Rodney J Bartlett

List of Publications by Year in Descending Order

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	Benchmarking isotropic hyperfine coupling constants using (QTP) DFT functionals and coupled cluster theory.. *Journal of Chemical Physics*, **2022**, 156, 094107	3.9	0
586	The Devil's Triangle of Kohn-Sham density functional theory and excited states. *Journal of Chemical Physics*, **2021**, 154, 074106	3.9	6
585	Equation of motion coupled-cluster study of core excitation spectra II: Beyond the dipole approximation. *Journal of Chemical Physics*, **2021**, 155, 094103	3.9	2
584	Basis Sets for Correlated Methods. *Lecture Notes in Quantum Chemistry II*, **2021**, 129-155	0.6	
583	Advanced concepts in electronic structure (ACES) software programs. *Journal of Chemical Physics*, **2020**, 152, 184105	3.9	12
582	A route to improving RPA excitation energies through its connection to equation-of-motion coupled cluster theory. *Journal of Chemical Physics*, **2020**, 153, 234101	3.9	4
581	Index of multi-determinantal and multi-reference character in coupled-cluster theory. *Journal of Chemical Physics*, **2020**, 153, 234103	3.9	5
580	Spin-orbit split ionized and electron-attached states using explicitly-correlated equation-of-motion coupled-cluster singles and doubles eigenvectors. *Chemical Physics Letters*, **2019**, 730, 372-377	2.5	3
579	Vertical valence ionization potential benchmarks from equation-of-motion coupled cluster theory and QTP functionals. *Journal of Chemical Physics*, **2019**, 150, 074108	3.9	25
578	Behind the success of modified coupled-cluster methods: addition by subtraction. *Molecular Physics* , **2019**, 117, 2201-2216	1.7	5
577	Adventures in DFT by a wavefunction theorist. *Journal of Chemical Physics*, **2019**, 151, 160901	3.9	16
576	Equation of motion coupled-cluster for core excitation spectra: Two complementary approaches. *Journal of Chemical Physics*, **2019**, 151, 164117	3.9	17
575	Similarity-transformed equation-of-motion coupled-cluster singles and doubles method with spin-orbit effects for excited states. *Journal of Chemical Physics*, **2019**, 151, 134110	3.9	7
574	Perturbation Improved Natural Linear-Scaled Coupled-Cluster Method and Its Application to Conformational Analysis. *Journal of Physical Chemistry A*, **2019**, 123, 371-381	2.8	1
573	Explicitly-correlated double ionization potentials and double electron attachment equation-of-motion coupled cluster methods. *Chemical Physics Letters*, **2018**, 692, 191-195	2.5	8
572	Reference dependence of the two-determinant coupled-cluster method for triplet and open-shell singlet states of biradical molecules. *Journal of Chemical Physics*, **2018**, 148, 164102	3.9	2
571	Vibrational Characterization of Radical Ion Adducts between Imidazole and CO. *Journal of Physical Chemistry A*, **2018**, 122, 3805-3810	2.8	3

570	Spin-orbit splitted excited states using explicitly-correlated equation-of-motion coupled-cluster singles and doubles eigenvectors. *Chemical Physics Letters*, **2018**, 698, 171-175	2.5	3
569	Non-empirical exchange-correlation parameterizations based on exact conditions from correlated orbital theory. *Journal of Chemical Physics*, **2018**, 148, 184106	3.9	17
568	Valence and charge-transfer optical properties for some SiC (m, n⁄12) clusters: Comparing TD-DFT, complete-basis-limit EOMCC, and benchmarks from spectroscopy. *Journal of Chemical Physics*, **2018**, 148, 174309	3.9	1
567	Accurate computation of X-ray absorption spectra with ionization potential optimized global hybrid functional. *Journal of Chemical Physics*, **2018**, 149, 064111	3.9	15
