Martin Head-Gordon

List of Publications by Year in Descending Order

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	Revisiting the Bonding Model for Gold(I) Species: The Importance of Pauli Repulsion Revealed in a Gold(I)-Cyclobutadiene Complex.. *Angewandte Chemie - International Edition*, **2022**,	16.4	3
413	Oxygen Isotope Exchange between Carbon Dioxide and Iron Oxides on Mars Surface.. *Journal of Physical Chemistry Letters*, **2022**, 2600-2606	6.4	
412	Relativistic Orbital-Optimized Density Functional Theory for Accurate Core-Level Spectroscopy.. *Journal of Physical Chemistry Letters*, **2022**, 3438-3449	6.4	5
411	Concerted Electron-Nuclear Motion in Proton-Coupled Electron Transfer-Driven Grotthuss-Type Proton Translocation.. *Journal of Physical Chemistry Letters*, **2022**, 4479-4485	6.4	0
410	A benchmark dataset for Hydrogen Combustion.. *Scientific Data*, **2022**, 9, 215	8.2	0
409	Regularized Second-Order Møller-Plesset Theory: A More Accurate Alternative to Conventional MP2 for Noncovalent Interactions and Transition Metal Thermochemistry for the Same Computational Cost.. *Journal of Physical Chemistry Letters*, **2021**, 12, 12084-12097	6.4	6
408	Stripping away ion hydration shells in electrical double-layer formation: Water networks matter. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	7
407	Dissociation of HCl in water nanoclusters: an energy decomposition analysis perspective. *Physical Chemistry Chemical Physics*, **2021**, 23, 26737-26749	3.6	0
406	Optimized Pseudopotentials and Basis Sets for Semiempirical Density Functional Theory for Electrocatalysis Applications. *Journal of Physical Chemistry Letters*, **2021**, 12, 10304-10309	6.4	3
405	Approaching the basis set limit in Gaussian-orbital-based periodic calculations with transferability: Performance of pure density functionals for simple semiconductors. *Journal of Chemical Physics*, **2021**, 155, 164102	3.9	4
404	Crossed Beam Experiments and Computational Studies of Pathways to the Preparation of Singlet Ethynylsilylene (HCCSiH; XA^1) The Silacarbene Counterpart of Triplet Propargylene (HCCCH; XB). *Journal of Physical Chemistry Letters*, **2021**, 12, 10768-10776	6.4	2
403	Ambient-Temperature Hydrogen Storage via Vanadium(II)-Dihydrogen Complexation in a Metal-Organic Framework. *Journal of the American Chemical Society*, **2021**, 143, 6248-6256	16.4	22
402	Controlled Single-Electron Transfer via Metal-Ligand Cooperativity Drives Divergent Nickel-Electrocatalyzed Radical Pathways. *Journal of the American Chemical Society*, **2021**, 143, 6990-7001	16.4	11
401	From Intermolecular Interaction Energies and Observable Shifts to Component Contributions and Back Again: A Tale of Variational Energy Decomposition Analysis. *Annual Review of Physical Chemistry*, **2021**, 72, 641-666	15.7	21
400	Assessment of Performance of Density Functionals for Predicting Potential Energy Curves in Hydrogen Storage Applications. *Journal of Physical Chemistry A*, **2021**, 125, 4245-4257	2.8	0
399	Revealing the nature of electron correlation in transition metal complexes with symmetry breaking and chemical intuition. *Journal of Chemical Physics*, **2021**, 154, 194109	3.9	9
398	Orbital Optimized Density Functional Theory for Electronic Excited States. *Journal of Physical Chemistry Letters*, **2021**, 12, 4517-4529	6.4	31

397	Two-Coordinate Iron(I) Complexes on the Edge of Stability: Influence of Dispersion and Steric Effects. *Organometallics*, **2021**, 40, 1758-1764	3.8	2
396	Modeling Molecules under Pressure with Gaussian Potentials. *Journal of Chemical Theory and Computation*, **2021**, 17, 583-597	6.4	5
395	A non-perturbative pairwise-additive analysis of charge transfer contributions to intermolecular interaction energies. *Physical Chemistry Chemical Physics*, **2021**, 23, 928-943	3.6	7
394	Siloxyaluminate and Siloxygallate Complexes as Models for Framework and Partially Hydrolyzed Framework Sites in Zeolites and Zeotypes. *Chemistry - A European Journal*, **2021**, 27, 307-315	4.8	2
393	Mechanistic Insights into Co and Fe Quaterpyridine-Based CO Reduction Catalysts: Metal-Ligand Orbital Interaction as the Key Driving Force for Distinct Pathways. *Journal of the American Chemical Society*, **2021**, 143, 744-763	16.4	19
392	Polishing the Gold Standard: The Role of Orbital Choice in CCSD(T) Vibrational Frequency Prediction. *Journal of Chemical Theory and Computation*, **2021**, 17, 742-755	6.4	6
391	Challenges for density functional theory: calculation of CO adsorption on electrocatalytically relevant metals. *Physical Chemistry Chemical Physics*, **2021**, 23, 9394-9406	3.6	8
390	Electron-Nuclear Dynamics Accompanying Proton-Coupled Electron Transfer. *Journal of the American Chemical Society*, **2021**, 143, 3104-3112	16.4	14
389	Mechanism and Kinetics of Light Alkane Dehydrogenation and Cracking over Isolated Ga Species in Ga/H-MFI. *ACS Catalysis*, **2021**, 11, 2062-2075	13.1	15
388	Too big, too small, or just right? A benchmark assessment of density functional theory for predicting the spatial extent of the electron density of small chemical systems. *Journal of Chemical Physics*, **2021**, 154, 074109	3.9	9
387	Critical Role of Thermal Fluctuations for CO Binding on Electrocatalytic Metal Surfaces. *Jacs Au*, **2021**, 1, 1708-1718		5
386	Exploring spin symmetry-breaking effects for static field ionization of atoms: Is there an analog to the Coulson-Fischer point in bond dissociation?. *Journal of Chemical Physics*, **2021**, 155, 014309	3.9	1
385	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. *Journal of Chemical Physics*, **2021**, 155, 084801	3.9	115
384	Effective Two-Body Interactions. *Journal of Physical Chemistry A*, **2021**, 125, 7750-7758	2.8	2
383	Exploring the Limits of Second- and Third-Order Møller-Plesset Perturbation Theories for Noncovalent Interactions: Revisiting MP2.5 and Assessing the Importance of Regularization and Reference Orbitals. *Journal of Chemical Theory and Computation*, **2021**, 17, 5582-5599	6.4	2
382	The Role of Roughening to Enhance Selectivity to C2+ Products during CO2 Electroreduction on Copper. *ACS Energy Letters*, **2021**, 6, 3252-3260	20.1	4
381	Observation of an Intermediate to H Binding in a Metal-Organic Framework. *Journal of the American Chemical Society*, **2021**, 143, 14884-14894	16.4	8
380	Computational Modeling Predicts the Stability of Both Pd and Pd Ion-Exchanged into H-CHA. *Journal of Materials Chemistry A*, **2021**, 9, 2161-2174	13	9

