Rodney J Bartlett

List of Publications by Citations

587 papers	52,921 citations	105 h-index	212 g-index
606 ext. papers	55,548 ext. citations	3.9 avg, IF	7.81 L-index

#	Paper	IF	Citations
587	A full coupled-cluster singles and doubles model: The inclusion of disconnected triples. *Journal of Chemical Physics*, **1982**, 76, 1910-1918	3.9	5133
586	Coupled-cluster theory in quantum chemistry. *Reviews of Modern Physics*, **2007**, 79, 291-352	40.5	2110
585	The equation of motion coupled-cluster method. A systematic biorthogonal approach to molecular excitation energies, transition probabilities, and excited state properties. *Journal of Chemical Physics*, **1993**, 98, 7029-7039	3.9	1895
584	Coupled-cluster methods with noniterative triple excitations for restricted open-shell Hartree–Fock and other general single determinant reference functions. Energies and analytical gradients. *Journal of Chemical Physics*, **1993**, 98, 8718-8733	3.9	1697
583	Many-body perturbation theory, coupled-pair many-electron theory, and the importance of quadruple excitations for the correlation problem. *International Journal of Quantum Chemistry*, **1978**, 14, 561-581	2.1	1321
582	Coupled-cluster approach to molecular structure and spectra: a step toward predictive quantum chemistry. *The Journal of Physical Chemistry*, **1989**, 93, 1697-1708		1101
581	The full CCSDT model for molecular electronic structure. *Journal of Chemical Physics*, **1987**, 86, 7041-7050	3.9	1009
580	Many-Body Methods in Chemistry and Physics: MBPT and Coupled-Cluster Theory **2009**,		879
579	Towards a full CCSDT model for electron correlation. *Journal of Chemical Physics*, **1985**, 83, 4041-4046	3.9	795
578	Non-iterative fifth-order triple and quadruple excitation energy corrections in correlated methods. *Chemical Physics Letters*, **1990**, 165, 513-522	2.5	736
577	A linear response, coupled-cluster theory for excitation energy. *International Journal of Quantum Chemistry*, **1984**, 26, 255-265	2.1	564
576	The equation-of-motion coupled-cluster method: Excitation energies of Be and CO. *Chemical Physics Letters*, **1989**, 164, 57-62	2.5	532
575	An open-shell spin-restricted coupled cluster method: application to ionization potentials in nitrogen. *The Journal of Physical Chemistry*, **1988**, 92, 3033-3036		486
574	Analytic energy derivatives in many-body methods. I. First derivatives. *Journal of Chemical Physics*, **1989**, 90, 1752-1766	3.9	484
573	Equation of motion coupled cluster method for electron attachment. *Journal of Chemical Physics*, **1995**, 102, 3629-3647	3.9	458
572	A coupled cluster approach with triple excitations. *Journal of Chemical Physics*, **1984**, 81, 5906-5912	3.9	401
571	The ACES II program system. *International Journal of Quantum Chemistry*, **1992**, 44, 879-894	2.1	390