566	Coupled-cluster based basis sets for valence correlation calculations. New primitives, frozen atomic natural orbitals, and basis sets from double to hextuple zeta for atoms H, He, and B-Ne. *Journal of Chemical Physics*, **2018**, 149, 064105	3.9	3
565	Rigorous and Empirical Approaches to Correlated Single-Particle Theories **2018**, 1-20		1
564	Low scaling EOM-CCSD and EOM-MBPT(2) method with natural transition orbitals. *Journal of Chemical Physics*, **2018**, 149, 184103	3.9	8
563	Communication: Can excitation energies be obtained from orbital energies in a correlated orbital theory?. *Journal of Chemical Physics*, **2018**, 149, 131101	3.9	23
562	Communication: Coupled cluster and many-body perturbation theory for fractional charges and spins. *Journal of Chemical Physics*, **2018**, 148, 221103	3.9	10
561	Explicitly-correlated coupled cluster method for long-range dispersion coefficients. *Chemical Physics Letters*, **2017**, 672, 133-136	2.5	2
560	Excited states from modified coupled cluster methods: Are they any better than EOM CCSD?. *Journal of Chemical Physics*, **2017**, 146, 144104	3.9	26
559	Does the ionization potential condition employed in QTP functionals mitigate the self-interaction error?. *Journal of Chemical Physics*, **2017**, 146, 034102	3.9	20
558	Towards core-excitation spectra in attosecond spectroscopy: A coupled-cluster study of ClF. *Chemical Physics Letters*, **2017**, 683, 68-75	2.5	11
557	Elementary reaction profile and chemical kinetics study of [C(1D)/(3P) + SiH4] with the CCSD(T) method. *Chemical Physics Letters*, **2017**, 680, 61-68	2.5	2
556	Automatic generation of reaction energy databases from highly accurate atomization energy benchmark sets. *Physical Chemistry Chemical Physics*, **2017**, 19, 9798-9805	3.6	23
555	The power of exact conditions in electronic structure theory. *Chemical Physics Letters*, **2017**, 669, 54-70	2.5	27
554	A note on the accuracy of KS-DFT densities. *Journal of Chemical Physics*, **2017**, 147, 204103	3.9	18
553	Single-reference coupled cluster theory for multi-reference problems. *Journal of Chemical Physics*, **2017**, 147, 184101	3.9	19

552	Excitation energies with spin-orbit couplings using equation-of-motion coupled-cluster singles and doubles eigenvectors. *Journal of Chemical Physics*, **2017**, 147, 164118	3.9	11
551	Determination of consistent semiempirical one-centre integrals based on coupled-cluster theory. *Molecular Physics*, **2017**, 115, 538-544	1.7	5
550	Aces4: A Platform for Computational Chemistry Calculations with Extremely Large Block-Sparse Arrays **2017**,		1
549	Gas phase RDX decomposition pathways using coupled cluster theory. *Physical Chemistry Chemical Physics*, **2016**, 18, 26069-26077	3.6	21
548	Predictive coupled-cluster isomer orderings for some SinCm (m, n≤12) clusters: A pragmatic comparison between DFT and complete basis limit coupled-cluster benchmarks. *Journal of Chemical Physics*, **2016**, 145, 024312	3.9	9
547	Ionization potential optimized double-hybrid density functional approximations. *Journal of Chemical Physics*, **2016**, 145, 104106	3.9	16
546	Increasing the applicability of density functional theory. V. X-ray absorption spectra with ionization potential corrected exchange and correlation potentials. *Journal of Chemical Physics*, **2016**, 145, 034108	3.9	20
545	Electric multipole moments calculation with explicitly correlated coupled-cluster wavefunctions. *Journal of Chemical Physics*, **2016**, 144, 234107	3.9	5
544	The QTP family of consistent functionals and potentials in Kohn-Sham density functional theory. *Journal of Chemical Physics*, **2016**, 145, 034107	3.9	55
543	Explicitly correlated coupled-cluster theory for static polarizabilities. *Journal of Chemical Physics*, **2016**, 145, 134104	3.9	5