379	Third-Order Møller-Plesset Theory Made More Useful? The Role of Density Functional Theory Orbitals. *Journal of Chemical Theory and Computation*, **2020**, 16, 7473-7489	6.4	16
378	Solvent Mediated Excited State Proton Transfer in Indigo Carmine. *Journal of Physical Chemistry Letters*, **2020**, 11, 4156-4162	6.4	17
377	Probing radical-molecule interactions with a second generation energy decomposition analysis of DFT calculations using absolutely localized molecular orbitals. *Physical Chemistry Chemical Physics*, **2020**, 22, 12867-12885	3.6	12
376	Computational Study of an Iron(II) Polypyridine Electrocatalyst for CO Reduction: Key Roles for Intramolecular Interactions in CO Binding and Proton Transfer. *Inorganic Chemistry*, **2020**, 59, 8146-8160	5.1	14
375	Bimetallic Mechanism for Alkyne Cyclotrimerization with a Two-Coordinate Fe Precatalyst. *ACS Catalysis*, **2020**, 10, 7800-7807	13.1	3
374	The rupture mechanism of rubredoxin is more complex than previously thought. *Chemical Science*, **2020**, 11, 6036-6044	9.4	0
373	Benchmarking the Performance of the ReaxFF Reactive Force Field on Hydrogen Combustion Systems. *Journal of Physical Chemistry A*, **2020**, 124, 5631-5645	2.8	14
372	Compressed intramolecular dispersion interactions. *Journal of Chemical Physics*, **2020**, 152, 024112	3.9	1
371	Modern Approaches to Exact Diagonalization and Selected Configuration Interaction with the Adaptive Sampling CI Method. *Journal of Chemical Theory and Computation*, **2020**, 16, 2139-2159	6.4	43
370	Experimental and Computational Studies of Carbon–Carbon Bond Formation via Ketonization and Aldol Condensation over Site-Isolated Zirconium Catalysts. *ACS Catalysis*, **2020**, 10, 4566-4579	13.1	14
369	Density Functionals for Hydrogen Storage: Defining the H2Bind275 Test Set with Ab Initio Benchmarks and Assessment of 55 Functionals. *Journal of Chemical Theory and Computation*, **2020**, 16, 4963-4982	6.4	7
368	Cation, Anion, and Radical Isomers of CHN: Computational Characterization and Implications for Astrophysical and Planetary Environments. *Journal of Physical Chemistry A*, **2020**, 124, 2001-2013	2.8	6
367	CASSCF with Extremely Large Active Spaces Using the Adaptive Sampling Configuration Interaction Method. *Journal of Chemical Theory and Computation*, **2020**, 16, 2340-2354	6.4	44
366	Heterogenized Pyridine-Substituted Cobalt(II) Phthalocyanine Yields Reduction of CO by Tuning the Electron Affinity of the Co Center. *ACS Applied Materials & Interfaces*, **2020**, 12, 5251-5258	9.5	22
365	Atomic-Scale Spacing between Copper Facets for the Electrochemical Reduction of Carbon Dioxide. *Advanced Energy Materials*, **2020**, 10, 1903423	21.8	22
364	Excited State Orbital Optimization via Minimizing the Square of the Gradient: General Approach and Application to Singly and Doubly Excited States via Density Functional Theory. *Journal of Chemical Theory and Computation*, **2020**, 16, 1699-1710	6.4	65
363	Generalized single excitation configuration interaction: an investigation into the impact of the inclusion of non-orthogonality on the calculation of core-excited states. *Physical Chemistry Chemical Physics*, **2020**, 22, 8182-8192	3.6	14
362	Clarifying the quantum mechanical origin of the covalent chemical bond. *Nature Communications*, **2020**, 11, 4893	17.4	9

