 8904-8912	3.9	195
374	Restricted active space spin-flip configuration interaction approach: theory, implementation and examples. *Physical Chemistry Chemical Physics*, **2009**, 11, 9779-90	3.6	187
373	Linear scaling computation of the Fock matrix. II. Rigorous bounds on exchange integrals and incremental Fock build. *Journal of Chemical Physics*, **1997**, 106, 9708-9717	3.9	186
372	Probing non-covalent interactions with a second generation energy decomposition analysis using absolutely localized molecular orbitals. *Physical Chemistry Chemical Physics*, **2016**, 18, 23067-79	3.6	184
371	Dispersion-corrected Møller-Plesset second-order perturbation theory. *Journal of Chemical Physics*, **2009**, 131, 094106	3.9	172
370	Configuration interaction singles, time-dependent Hartree–Fock, and time-dependent density functional theory for the electronic excited states of extended systems. *Journal of Chemical Physics*, **1999**, 111, 10774-10786	3.9	169
369	An efficient self-consistent field method for large systems of weakly interacting components. *Journal of Chemical Physics*, **2006**, 124, 204105	3.9	166
368	Mechanistic insights into electrochemical reduction of CO over Ag using density functional theory and transport models. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E8812-E8821	11.5	163
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365	Closely approximating second-order Mo/llerPlesset perturbation theory with a local triatomics in molecules model. *Journal of Chemical Physics*, **2000**, 112, 3592-3601	3.9	158
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363	Vibronically coherent ultrafast triplet-pair formation and subsequent thermally activated dissociation control efficient endothermic singlet fission. *Nature Chemistry*, **2017**, 9, 1205-1212	17.6	151
362	Second-order perturbation corrections to singles and doubles coupled-cluster methods: General theory and application to the valence optimized doubles model. *Journal of Chemical Physics*, **2000**, 113, 3548-3560	3.9	151

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359	Catalytic proton reduction with transition metal complexes of the redox-active ligand bpy2PYMe. *Chemical Science*, **2013**, 4, 3934	9.4	141
358	Orbital-optimized opposite-spin scaled second-order correlation: an economical method to improve the description of open-shell molecules. *Journal of Chemical Physics*, **2007**, 126, 164101	3.9	137
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306	Hartree-Fock solutions as a quasidiabatic basis for nonorthogonal configuration interaction. *Journal of Chemical Physics*, **2009**, 131, 124113	3.9	67
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List of Publications

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