570	Multi-reference averaged quadratic coupled-cluster method: a size-extensive modification of multi-reference CI. *Chemical Physics Letters*, **1993**, 214, 481-488	2.5	386
569	The equation-of-motion coupled-cluster method. Applications to open- and closed-shell reference states. *Chemical Physics Letters*, **1993**, 207, 414-423	2.5	370
568	The coupled-cluster single, double, triple, and quadruple excitation method. *Journal of Chemical Physics*, **1992**, 97, 4282-4288	3.9	355
567	Multireference nature of chemistry: the coupled-cluster view. *Chemical Reviews*, **2012**, 112, 182-243	68.1	349
566	Molecular Applications of Coupled Cluster and Many-Body Perturbation Methods. *Physica Scripta*, **1980**, 21, 255-265	2.6	342
565	Frequency dependent nonlinear optical properties of molecules. *Journal of Chemical Physics*, **1986**, 85, 976-989	3.9	338
564	Many-body perturbation theory applied to electron pair correlation energies. I. Closed-shell first-row diatomic hydrides. *Journal of Chemical Physics*, **1975**, 62, 3258-3268	3.9	337
563	Molecular hyperpolarizabilities. *Journal of Chemical Physics*, **1993**, 98, 3022-3037	3.9	311
562	The description of N2 and F2 potential energy surfaces using multireference coupled cluster theory. *Journal of Chemical Physics*, **1987**, 86, 887-907	3.9	306
561	The coupled-cluster single, double, and triple excitation model for open-shell single reference functions. *Journal of Chemical Physics*, **1990**, 93, 6104-6105	3.9	304
560	COUPLED-CLUSTER THEORY: AN OVERVIEW OF RECENT DEVELOPMENTS. *Advanced Series in Physical Chemistry*, **1995**, 1047-1131		283
559	Similarity transformed equation-of-motion coupled-cluster theory: Details, examples, and comparisons. *Journal of Chemical Physics*, **1997**, 107, 6812-6830	3.9	263
558	Open-shell analytical energy gradients for triple excitation many-body, coupled-cluster methods: MBPT(4), CCSD+T(CCSD), CCSD(T),and QCISD(T). *Chemical Physics Letters*, **1992**, 200, 1-7	2.5	263
557	Exact Exchange Treatment for Molecules in Finite-Basis-Set Kohn-Sham Theory. *Physical Review Letters*, **1999**, 83, 5455-5458	7.4	252
556	Electron correlation effects on the theoretical calculation of nuclear magnetic resonance spin□spin coupling constants. *Journal of Chemical Physics*, **1996**, 104, 3290-3305	3.9	250
555	Towards a full CCSDT model for electron correlation. CCSDT-n models. *Chemical Physics Letters*, **1987**, 134, 126-132	2.5	247
554	Coupled-cluster calculations of indirect nuclear coupling constants: The importance of non-Fermi contact contributions. *Journal of Chemical Physics*, **1994**, 101, 2186-2191	3.9	241
553	Fifth-Order Many-Body Perturbation Theory and Its Relationship to Various Coupled-Cluster Approaches. *Advances in Quantum Chemistry*, **1986**, 281-344	1.4	241

552	A theoretical study of the water dimer interaction. *Journal of Chemical Physics*, **1988**, 89, 3662-3673	3.9	240
551	The quartic force field of H2O determined by many-body methods that include quadruple excitation effects. *Journal of Chemical Physics*, **1979**, 71, 281-291	3.9	236
550	Full configuration interaction and state of the art correlation calculations on water in a valence double-zeta basis with polarization functions. *Journal of Chemical Physics*, **1996**, 104, 8007-8015	3.9	235
549	Coupled-cluster theory and its equation-of-motion extensions. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 126-138	7.9	231
548	Applications of Post-Hartree–Fock Methods: A Tutorial. *Reviews in Computational Chemistry*, **2007**, 65-169		230
547	Coupled-cluster open-shell analytic gradients: Implementation of the direct product decomposition approach in energy gradient calculations. *Journal of Chemical Physics*, **1991**, 95, 2623-2638	3.9	229
546	Economical triple excitation equation-of-motion coupled-cluster methods for excitation energies. *Chemical Physics Letters*, **1995**, 233, 81-87	2.5	228
545	A new method for excited states: Similarity transformed equation-of-motion coupled-cluster theory. *Journal of Chemical Physics*, **1997**, 106, 6441-6448	3.9	225
544	Recursive intermediate factorization and complete computational linearization of the coupled-cluster single, double, triple, and quadruple excitation equations. *Theoretica Chimica Acta*, **1991**, 80, 387-405		222
543	A direct product decomposition approach for symmetry exploitation in many-body methods. I. Energy calculations. *Journal of Chemical Physics*, **1991**, 94, 4334-4345	3.9	220
542	Coupled-cluster methods with internal and semi-internal triply and quadruply excited clusters: CCSDt and CCSDtq approaches. *Journal of Chemical Physics*, **1999**, 110, 6103-6122	3.9	219
541	Molecular applications of multireference coupled-cluster methods using an incomplete model space: Direct calculation of excitation energies. *Journal of Chemical Physics*, **1988**, 88, 4357-4366	3.9	219
540	Many-body perturbation theory with a restricted open-shell Hartree–Fock reference. *Chemical Physics Letters*, **1991**, 187, 21-28	2.5	213
539	Molecular hyperpolarizabilities. I. Theoretical calculations including correlation. *Physical Review A*, **1979**, 20, 1313-1322	2.6	211
538	Coupled-cluster theory for excited electronic states: The full equation-of-motion coupled-cluster single, double, and triple excitation method. *Journal of Chemical Physics*, **2001**, 115, 8263-8266	3.9	206
537	Comparison of high-order many-body perturbation theory and configuration interaction for H2O. *Chemical Physics Letters*, **1977**, 50, 190-198	2.5	206
536	Approximately extensive modifications of the multireference configuration interaction method: A theoretical and practical analysis. *Journal of Chemical Physics*, **1995**, 103, 3600-3612	3.9	205
535	A multi-reference coupled-cluster method for molecular applications. *Chemical Physics Letters*, **1984**, 104, 424-430	2.5	204