361	Highly Accurate Prediction of Core Spectra of Molecules at Density Functional Theory Cost: Attaining Sub-electronvolt Error from a Restricted Open-Shell Kohn-Sham Approach. *Journal of Physical Chemistry Letters*, **2020**, 11, 775-786	6.4	43
360	Variational Forward-Backward Charge Transfer Analysis Based on Absolutely Localized Molecular Orbitals: Energetics and Molecular Properties. *Journal of Chemical Theory and Computation*, **2020**, 16, 1073-1089	6.4	15
359	Electronic structure calculations permit identification of the driving forces behind frequency shifts in transition metal monocarbonyls. *Physical Chemistry Chemical Physics*, **2020**, 22, 781-798	3.6	15
358	Systematically Improvable Tensor Hypercontraction: Interpolative Separable Density-Fitting for Molecules Applied to Exact Exchange, Second- and Third-Order Møller-Plesset Perturbation Theory. *Journal of Chemical Theory and Computation*, **2020**, 16, 243-263	6.4	25
357	Facing the Challenges of Borderline Oxidation State Assignments Using State-of-the-Art Computational Methods. *Inorganic Chemistry*, **2020**, 59, 15410-15420	5.1	8
356	The Ground State Electronic Energy of Benzene. *Journal of Physical Chemistry Letters*, **2020**, 11, 8922-8929	6.4	52
355	Accurate prediction of core-level spectra of radicals at density functional theory cost via square gradient minimization and recoupling of mixed configurations. *Journal of Chemical Physics*, **2020**, 153, 134108	3.9	19
354	Metal-Ligand Cooperativity via Exchange Coupling Promotes Iron- Catalyzed Electrochemical CO Reduction at Low Overpotentials. *Journal of the American Chemical Society*, **2020**, 142, 20489-20501	16.4	33
353	Predicting Excitation Energies of Twisted Intramolecular Charge-Transfer States with the Time-Dependent Density Functional Theory: Comparison with Experimental Measurements in the Gas Phase and Solvents Ranging from Hexanes to Acetonitrile. *Journal of Chemical Theory and Computation*, **2020**, 16, 6244-6255	6.4	10
352	Molecular growth upon ionization of van der Waals clusters containing HCCH and HCN is a pathway to prebiotic molecules. *Physical Chemistry Chemical Physics*, **2020**, 22, 20337-20348	3.6	5
351	Consistent inclusion of continuum solvation in energy decomposition analysis: theory and application to molecular CO reduction catalysts. *Chemical Science*, **2020**, 12, 1398-1414	9.4	24
350	What Levels of Coupled Cluster Theory Are Appropriate for Transition Metal Systems? A Study Using Near-Exact Quantum Chemical Values for 3d Transition Metal Binary Compounds. *Journal of Chemical Theory and Computation*, **2019**, 15, 5370-5385	6.4	22
349	Kohn-Sham Density Functional Theory with Complex, Spin-Restricted Orbitals: Accessing a New Class of Densities without the Symmetry Dilemma. *Physical Review Letters*, **2019**, 123, 113001	7.4	13
348	Probing solvation and reactivity in ionized polycyclic aromatic hydrocarbon-water clusters with photoionization mass spectrometry and electronic structure calculations. *Faraday Discussions*, **2019**, 217, 414-433	3.6	9
347	Chemoenzymatic Platform for Synthesis of Chiral Organofluorines Based on Type II Aldolases. *Angewandte Chemie - International Edition*, **2019**, 58, 11841-11845	16.4	23
346	Assessing Electronic Structure Methods for Long-Range Three-Body Dispersion Interactions: Analysis and Calculations on Well-Separated Metal Atom Trimers. *Journal of Chemical Theory and Computation*, **2019**, 15, 4351-4361	6.4	6
345	Probing Blue-Shifting Hydrogen Bonds with Adiabatic Energy Decomposition Analysis. *Journal of Physical Chemistry Letters*, **2019**, 10, 3899-3905	6.4	19
344	Zeolite-Catalyzed Isobutene Amination: Mechanism and Kinetics. *ACS Catalysis*, **2019**, 9, 7012-7022	13.1	8

343	Non-Orthogonal Configuration Interaction with Single Substitutions for Core-Excited States: An Extension to Doublet Radicals. *Journal of Chemical Theory and Computation*, **2019**, 15, 2966-2973	6.4	29
342	Tracing the 267 nm-Induced Radical Formation in Dimethyl Disulfide Using Time-Resolved X-ray Absorption Spectroscopy. *Journal of Physical Chemistry Letters*, **2019**, 10, 1382-1387	6.4	17
341	Mutually polarizable QM/MM model with in situ optimized localized basis functions. *Journal of Chemical Physics*, **2019**, 150, 074103	3.9	14
340	Well-behaved versus ill-behaved density functionals for single bond dissociation: Separating success from disaster functional by functional for stretched H. *Journal of Chemical Physics*, **2019**, 150, 094115	3.9	18
339	Distinguishing artificial and essential symmetry breaking in a single determinant: approach and application to the C, C, and C fullerenes. *Physical Chemistry Chemical Physics*, **2019**, 21, 4763-4778	3.6	31
338	Explaining the Incorporation of Oxygen Derived from Solvent Water into the Oxygenated Products of CO Reduction over Cu. *Journal of the American Chemical Society*, **2019**, 141, 4191-4193	16.4	18
337	Development of an Advanced Force Field for Water Using Variational Energy Decomposition Analysis. *Journal of Chemical Theory and Computation*, **2019**, 15, 5001-5013	6.4	27
336	Two single-reference approaches to singlet biradicaloid problems: Complex, restricted orbitals and approximate spin-projection combined with regularized orbital-optimized M□ller-Plesset perturbation theory. *Journal of Chemical Physics*, **2019**, 150, 244106	3.9	30
335	Multiresolution 3D-DenseNet for Chemical Shift Prediction in NMR Crystallography. *Journal of Physical Chemistry Letters*, **2019**, 10, 4558-4565	6.4	17
334	Chemoenzymatic Platform for Synthesis of Chiral Organofluorines Based on Type II Aldolases. *Angewandte Chemie*, **2019**, 131, 11967-11971	3.6	7
333	Gas phase formation of c-SiC molecules in the circumstellar envelope of carbon stars. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 14471-14478	11.5	11
332	Third-Order M□ller-Plesset Perturbation Theory Made Useful? Choice of Orbitals and Scaling Greatly Improves Accuracy for Thermochemistry, Kinetics, and Intermolecular Interactions. *Journal of Physical Chemistry Letters*, **2019**, 10, 4170-4176	6.4	24
331	Energy Decomposition Analysis for Interactions of Radicals: Theory and Implementation at the MP2 Level with Application to Hydration of Halogenated Benzene Cations and Complexes between CO□ and Pyridine and Imidazole. *Journal of Physical Chemistry A*, **2019**, 123, 9621-9633	2.8	8
330	Quantum Chemical Modeling of Pressure-Induced Spin Crossover in Octahedral Metal-Ligand Complexes. *ChemPhysChem*, **2019**, 20, 2742-2747	3.2	9
329	The Poisson-Boltzmann model for implicit solvation of electrolyte solutions: Quantum chemical implementation and assessment via Sechenov coefficients. *Journal of Chemical Physics*, **2019**, 151, 224111	3.9	20
328	Beyond the Coulson-Fischer point: characterizing single excitation CI and TDDFT for excited states in single bond dissociations. *Physical Chemistry Chemical Physics*, **2019**, 21, 21761-21775	3.6	12
327	Making many-body interactions nearly pairwise additive: The polarized many-body expansion approach. *Journal of Chemical Physics*, **2019**, 151, 194101	3.9	10
326	Excited states via coupled cluster theory without equation-of-motion methods: Seeking higher roots with application to doubly excited states and double core hole states. *Journal of Chemical Physics*, **2019**, 151, 214103	3.9	26