542	Assessing the distinguishable cluster approximation based on the triple bond-breaking in the nitrogen molecule. *Journal of Chemical Physics*, **2016**, 144, 124117	3.9	15
541	Coupled-cluster based basis sets for valence correlation calculations. *Journal of Chemical Physics*, **2016**, 144, 104106	3.9	10
540	Facile C(sp(2))-C(sp(2)) bond cleavage in oxalic acid-derived radicals. *Journal of the American Chemical Society*, **2015**, 137, 3248-52	16.4	10
539	The benzene radical anion: A computationally demanding prototype for aromatic anions. *Journal of Chemical Physics*, **2015**, 142, 204304	3.9	18
538	Coupled cluster geometries and energies of C20 carbon cluster isomers □A new benchmark study. *Chemical Physics Letters*, **2015**, 629, 76-80	2.5	24
537	Spectroscopic analysis of diphosphatriazolate anion (P2N3)□by coupled-cluster methods as a step toward N5□*Chemical Physics Letters*, **2015**, 640, 68-71	2.5	6
536	Molecular cluster perturbation theory. I. Formalism. *Molecular Physics*, **2015**, 113, 3459-3470	1.7	5
535	Explicitly correlated similarity transformed equation-of-motion coupled-cluster method. *Journal of Chemical Physics*, **2015**, 143, 074111	3.9	11

534	Approximating electronically excited states with equation-of-motion linear coupled-cluster theory. *Journal of Chemical Physics*, **2015**, 143, 164103	3.9	17
533	Algebraic connectivity analysis in molecular electronic structure theory II: total exponential formulation of second-quantised correlated methods. *Molecular Physics*, **2014**, 112, 213-260	1.7	8
532	Gas-Phase Synthesis of Boronylallene (HCCCH(BO)) under Single Collision Conditions: A Crossed Molecular Beams and Computational Study. *Journal of Physical Chemistry A*, **2014**, 118, 3810-3819	2.8	6
531	Equation-of-motion coupled cluster method for ionized states with partial inclusion of connected triples: Assessment of the accuracy in regular and explicitly-correlated approaches. *Chemical Physics Letters*, **2014**, 610-611, 173-178	2.5	3
530	Transition metal atomic multiplet states through the lens of single-reference coupled-cluster and the equation-of-motion coupled-cluster methods. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	9
529	At what chain length do unbranched alkanes prefer folded conformations?. *Journal of Physical Chemistry A*, **2014**, 118, 1706-12	2.8	50
528	Singlet–triplet separations of di-radicals treated by the DEA/DIP-EOM-CCSD methods. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	20
527	Relaxed active space: fixing tailored-CC with high order coupled cluster. II. *Journal of Chemical Physics*, **2014**, 140, 064113	3.9	19
526	Complex absorbing potential based equation-of-motion coupled cluster method for the potential energy curve of CO_2^- anion. *Journal of Chemical Physics*, **2014**, 141, 164113	3.9	16
525	Correlation correction to configuration interaction singles from coupled cluster perturbation theory. *Journal of Chemical Physics*, **2014**, 140, 234108	3.9	3
524	Monte Carlo configuration interaction with perturbation corrections for dissociation energies of first row diatomic molecules: C2, N2, O2, CO, and NO. *Journal of Chemical Physics*, **2014**, 140, 084114	3.9	19
523	Increasing the applicability of density functional theory. IV. Consequences of ionization-potential improved exchange-correlation potentials. *Journal of Chemical Physics*, **2014**, 140, 18A534	3.9	56
522	Theoretical study of low-lying excited states of HSX (X = F, Cl, Br, I). *Chemical Physics Letters*, **2014**, 602, 34-39	2.5	1
521	Geometric Metastability in Molecules as a Way to Enhance Energy Storage. *Advances in Quantum Chemistry*, **2014**, 69, 147-170	1.4	2
520	Pragmatic ab initio prediction of enthalpies of formation for large molecules: accuracy of MP2 geometries and frequencies using CCSD(T) correlation energies. *Journal of Molecular Modeling*, **2013**, 19, 2821-4	2	