534	Iterative and non-iterative triple excitation corrections in coupled-cluster methods for excited electronic states: the EOM-CCSDT-3 and EOM-CCSD(T) methods. *Chemical Physics Letters*, **1996**, 258, 581-588	2.5	201
533	Analytic energy gradients for open-shell coupled-cluster singles and doubles (CCSD) calculations using restricted open-shell HartreeFock (ROHF) reference functions. *Chemical Physics Letters*, **1991**, 182, 207-215	2.5	195
532	Accurate binding energies of diborane, borane carbonyl, and borazane determined by many-body perturbation theory. *Journal of the American Chemical Society*, **1979**, 101, 2856-2862	16.4	195
531	A systematic comparison of molecular properties obtained using HartreeFock, a hybrid HartreeFock density-functional-theory, and coupled-cluster methods. *Journal of Chemical Physics*, **1994**, 100, 6550-6561	3.9	188
530	Hyperpolarizabilities of the hydrogen fluoride molecule: A discrepancy between theory and experiment?. *Journal of Chemical Physics*, **1986**, 84, 2726-2733	3.9	187
529	Noniterative energy corrections through fifth-order to the coupled cluster singles and doubles method. *Journal of Chemical Physics*, **1998**, 108, 5243-5254	3.9	185
528	Multireference coupled-cluster methods using an incomplete model space: Application to ionization potentials and excitation energies of formaldehyde. *Chemical Physics Letters*, **1987**, 137, 273-278	2.5	180
527	Can optimized effective potentials be determined uniquely?. *Journal of Chemical Physics*, **2001**, 115, 1635-1649	3.9	178
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522	The reduced linear equation method in coupled cluster theory.. *Journal of Chemical Physics*, **1981**, 75, 1284-1292	3.9	169
521	Stability and energetics of metastable molecules: tetraazatetrahedrane (N4), hexaazabenzene (N6), and octaazacubane (N8). *The Journal of Physical Chemistry*, **1992**, 96, 1173-1178		168
520	Equation-of-motion coupled cluster method with full inclusion of the connected triple excitations for ionized states: IP-EOM-CCSDT. *Journal of Chemical Physics*, **2003**, 118, 1128-1136	3.9	164
519	Perturbative corrections to coupled-cluster and equation-of-motion coupled-cluster energies: A determinantal analysis. *Journal of Chemical Physics*, **2001**, 114, 3919-3928	3.9	160
518	Improving upon CCSD(T): LambdaCCSD(T). I. Potential energy surfaces. *Journal of Chemical Physics*, **2008**, 128, 044110	3.9	157
517	Property evaluation and orbital relaxation in coupled cluster methods. *Journal of Chemical Physics*, **1987**, 87, 502-509	3.9	155