325	Mechanism and Kinetics of Propane Dehydrogenation and Cracking over Ga/H-MFI Prepared via Vapor-Phase Exchange of H-MFI with GaCl. *Journal of the American Chemical Society*, **2019**, 141, 1614-1627	16.4	58
324	Push it to the limit: comparing periodic and local approaches to density functional theory for intermolecular interactions. *Molecular Physics*, **2019**, 117, 1298-1305	1.7	3
323	Challenges in Modeling Electrochemical Reaction Energetics with Polarizable Continuum Models. *ACS Catalysis*, **2019**, 9, 920-931	13.1	100
322	Generalized Unitary Coupled Cluster Wave functions for Quantum Computation. *Journal of Chemical Theory and Computation*, **2019**, 15, 311-324	6.4	118
321	Understanding Brønsted-Acid Catalyzed Monomolecular Reactions of Alkanes in Zeolite Pores by Combining Insights from Experiment and Theory. *ChemPhysChem*, **2018**, 19, 338-338	3.2	
320	On the Computational Characterization of Charge-Transfer Effects in Noncovalently Bound Molecular Complexes. *Journal of Chemical Theory and Computation*, **2018**, 14, 2401-2417	6.4	37
319	Energy decomposition analysis for exciplexes using absolutely localized molecular orbitals. *Journal of Chemical Physics*, **2018**, 148, 064105	3.9	20
318	Impact of long-range electrostatic and dispersive interactions on theoretical predictions of adsorption and catalysis in zeolites. *Catalysis Today*, **2018**, 312, 51-65	5.3	22
317	Is Subsurface Oxygen Necessary for the Electrochemical Reduction of CO on Copper?. *Journal of Physical Chemistry Letters*, **2018**, 9, 601-606	6.4	93
316	Mechanism of CO2 Reduction at Copper Surfaces: Pathways to C2 Products. *ACS Catalysis*, **2018**, 8, 1490-1499	13.1	377
315	How Accurate Is Density Functional Theory at Predicting Dipole Moments? An Assessment Using a New Database of 200 Benchmark Values. *Journal of Chemical Theory and Computation*, **2018**, 14, 1969-1981	6.4	119
314	Non-orthogonal configuration interaction with single substitutions for the calculation of core-excited states. *Journal of Chemical Physics*, **2018**, 149, 044116	3.9	36
313	Efficient Implementation of NOCI-MP2 Using the Resolution of the Identity Approximation with Application to Charged Dimers and Long C-C Bonds in Ethane Derivatives. *Journal of Chemical Theory and Computation*, **2018**, 14, 4791-4805	6.4	13
312	How accurate are static polarizability predictions from density functional theory? An assessment over 132 species at equilibrium geometry. *Physical Chemistry Chemical Physics*, **2018**, 20, 19800-19810	3.6	60
311	Understanding Non-Covalent Interactions: Correlated Energy Decomposition Analysis and Applications to Halogen Bonding. *Chimia*, **2018**, 72, 193-198	1.3	6
310	Nonempirical Meta-Generalized Gradient Approximations for Modeling Chemisorption at Metal Surfaces. *Journal of Chemical Theory and Computation*, **2018**, 14, 3083-3090	6.4	13
309	Communication: xDH double hybrid functionals can be qualitatively incorrect for non-equilibrium geometries: Dipole moment inversion and barriers to radical-radical association using XYG3 and XYGJ-OS. *Journal of Chemical Physics*, **2018**, 148, 171102	3.9	17
308	An assessment of strategies for the development of solid-state adsorbents for vehicular hydrogen storage. *Energy and Environmental Science*, **2018**, 11, 2784-2812	35.4	97