519	The great diversity of HMX conformers: probing the potential energy surface using CCSD(T). *Journal of Physical Chemistry A*, **2013**, 117, 3467-74	2.8	12
518	Benchmarking for perturbative triple-excitations in EE-EOM-CC methods. *Journal of Physical Chemistry A*, **2013**, 117, 2569-79	2.8	51
517	Benchmark studies on the building blocks of DNA. 3. Watson-Crick and stacked base pairs. *Journal of Physical Chemistry A*, **2013**, 117, 3149-57	2.8	35

516	Potential energy curves via double electron-attachment calculations: dissociation of alkali metal dimers. *Journal of Chemical Physics*, **2013**, 138, 194103	3.9	36
515	A crossed molecular beam and ab-initio investigation of the reaction of boron monoxide (BO; X2□) with methylacetylene (CH3CCH; X1A1): competing atomic hydrogen and methyl loss pathways. *Journal of Physical Chemistry A*, **2013**, 117, 11794-807	2.8	13
514	Infinite order relaxation effects for core ionization energies with a variational coupled cluster ansatz. *Chemical Physics Letters*, **2013**, 555, 235-238	2.5	12
513	Increasing the applicability of DFT I: Non-variational correlation corrections from Hartree□ock DFT for predicting transition states. *Chemical Physics Letters*, **2012**, 524, 10-15	2.5	61
512	The equation-of-motion coupled cluster method for triple electron attached states. *Journal of Chemical Physics*, **2012**, 137, 174102	3.9	21
511	Conformers of CL-20 explosive and ab initio refinement using perturbation theory: implications to detonation mechanisms. *Journal of Physical Chemistry A*, **2012**, 116, 12129-35	2.8	18
510	Relaxed active space: fixing tailored-CC with high order coupled cluster. I. *Journal of Chemical Physics*, **2012**, 137, 214103	3.9	23
509	Benchmark studies on the building blocks of DNA. 2. Effect of biological environment on the electronic excitation spectrum of nucleobases. *Journal of Physical Chemistry A*, **2012**, 116, 8851-60	2.8	31
508	Benchmark studies on the building blocks of DNA. 1. Superiority of coupled cluster methods in describing the excited states of nucleobases in the Franck-Condon region. *Journal of Physical Chemistry A*, **2012**, 116, 6702-10	2.8	80
507	Increasing the applicability of density functional theory. III. Do consistent Kohn-Sham density functional methods exist?. *Journal of Chemical Physics*, **2012**, 137, 134102	3.9	31
506	Coupled-cluster theory and its equation-of-motion extensions. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 126-138	7.9	231
505	Multireference nature of chemistry: the coupled-cluster view. *Chemical Reviews*, **2012**, 112, 182-243	68.1	349
504	Increasing the applicability of density functional theory. II. Correlation potentials from the random phase approximation and beyond. *Journal of Chemical Physics*, **2012**, 136, 044105	3.9	63
503	A remark on the disconnected nature of Lagrange equations in the context of a linear-scaling implementation of the coupled-cluster energy gradients. *Molecular Physics*, **2012**, 110, 2343-2348	1.7	2
502	Multireference coupled-cluster theory: the easy way. *Journal of Chemical Physics*, **2011**, 134, 114108	3.9	104
501	RDX geometries, excited states, and revised energy ordering of conformers via MP2 and CCSD(T) methodologies: insights into decomposition mechanism. *Journal of Physical Chemistry A*, **2011**, 115, 884-90	2.8	28
500	Multireference Double Electron Attached Coupled Cluster Method with Full Inclusion of the Connected Triple Excitations: MR-DA-CCSDT. *Journal of Chemical Theory and Computation*, **2011**, 7, 3088-96	6.4	47
499	Comparing ab initio density-functional and wave function theories: the impact of correlation on the electronic density and the role of the correlation potential. *Journal of Chemical Physics*, **2011**, 135, 114111	3.9	36