516	The exchange-correlation potential in ab initio density functional theory. *Journal of Chemical Physics*, **2005**, 122, 34104	3.9	150
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514	A CCSD (T) investigation of carbonyl oxide and dioxirane. Equilibrium geometries, dipole moments, infrared spectra, heats of formation and isomerization energies. *Chemical Physics Letters*, **1993**, 209, 547-556	2.5	150
513	An efficient way to include connected quadruple contributions into the coupled cluster method. *Journal of Chemical Physics*, **1998**, 108, 9221-9226	3.9	147
512	Alternative coupled-cluster ansätze II. The unitary coupled-cluster method. *Chemical Physics Letters* , **1989**, 155, 133-140	2.5	147
511	Ab initio density functional theory: the best of both worlds?. *Journal of Chemical Physics*, **2005**, 123, 62205	3.9	143
510	Description of core-excitation spectra by the open-shell electron-attachment equation-of-motion coupled cluster method. *Journal of Chemical Physics*, **1995**, 102, 6735-6756	3.9	142
509	A theoretical study of linear carbon cluster monoanions, C□, and dianions, C2□ (n=2□10). *Journal of Chemical Physics*, **1992**, 97, 3445-3457	3.9	142
508	Second-order many-body perturbation-theory calculations in extended systems. *Journal of Chemical Physics*, **1996**, 104, 8553-8565	3.9	139
507	A general model-space coupled-cluster method using a Hilbert-space approach. *Journal of Chemical Physics*, **1990**, 92, 561-567	3.9	139
506	A multireference coupled-cluster method for special classes of incomplete model spaces. *Journal of Chemical Physics*, **1989**, 91, 6187-6194	3.9	137
505	Electron affinities of CO2, OCS, and CS2. *Journal of Chemical Physics*, **1998**, 108, 6756-6762	3.9	135
504	Similarity transformed equation-of-motion coupled-cluster study of ionized, electron attached, and excited states of free base porphin. *Journal of Chemical Physics*, **1997**, 106, 6449-6455	3.9	133
503	Ab initio density functional theory: OEP-MBPT(2). A new orbital-dependent correlation functional. *Journal of Chemical Physics*, **2002**, 116, 4415-4425	3.9	132
502	Coupled-cluster calculations of the excitation energies of ethylene, butadiene, and cyclopentadiene. *Journal of Chemical Physics*, **1996**, 105, 6979-6988	3.9	132
501	C2V Insertion pathway for BeH2: A test problem for the coupled-cluster single and double excitation model. *International Journal of Quantum Chemistry*, **1983**, 23, 835-845	2.1	132
500	Coupled-cluster calculations on the C2 molecule and the C+2 and C□ molecular ions. *Journal of Chemical Physics*, **1992**, 96, 6073-6084	3.9	130
499	The inclusion of connected triple excitations in the equation-of-motion coupled-cluster method. *Journal of Chemical Physics*, **1994**, 101, 3073-3078	3.9	129

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496	The expectation value coupled-cluster method and analytical energy derivatives. *Chemical Physics Letters*, **1988**, 150, 29-36	2.5	122
495	A Hilbert space multi-reference coupled-cluster study of the H4 model system. *Theoretica Chimica Acta*, **1991**, 80, 335-348		120
494	Isomers and excitation energies of C4. *Journal of Chemical Physics*, **1986**, 84, 3284-3290	3.9	120
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489	A theoretical study of the valence- and dipole-bound states of the nitromethane anion. *Journal of Chemical Physics*, **1996**, 105, 8785-8792	3.9	112
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486	On the Stability of N5+N5-. *Journal of Physical Chemistry A*, **2002**, 106, 4639-4644	2.8	108
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479	Simplified methods for equation-of-motion coupled-cluster excited state calculations. *Chemical Physics Letters*, **1996**, 248, 189-198	2.5	104
478	Theory and implementation of the MBPT density matrix. An application to one-electron properties. *Chemical Physics Letters*, **1988**, 147, 359-366	2.5	104
477	Predicted NMR Spectra for Ethyl Carbocations: A Fingerprint for Nonclassical Hydrogen-Bridged Structures. *Journal of the American Chemical Society*, **1995**, 117, 8476-8477	16.4	103
476	New perspectives on unitary coupled-cluster theory. *International Journal of Quantum Chemistry*, **2006**, 106, 3393-3401	2.1	102
475	Coupled-cluster method tailored by configuration interaction. *Journal of Chemical Physics*, **2005**, 123, 074106	3.9	101
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472	EOMXCC: A New Coupled-Cluster Method for Electronic Excited States. *Advances in Quantum Chemistry*, **1999**, 34, 295-380	1.4	99
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459	Time-dependent density functional theory employing optimized effective potentials. *Journal of Chemical Physics*, **2002**, 116, 6468-6481	3.9	92
458	High-order determinantal equation-of-motion coupled-cluster calculations for electronic excited states. *Chemical Physics Letters*, **2000**, 326, 255-262	2.5	92
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455	Analytic evaluation of energy gradients at the coupled-cluster singles and doubles level using quasi-restricted Hartree–Fock open-shell reference functions. *Journal of Chemical Physics*, **1991**, 95, 2639-2645	3.9	90
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427	Coupled-cluster calculations of Raman intensities and their application to N4 and N5 *Chemical Physics Letters*, **1999**, 314, 381-387	2.5	72

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