307	Bimolecular Reaction Dynamics in the Phenyl-Silane System: Exploring the Prototype of a Radical Substitution Mechanism. *Journal of Physical Chemistry Letters*, **2018**, 9, 5135-5142	6.4	2
306	Regularized Orbital-Optimized Second-Order Møller-Plesset Perturbation Theory: A Reliable Fifth-Order-Scaling Electron Correlation Model with Orbital Energy Dependent Regularizers. *Journal of Chemical Theory and Computation*, **2018**, 14, 5203-5219	6.4	56
305	Survival of the most transferable at the top of Jacob's ladder: Defining and testing the B97M(2) double hybrid density functional. *Journal of Chemical Physics*, **2018**, 148, 241736	3.9	97
304	Understanding Brønsted-Acid Catalyzed Monomolecular Reactions of Alkanes in Zeolite Pores by Combining Insights from Experiment and Theory. *ChemPhysChem*, **2018**, 19, 341-358	3.2	18
303	Characterizing the interplay of Pauli repulsion, electrostatics, dispersion and charge transfer in halogen bonding with energy decomposition analysis. *Physical Chemistry Chemical Physics*, **2018**, 20, 905-915	3.6	123
302	Orbital optimisation in the perfect pairing hierarchy: applications to full-valence calculations on linear polyacenes. *Molecular Physics*, **2018**, 116, 547-560	1.7	10
301	Independent amplitude approximations in coupled cluster valence bond theory: Incorporation of 3-electron-pair correlation and application to spin frustration in the low-lying excited states of a ferredoxin-type tetrametallic iron-sulfur cluster. *Journal of Chemical Physics*, **2018**, 149, 144103	3.9	5
300	Open-shell coupled-cluster valence-bond theory augmented with an independent amplitude approximation for three-pair correlations: Application to a model oxygen-evolving complex and single molecular magnet. *Journal of Chemical Physics*, **2018**, 149, 244121	3.9	11
299	Delocalization Errors in Density Functional Theory Are Essentially Quadratic in Fractional Occupation Number. *Journal of Physical Chemistry Letters*, **2018**, 9, 6280-6288	6.4	45
298	Energy Decomposition Analysis for Excimers Using Absolutely Localized Molecular Orbitals within Time-Dependent Density Functional Theory and Configuration Interaction with Single Excitations. *Journal of Chemical Theory and Computation*, **2018**, 14, 5156-5168	6.4	12
297	Resonance-stabilized hydrocarbon-radical chain reactions may explain soot inception and growth. *Science*, **2018**, 361, 997-1000	33.3	286
296	Reaction mechanism of the selective reduction of CO to CO by a tetraaza [CoNH] complex in the presence of protons. *Physical Chemistry Chemical Physics*, **2018**, 20, 24058-24064	3.6	11
295	Unraveling substituent effects on frontier orbitals of conjugated molecules using an absolutely localized molecular orbital based analysis. *Chemical Science*, **2018**, 9, 8598-8607	9.4	29
294	Characterization of Isolated Ga3+Cations in Ga/H-MFI Prepared by Vapor-Phase Exchange of H-MFI Zeolite with GaCl3. *ACS Catalysis*, **2018**, 8, 6106-6126	13.1	48
293	Computational Modeling of the Nature and Role of Ga Species for Light Alkane Dehydrogenation Catalyzed by Ga/H-MFI. *ACS Catalysis*, **2018**, 8, 6146-6162	13.1	53
292	Coupled-Cluster Valence-Bond Singles and Doubles for Strongly Correlated Systems: Block-Tensor Based Implementation and Application to Oligoacenes. *Journal of Chemical Theory and Computation* , **2017**, 13, 602-615	6.4	46
291	A General Sparse Tensor Framework for Electronic Structure Theory. *Journal of Chemical Theory and Computation*, **2017**, 13, 1108-1116	6.4	8
290	molecular dynamics simulations of liquid water using high quality meta-GGA functionals. *Chemical Science*, **2017**, 8, 3554-3565	9.4	60

289	Theoretical Analysis of the Influence of Pore Geometry on Monomolecular Cracking and Dehydrogenation of n-Butane in Br□sted Acidic Zeolites. *ACS Catalysis*, **2017**, 7, 2685-2697	13.1	33
288	Energy decomposition analysis in an adiabatic picture. *Physical Chemistry Chemical Physics*, **2017**, 19, 5944-5958	3.6	43
287	Simulating the absorption spectra of helium clusters (N = 70, 150, 231, 300) using a charge transfer correction to superposition of fragment single excitations. *Journal of Chemical Physics*, **2017**, 146, 044111	3.9	10
286	Assessing DFT-D3 Damping Functions Across Widely Used Density Functionals: Can We Do Better?. *Journal of Chemical Theory and Computation*, **2017**, 13, 2043-2052	6.4	48
285	Stabilizing potentials in bound state analytic continuation methods for electronic resonances in polyatomic molecules. *Journal of Chemical Physics*, **2017**, 146, 044112	3.9	11
284	Performance of the AMOEBA Water Model in the Vicinity of QM Solutes: A Diagnosis Using Energy Decomposition Analysis. *Journal of Chemical Theory and Computation*, **2017**, 13, 1963-1979	6.4	22
283	Quantifying the Role of Orbital Contraction in Chemical Bonding. *Journal of Physical Chemistry Letters*, **2017**, 8, 1967-1972	6.4	16
282	Ab initio dynamics and photoionization mass spectrometry reveal ion-molecule pathways from ionized acetylene clusters to benzene cation. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E4125-E4133	11.5	16
281	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
280	Methane Storage: Molecular Mechanisms Underlying Room-Temperature Adsorption in Zn4O(BDC)3 (MOF-5). *Journal of Physical Chemistry C*, **2017**, 121, 12091-12100	3.8	20
279	Addressing first derivative discontinuities in orbital-optimised opposite-spin scaled second-order perturbation theory with regularisation. *Molecular Physics*, **2017**, 115, 2102-2109	1.7	10
278	Efficient Implementation of Energy Decomposition Analysis for Second-Order M□ller-Plesset Perturbation Theory and Application to Anion-□nteractions. *Journal of Physical Chemistry A*, **2017**, 121, 717-728	2.8	24
277	Use of the rVV10 Nonlocal Correlation Functional in the B97M-V Density Functional: Defining B97M-rV and Related Functionals. *Journal of Physical Chemistry Letters*, **2017**, 8, 35-40	6.4	62
276	Second order M□ller-Plesset and coupled cluster singles and doubles methods with complex basis functions for resonances in electron-molecule scattering. *Journal of Chemical Physics*, **2017**, 146, 234107	3.9	22
275	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
274	Compressed representation of dispersion interactions and long-range electronic correlations. *Journal of Chemical Physics*, **2017**, 147, 144110	3.9	6
273	A celebration of the Swedish school. *Molecular Physics*, **2017**, 115, 1993-1994	1.7	1
272	Cluster decomposition of full configuration interaction wave functions: A tool for chemical interpretation of systems with strong correlation. *Journal of Chemical Physics*, **2017**, 147, 154105	3.9	20