498	Multi-reference Fock space coupled-cluster method in the intermediate Hamiltonian formulation for potential energy surfaces. *Journal of Chemical Physics*, **2011**, 135, 044121	3.9	40
497	Software design of ACES III with the super instruction architecture. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 895-901	7.9	46
496	The Tailored CCSD(T) description of the automerization of cyclobutadiene. *Chemical Physics Letters*, **2011**, 501, 166-171	2.5	44
495	Gas phase solvatochromic effects of phenol and naphthol photoacids. *Journal of Chemical Physics*, **2011**, 134, 244303	3.9	5
494	Charge-transfer separability and size-extensivity in the equation-of-motion coupled cluster method: EOM-CCx. *Journal of Chemical Physics*, **2011**, 134, 034106	3.9	32
493	External coupled-cluster perturbation theory: description and application to weakly interaction dimers. Corrections to the random phase approximation. *Journal of Chemical Physics*, **2011**, 134, 184108	3.9	18
492	The Super Instruction Architecture: A Framework for High-Productivity Parallel Implementation of Coupled-Cluster Methods on Petascale Computers. *Annual Reports in Computational Chemistry*, **2011**, 7, 179-191	1.8	7
491	A personal history of the Quantum Theory Project and the Sanibel meeting on the occasion of their fiftieth anniversary. *Molecular Physics*, **2010**, 108, 2823-2839	1.7	1
490	Improving upon CCSD(TQ(f)) for potential energy surfaces: CCSD(TQ(f)) models. *Journal of Chemical Physics*, **2010**, 133, 104102	3.9	23
489	Introduction to proceedings of Molecular Quantum Mechanics 2010: from methylene to DNA and beyond. *Molecular Physics*, **2010**, 108, 2437-2438	1.7	
488	Ab initio DFT and its role in electronic structure theory. *Molecular Physics*, **2010**, 108, 3299-3311	1.7	39
487	The coupled-cluster revolution. *Molecular Physics*, **2010**, 108, 2905-2920	1.7	105
486	On the directed gas phase synthesis of the imidoborane molecule (HNBH)--an isoelectronic molecule of acetylene (HCCH). *Journal of Physical Chemistry A*, **2010**, 114, 12148-54	2.8	10
485	Accuracy of Computed 15N Nuclear Magnetic Resonance Chemical Shifts. *Journal of Chemical Theory and Computation*, **2010**, 6, 1228-1239	6.4	22
484	Ab initio simulation of UV/vis absorption spectra for atmospheric modeling: method design for medium-sized molecules. *Physical Chemistry Chemical Physics*, **2010**, 12, 9726-35	3.6	4
483	An adaptive coupled-cluster theory: @CC approach. *Journal of Chemical Physics*, **2010**, 133, 244112	3.9	24
482	The Yearn to be Hermitian. *Challenges and Advances in Computational Chemistry and Physics*, **2010**, 1-36	0.7	7
481	Rethinking linearized coupled-cluster theory. *Journal of Chemical Physics*, **2009**, 130, 144112	3.9	67

480	Improving upon the accuracy for doubly excited states within the coupled cluster singles and doubles theory. *Journal of Chemical Physics*, **2009**, 131, 124310	3.9	6
479	Parallel implementation of the equation-of-motion coupled-cluster singles and doubles method and application for radical adducts of cytosine. *Journal of Chemical Physics*, **2009**, 130, 124122	3.9	25
478	An ab initio study of the (H2O)20H+ and (H2O)21H+ water clusters. *Journal of Chemical Physics*, **2009**, 131, 104313	3.9	27
477	Excited and ionized states of the ozone molecule with full triples coupled cluster methods. *Journal of Chemical Physics*, **2009**, 131, 194104	3.9	20
476	An infrastructure for scalable and portable parallel programs for computational chemistry **2009**,		8
475	Determination of the size-consistency error in the single and double excitation configuration interaction model. *International Journal of Quantum Chemistry*, **2009**, 12, 165-173	2.1	3