271	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
270	Coupled cluster valence bond theory for open-shell systems with application to very long range strong correlation in a polycarbene dimer. *Journal of Chemical Physics*, **2017**, 147, 024107	3.9	6
269	Nucleophilic Aromatic Addition in Ionizing Environments: Observation and Analysis of New C-N Valence Bonds in Complexes between Naphthalene Radical Cation and Pyridine. *Journal of the American Chemical Society*, **2017**, 139, 11923-11932	16.4	7
268	Mechanisms of the Formation of Adenine, Guanine, and Their Analogues in UV-Irradiated Mixed NH:HO Molecular Ices Containing Purine. *Astrobiology*, **2017**, 17, 771-785	3.7	17
267	Energy decomposition analysis of single bonds within Kohn-Sham density functional theory. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 12649-12656	11.5	51
266	Effective empirical corrections for basis set superposition error in the def2-SVPD basis: gCP and DFT-C. *Journal of Chemical Physics*, **2017**, 146, 234105	3.9	21
265	High-Temperature Hydrogen Storage of Multiple Molecules: Theoretical Insights from Metalated Catechols. *ChemPhysChem*, **2017**, 18, 184-188	3.2	17
264	Assessing many-body contributions to intermolecular interactions of the AMOEBA force field using energy decomposition analysis of electronic structure calculations. *Journal of Chemical Physics*, **2017**, 147, 161721	3.9	31
263	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
262	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
261	A systematic study on Pt based, subnanometer-sized alloy cluster catalysts for alkane dehydrogenation: effects of intermetallic interaction. *Physical Chemistry Chemical Physics*, **2016**, 18, 10906-17	3.6	26
260	Computation of high-harmonic generation spectra of the hydrogen molecule using time-dependent configuration-interaction. *Molecular Physics*, **2016**, 114, 947-956	1.7	32
259	Computational Characterization of Redox Non-Innocence in Cobalt-Bis(Diaryldithiolene)-Catalyzed Proton Reduction. *Journal of Chemical Theory and Computation*, **2016**, 12, 223-30	6.4	23
258	Theoretical Study of 4-(Hydroxymethyl)benzoic Acid Synthesis from Ethylene and 5-(Hydroxymethyl)furoic Acid Catalyzed by Sn-BEA. *ACS Catalysis*, **2016**, 6, 5052-5061	13.1	11
257	Alternative definitions of the frozen energy in energy decomposition analysis of density functional theory calculations. *Journal of Chemical Physics*, **2016**, 144, 084118	3.9	36
256	Self-consistent implementation of meta-GGA functionals for the ONETEP linear-scaling electronic structure package. *Journal of Chemical Physics*, **2016**, 145, 204114	3.9	11
255	TINKTEP: A fully self-consistent, mutually polarizable QM/MM approach based on the AMOEBA force field. *Journal of Chemical Physics*, **2016**, 145, 124106	3.9	38
254	A deterministic alternative to the full configuration interaction quantum Monte Carlo method. *Journal of Chemical Physics*, **2016**, 145, 044112	3.9	161

253	Size consistent formulations of the perturb-then-diagonalize Møller-Plesset perturbation theory correction to non-orthogonal configuration interaction. *Journal of Chemical Physics*, **2016**, 145, 054105	3.9	24
252	Note: The performance of new density functionals for a recent blind test of non-covalent interactions. *Journal of Chemical Physics*, **2016**, 145, 186101	3.9	9
251	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
250	Cost-effective description of strong correlation: Efficient implementations of the perfect quadruples and perfect hextuples models. *Journal of Chemical Physics*, **2016**, 145, 134110	3.9	15
249	Defining the contributions of permanent electrostatics, Pauli repulsion, and dispersion in density functional theory calculations of intermolecular interaction energies. *Journal of Chemical Physics*, **2016**, 144, 114107	3.9	93
248	Approaching the basis set limit for DFT calculations using an environment-adapted minimal basis with perturbation theory: Formulation, proof of concept, and a pilot implementation. *Journal of Chemical Physics*, **2016**, 145, 044109	3.9	12
247	Push it to the limit: Characterizing the convergence of common sequences of basis sets for intermolecular interactions as described by density functional theory. *Journal of Chemical Physics*, **2016**, 144, 194306	3.9	29
246	A computational study of CH storage in porous framework materials with metalated linkers: connecting the atomistic character of CH binding sites to usable capacity. *Chemical Science*, **2016**, 7, 4503-4518	9.4	19
245	A Combined Experimental and Theoretical Study on the Formation of the 2-Methyl-1-silacycloprop-2-enylidene Molecule via the Crossed Beam Reactions of the Silylidyne Radical (SiH; X(2)Π) with Methylacetylene (CH3CCH; X(1)A1) and D4-Methylacetylene (CD3CCD; X(1)A1). *Journal of Physical Chemistry A*, **2016**, 120, 4872-83	2.8	5
244	Thermodynamics of Anharmonic Systems: Uncoupled Mode Approximations for Molecules. *Journal of Chemical Theory and Computation*, **2016**, 12, 2861-70	6.4	22
243	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
242	Experimental and Computational Evidence of Highly Active Fe Impurity Sites on the Surface of Oxidized Au for the Electrocatalytic Oxidation of Water in Basic Media. *ChemElectroChem*, **2016**, 3, 66-73	4.3	34
241	Probing Ionic Complexes of Ethylene and Acetylene with Vacuum-Ultraviolet Radiation. *Journal of Physical Chemistry A*, **2016**, 120, 5053-64	2.8	8
240	Variational Energy Decomposition Analysis of Chemical Bonding. 1. Spin-Pure Analysis of Single Bonds. *Journal of Chemical Theory and Computation*, **2016**, 12, 4812-4820	6.4	40
239	Assessing Ion-Water Interactions in the AMOEBA Force Field Using Energy Decomposition Analysis of Electronic Structure Calculations. *Journal of Chemical Theory and Computation*, **2016**, 12, 5422-5437	6.4	62
238	Advanced Potential Energy Surfaces for Molecular Simulation. *Journal of Physical Chemistry B*, **2016**, 120, 9811-32	3.4	66
237	What Is the Structure of the Naphthalene-Benzene Heterodimer Radical Cation? Binding Energy, Charge Delocalization, and Unexpected Charge-Transfer Interaction in Stacked Dimer and Trimer Radical Cations. *Journal of Physical Chemistry Letters*, **2015**, 6, 1111-8	6.4	15
236	What Is the Price of Open-Source Software?. *Journal of Physical Chemistry Letters*, **2015**, 6, 2751-4	6.4	8

235	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
234	A simple way to test for collinearity in spin symmetry broken wave functions: general theory and application to generalized Hartree Fock. *Journal of Chemical Physics*, **2015**, 142, 094112	3.9	12
233	Beyond Energies: Geometries of Nonbonded Molecular Complexes as Metrics for Assessing Electronic Structure Approaches. *Journal of Chemical Theory and Computation*, **2015**, 11, 1481-92	6.4	63
232	Tailoring Metal-Porphyrin-Like Active Sites on Graphene to Improve the Efficiency and Selectivity of Electrochemical CO2 Reduction. *Journal of Physical Chemistry C*, **2015**, 119, 21345-21352	3.8	67
231	Attenuated MP2 with a Long-Range Dispersion Correction for Treating Nonbonded Interactions. *Journal of Chemical Theory and Computation*, **2015**, 11, 4159-68	6.4	15
230	Complex basis functions revisited: implementation with applications to carbon tetrafluoride and aromatic N-containing heterocycles within the static-exchange approximation. *Journal of Chemical Physics*, **2015**, 142, 054103	3.9	33
229	Wavefunction stability analysis without analytical electronic Hessians: application to orbital-optimised second-order Møller–Plesset theory and VV10-containing density functionals. *Molecular Physics*, **2015**, 113, 1802-1808	1.7	20
228	Bioinspired design of redox-active ligands for multielectron catalysis: effects of positioning pyrazine reservoirs on cobalt for electro- and photocatalytic generation of hydrogen from water. *Chemical Science*, **2015**, 6, 4954-4972	9.4	77
227	Superposition of Fragment Excitations for Excited States of Large Clusters with Application to Helium Clusters. *Journal of Chemical Theory and Computation*, **2015**, 11, 5791-803	6.4	13
226	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics*, **2015**, 113, 184-215	1.7	2068
225	Fast, accurate evaluation of exact exchange: The occ-RI-K algorithm. *Journal of Chemical Physics*, **2015**, 143, 024113	3.9	38
224	Polarization contributions to intermolecular interactions revisited with fragment electric-field response functions. *Journal of Chemical Physics*, **2015**, 143, 114111	3.9	69
223	An energy decomposition analysis for second-order Møller-Plesset perturbation theory based on absolutely localized molecular orbitals. *Journal of Chemical Physics*, **2015**, 143, 084124	3.9	46
222	Restricted and unrestricted non-Hermitian Hartree-Fock: Theory, practical considerations, and applications to metastable molecular anions. *Journal of Chemical Physics*, **2015**, 143, 074103	3.9	24
221	Catalytic Upgrading of Biomass-Derived Methyl Ketones to Liquid Transportation Fuel Precursors by an Organocatalytic Approach. *Angewandte Chemie*, **2015**, 127, 4756-4760	3.6	9
220	Adsorption Thermodynamics and Intrinsic Activation Parameters for Monomolecular Cracking of n-Alkanes on Brønsted Acid Sites in Zeolites. *Journal of Physical Chemistry C*, **2015**, 119, 10427-10438	3.8	42
219	Computational Quantum Chemistry for Multiple-Site Heisenberg Spin Couplings Made Simple: Still Only One Spin-Flip Required. *Journal of Physical Chemistry Letters*, **2015**, 6, 1982-8	6.4	44
218	Similarity-transformed perturbation theory on top of truncated local coupled cluster solutions: Theory and applications to intermolecular interactions. *Journal of Chemical Physics*, **2015**, 142, 204101	3.9	4

217	Combined Experimental and Theoretical Study on the Formation of the Elusive 2-Methyl-1-silacycloprop-2-enylidene Molecule under Single Collision Conditions via Reactions of the Silylidyne Radical (SiH; X(2)Π) with Allene (H2CCCH2; X(1)A1) and D4-Allene (D2CCCD2; X(1)A1). *Journal of Physical Chemistry A*, **2015**, 119, 12562-78	2.8	10
216	Restricted Hartree Fock using complex-valued orbitals: a long-known but neglected tool in electronic structure theory. *Journal of Chemical Physics*, **2015**, 142, 024104	3.9	24
215	Improved Force-Field Parameters for QM/MM Simulations of the Energies of Adsorption for Molecules in Zeolites and a Free Rotor Correction to the Rigid Rotor Harmonic Oscillator Model for Adsorption Enthalpies. *Journal of Physical Chemistry C*, **2015**, 119, 1840-1850	3.8	59
214	Hydrocarbon growth via ion-molecule reactions: computational studies of the isomers of CH2+, CH3+ and CH5+ and their formation paths from acetylene and its fragments. *Physical Chemistry Chemical Physics*, **2015**, 17, 1859-69	3.6	17
213	Efficient implementation of the pair atomic resolution of the identity approximation for exact exchange for hybrid and range- separated density functionals. *Journal of Chemical Theory and Computation*, **2015**, 11, 518-27	6.4	41
212	Tailoring the Cooperative Acid–Base Effects in Silica-Supported Amine Catalysts: Applications in the Continuous Gas-Phase Self-Condensation of n-Butanal. *ChemCatChem*, **2014**, 6, n/a-n/a	5.2	17
211	Assessing electronic structure approaches for gas-ligand interactions in metal-organic frameworks: the CO2-benzene complex. *Journal of Chemical Physics*, **2014**, 140, 104707	3.9	18
210	Achieving High-Accuracy Intermolecular Interactions by Combining Coulomb-Attenuated Second-Order Møller-Plesset Perturbation Theory with Coupled Kohn-Sham Dispersion. *Journal of Chemical Theory and Computation*, **2014**, 10, 2054-63	6.4	13
209	Exploring the limit of accuracy for density functionals based on the generalized gradient approximation: local, global hybrid, and range-separated hybrid functionals with and without dispersion corrections. *Journal of Chemical Physics*, **2014**, 140, 18A527	3.9	33
208	Spin-flip non-orthogonal configuration interaction: a variational and almost black-box method for describing strongly correlated molecules. *Physical Chemistry Chemical Physics*, **2014**, 16, 22694-705	3.6	31
207	Reaction Dynamics of Zeolite-Catalyzed Alkene Methylation by Methanol. *Journal of Physical Chemistry C*, **2014**, 118, 21409-21419	3.8	25
206	Electrostatic Domination of the Effect of Electron Correlation in Intermolecular Interactions. *Journal of Physical Chemistry Letters*, **2014**, 5, 1380-5	6.4	26
205	Experimental and Theoretical Study of n-Butanal Self-Condensation over Ti Species Supported on Silica. *ACS Catalysis*, **2014**, 4, 2908-2916	13.1	30
204	Computational Study of p-Xylene Synthesis from Ethylene and 2,5-Dimethylfuran Catalyzed by H-BEA. *Journal of Physical Chemistry C*, **2014**, 118, 22090-22095	3.8	50
203	ωB97X-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
202	A Quasidegenerate Second-Order Perturbation Theory Approximation to RAS-nSF for Excited States and Strong Correlations. *Journal of Chemical Theory and Computation*, **2014**, 10, 589-99	6.4	41
201	Coupled Cluster Valence Bond Method: Efficient Computer Implementation and Application to Multiple Bond Dissociations and Strong Correlations in the Acenes. *Journal of Chemical Theory and Computation*, **2014**, 10, 2027-40	6.4	39
200	Complex absorbing potentials within EOM-CC family of methods: theory, implementation, and benchmarks. *Journal of Chemical Physics*, **2014**, 141, 024102	3.9	84