474	Localized orbitals in the coupled cluster singles and doubles model. *International Journal of Quantum Chemistry*, **2009**, 22, 561-573	2.1	5
473	A multireference many-body perturbation theory study of Be + H2 -HBeH2. *International Journal of Quantum Chemistry*, **2009**, 24, 347-356	2.1	
472	Direct coupled cluster calculations on excited states. *International Journal of Quantum Chemistry*, **2009**, 28, 217-220	2.1	2
471	Geometric sumrule and the reduced partitioning procedure. *International Journal of Quantum Chemistry*, **2009**, 5, 151-159	2.1	12
470	The treatment of correlation effects in second-order properties. *International Journal of Quantum Chemistry*, **2009**, 7, 449-462	2.1	6
469	Correlation energy in LiH, BH, and HF with many-body perturbation theory using slater-type atomic orbitals. *International Journal of Quantum Chemistry*, **2009**, 8, 271-276	2.1	28
468	Some aspects of diagrammatic perturbation theory. *International Journal of Quantum Chemistry*, **2009**, 9, 183-198	2.1	81
467	Towards an exact correlated orbital theory for electrons. *Chemical Physics Letters*, **2009**, 484, 1-9	2.5	50
466	First calculations of 15N-15N J values and new calculations of chemical shifts for high nitrogen systems: a comment on the long search for HN5 and its pentazole anion. *Journal of Physical Chemistry A*, **2009**, 113, 3197-201	2.8	34
465	Many-Body Methods in Chemistry and Physics: MBPT and Coupled-Cluster Theory **2009**,		879
464	Improving upon CCSD(T): LambdaCCSD(T). I. Potential energy surfaces. *Journal of Chemical Physics*, **2008**, 128, 044110	3.9	157
463	Intermediate Hamiltonian Fock-space multireference coupled-cluster method with full triples for calculation of excitation energies. *Journal of Chemical Physics*, **2008**, 129, 044101	3.9	63

462	Multireference Fock-space coupled-cluster and equation-of-motion coupled-cluster theories: the detailed interconnections. *Journal of Chemical Physics*, **2008**, 129, 134105	3.9	69
461	Natural linear-scaled coupled-cluster theory with local transferable triple excitations: applications to peptides. *Journal of Physical Chemistry A*, **2008**, 112, 5994-6003	2.8	58
460	Ground state potential energy surfaces and bound states of M-He dimers (M=Cu,Ag,Au): a theoretical investigation. *Journal of Chemical Physics*, **2008**, 129, 204307	3.9	28
459	Improving upon CCSD(T): LambdaCCSD(T). II. Stationary formulation and derivatives. *Journal of Chemical Physics*, **2008**, 128, 044111	3.9	65
458	Transferability in the natural linear-scaled coupled-cluster effective Hamiltonian approach: Applications to dynamic polarizabilities and dispersion coefficients. *Journal of Chemical Physics*, **2008**, 129, 054105	3.9	14
457	Effect of the nonlocal exchange on the performance of the orbital-dependent correlation functionals from second-order perturbation theory. *Journal of Chemical Physics*, **2008**, 129, 124109	3.9	17
456	Different equation-of-motion coupled cluster methods with different reference functions: the formyl radical. *Journal of Chemical Physics*, **2008**, 129, 104301	3.9	11
455	Spin-free intermediate Hamiltonian Fock space coupled-cluster theory with full inclusion of triple excitations for restricted Hartree Fock based triplet states. *Journal of Chemical Physics*, **2008**, 129, 244111	3.9	35
454	Frozen natural orbital coupled-cluster theory: forces and application to decomposition of nitroethane. *Journal of Chemical Physics*, **2008**, 128, 164101	3.9	82
453	Structure and properties of disiloxane: An ab initio and post-Hartree–Fock study. *International Journal of Quantum Chemistry*, **2008**, 108, 2088-2096	2.1	12
452	Benchmark calculations of the Fock-space coupled cluster single, double, triple excitation method in the intermediate Hamiltonian formulation for electronic excitation energies. *Chemical Physics Letters*, **2008**, 457, 267-270	2.5	39
451	Structure, spectra, and rearrangement mechanism of PH2F3: revisiting a classic problem in structural inorganic chemistry. *Journal of Physical Chemistry A*, **2007**, 111, 2220-8	2.8	2
450	HNNC radical and its role in the CH+N2 reaction. *Journal of Physical Chemistry A*, **2007**, 111, 6894-9	2.8	22
449	Coupled-cluster theory in quantum chemistry. *Reviews of Modern Physics*, **2007**, 79, 291-352	40.5	2110
448	Applications of Post-Hartree–Fock Methods: A Tutorial. *Reviews in Computational Chemistry*, **2007**, 65-169		230
447	Theoretical study of the electronic structure of MCH(2)(+)(M=Fe,Co,Ni). *Journal of Chemical Physics*, **2007**, 126, 154318	3.9	8
446	Addition by subtraction in coupled cluster theory. II. Equation-of-motion coupled cluster method for excited, ionized, and electron-attached states based on the nCC ground state wave function. *Journal of Chemical Physics*, **2007**, 127, 024106	3.9	25
445	Ab initio density functional theory applied to quasidegenerate problems. *Journal of Chemical Physics*, **2007**, 127, 154111	3.9	34

444	Exact-exchange density functional theory for hyperpolarizabilities. *Journal of Chemical Physics*, **2007**, 127, 174102	3.9	12
443	A coupled cluster study of the electronic spectroscopy and photochemistry of Cr(CO)6. *Physical Chemistry Chemical Physics*, **2007**, 9, 6115-22	3.6	40
442	Making More Extensive Use of the Coupled-cluster Wave Function: from the Standard Energy Expression to the Energy Expectation Value. *Theoretical Chemistry Accounts*, **2006**, 116, 440-449	1.9	4
441	Addition by subtraction in coupled-cluster theory: a reconsideration of the CC and CI interface and the nCC hierarchy. *Journal of Chemical Physics*, **2006**, 125, 204105	3.9	60
440	Ab initio correlation functionals from second-order perturbation theory. *Journal of Chemical Physics* , **2006**, 125, 104108	3.9	54
439	Tailored coupled cluster singles and doubles method applied to calculations on molecular structure and harmonic vibrational frequencies of ozone. *Journal of Chemical Physics*, **2006**, 124, 114311	3.9	71
438	Adiabatic ab initio time-dependent density-functional theory employing optimized-effective-potential many-body perturbation theory potentials. *Physical Review A*, **2006**, 73,	2.6	16
437	Computational design of Si–SiO2 interfaces: Stress and strain on the atomic scale. *Physical Review B*, **2006**, 73,	3.3	32
436	High-level coupled-cluster methods for electron spin resonance spectra: on the experimental spectrum of the silacyclobutane radical cation. *Journal of Physical Chemistry A*, **2006**, 110, 4473-8	2.8	4
435	Hidden symmetry in Fermi-contact NMR spin–spin coupling constants. *Molecular Physics*, **2006**, 104, 2403-2411	1.7	3
434	New perspectives on unitary coupled-cluster theory. *International Journal of Quantum Chemistry*, **2006**, 106, 3393-3401	2.1	102
433	Ab initio density functional theory for spin-polarized systems. *Chemical Physics Letters*, **2006**, 427, 466-471	2.5	21
432	Ab initio DFT: Getting the right answer for the right reason. *Computational and Theoretical Chemistry*, **2006**, 771, 1-8		48
431	Accurate calculation of vibrational frequencies in excited states with the full EOM-CCSDT method. *Computational and Theoretical Chemistry*, **2006**, 768, 103-109		10
430	Computational Design of Silicon Suboxides: Chemical and Mechanical Forces on the Atomic Scale. *Journal of Computer-Aided Materials Design*, **2006**, 13, 185-200		3
429	Quantum mechanics at the core of multi-scale simulations. *Journal of Computer-Aided Materials Design*, **2006**, 13, 89-109		5
428	Frozen Natural Orbitals: Systematic Basis Set Truncation for Coupled-Cluster Theory. *Collection of Czechoslovak Chemical Communications*, **2005**, 70, 837-850		92
427	A Reinvestigation of Ramsey's Theory of NMR Coupling. *Advances in Quantum Chemistry*, **2005**, 48, 434-467	1.4	3

426	Critical comparison of various connected quadruple excitation approximations in the coupled-cluster treatment of bond breaking. *Journal of Chemical Physics*, **2005**, 122, 224102	3.9	48
425	Improving the performance of direct coupled cluster analytical gradients algorithms. *Molecular Physics*, **2005**, 103, 2081-2083	1.7	1
424	Interconnection between functional derivative and effective operator approaches to ab initio density functional theory. *Molecular Physics*, **2005**, 103, 2299-2307	1.7	8
423	Study of the effect of hydration on the tensile strength of a silica nanotube. *Molecular Physics*, **2005** , 103, 2019-2026	1.7	8
422	Theory of the short-range correlation hole model. *Molecular Physics*, **2005**, 103, 2093-2103	1.7	2
421	Quantum chemical study of the electronic structure of NiCH2 + in its ground state and low-lying electronic excited states. *Journal of Chemical Physics*, **2005**, 122, 44313	3.9	22
420	The exchange-correlation potential in ab initio density functional theory. *Journal of Chemical Physics*, **2005**, 122, 34104	3.9	150
419	Intermolecular potential energy surfaces of weakly bound dimers computed from ab initio density functional theory: The right answer for the right reason. *Chemical Physics Letters*, **2005**, 405, 43-48	2.5	59
418	Achieving Predictive Simulations with Quantum Mechanical Forces Via the Transfer Hamiltonian: Problems and Prospects **2005**, 27-57		3
417	Application of the transfer Hamiltonian formalism to high-energy model systems. *International Journal of Quantum Chemistry*, **2005**, 105, 914-920	2.1	4
416	How and why coupled-cluster theory became the pre-eminent method in an ab into quantum chemistry **2005**, 1191-1221		55
415	Ab initio density functional theory: the best of both worlds?. *Journal of Chemical Physics*, **2005**, 123, 62205	3.9	143
414	Correlated one-particle method: numerical results. *Journal of Chemical Physics*, **2005**, 123, 154103	3.9	17
413	Molecular applications of the intermediate Hamiltonian Fock-space coupled-cluster method for calculation of excitation energies. *Journal of Chemical Physics*, **2005**, 122, 224110	3.9	74
412	Coupled-cluster method tailored by configuration interaction. *Journal of Chemical Physics*, **2005**, 123, 074106	3.9	101
411	Exact-exchange time-dependent density-functional theory for static and dynamic polarizabilities. *Physical Review A*, **2005**, 71,	2.6	23
410	Achieving Predictive Simulations with Quantum Mechanical Forces Via the Transfer Hamiltonian: Problems and Prospects **2005**, 27-57		
409	Singular value decomposition applied to the compression of T3 amplitude for the coupled cluster method. *Journal of Chemical Physics*, **2004**, 121, 1206-13	3.9	24

408	EOM-CCSDT study of the low-lying ionization potentials of ethylene, acetylene and formaldehyde. *Chemical Physics Letters*, **2004**, 384, 210-214	2.5	63
407	Fock space multireference coupled cluster method with full inclusion of connected triples for excitation energies. *Journal of Chemical Physics*, **2004**, 121, 1670-5	3.9	72
406	Independent particle theory with electron correlation. *Journal of Chemical Physics*, **2004**, 120, 8395-404	3.9	34
405	Toward a computational description of nitrile hydratase: studies of the ground state bonding and spin-dependent energetics of mononuclear, non-heme Fe(III) complexes. *Inorganic Chemistry*, **2004**, 43, 458-72	5.1	30
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