199	Analysis of the Reaction Mechanism and Catalytic Activity of Metal-Substituted Beta Zeolite for the Isomerization of Glucose to Fructose. *ACS Catalysis*, **2014**, 4, 1537-1545	13.1	129
198	Mechanism of the electrocatalytic reduction of protons with diaryldithiolene cobalt complexes. *Journal of the American Chemical Society*, **2014**, 136, 9364-76	16.4	85
197	Convergence of attenuated second order Møller-Plesset perturbation theory towards the complete basis set limit. *Chemical Physics Letters*, **2014**, 608, 249-254	2.5	5
196	M2(m-dobdc) (M = Mg, Mn, Fe, Co, Ni) metal-organic frameworks exhibiting increased charge density and enhanced H2 binding at the open metal sites. *Journal of the American Chemical Society*, **2014**, 136, 12119-29	16.4	160
195	Separate electronic attenuation allowing a spin-component-scaled second-order Møller-Plesset theory to be effective for both thermochemistry and noncovalent interactions. *Journal of Physical Chemistry B*, **2014**, 118, 6519-25	3.4	13
194	Shared memory multiprocessing implementation of resolution-of-the-identity second-order Møller-Plesset perturbation theory with attenuated and unattenuated results for intermolecular interactions between large molecules. *Molecular Physics*, **2014**, 112, 836-843	1.7	10
193	Simulations of the dissociation of small helium clusters with ab initio molecular dynamics in electronically excited states. *Journal of Chemical Physics*, **2014**, 140, 134306	3.9	25
192	Computational quantum chemistry for single Heisenberg spin couplings made simple: just one spin flip required. *Journal of Chemical Physics*, **2014**, 141, 134111	3.9	27
191	Non-orthogonal configuration interaction for the calculation of multielectron excited states. *Journal of Chemical Physics*, **2014**, 140, 114103	3.9	51
190	Increasing spin-flips and decreasing cost: Perturbative corrections for external singles to the complete active space spin flip model for low-lying excited states and strong correlation. *Journal of Chemical Physics*, **2014**, 141, 044112	3.9	24
189	A finite difference Davidson procedure to sidestep full ab initio hessian calculation: application to characterization of stationary points and transition state searches. *Journal of Chemical Physics*, **2014**, 140, 164115	3.9	20
188	Hydrogen physisorption on metal-organic framework linkers and metalated linkers: a computational study of the factors that control binding strength. *Journal of the American Chemical Society*, **2014**, 136, 17827-35	16.4	62
187	Funktionalisiertes Graphen als Träger für chirale Moleküle: ein alternatives Konzept zur Racematspaltung. *Angewandte Chemie*, **2014**, 126, 10117-10120	3.6	5
186	Innentitelbild: Funktionalisiertes Graphen als Träger für chirale Moleküle: ein alternatives Konzept zur Racematspaltung (Angew. Chem. 37/2014). *Angewandte Chemie*, **2014**, 126, 9832-9832	3.6	
185	ON THE FORMATION OF SILACYCLOPROPENYLIDENE (c-SiC2H2) AND ITS ROLE IN THE ORGANOSILICON CHEMISTRY IN THE INTERSTELLAR MEDIUM. *Astrophysical Journal*, **2013**, 770, 33	4.7	19
184	Attenuated second-order Møller-Plesset perturbation theory: performance within the aug-cc-pVTZ basis. *Physical Chemistry Chemical Physics*, **2013**, 15, 15869-75	3.6	38
183	Catalytic proton reduction with transition metal complexes of the redox-active ligand bpy2PYMe. *Chemical Science*, **2013**, 4, 3934	9.4	141
182	Regularized orbital-optimized second-order perturbation theory. *Journal of Chemical Physics*, **2013**, 139, 244109	3.9	32

181	Dissociative photoionization of glycerol and its dimer occurs predominantly via a ternary hydrogen-bridged ion-molecule complex. *Journal of the American Chemical Society*, **2013**, 135, 14229-39	16.4	32
180	Impact of metal and anion substitutions on the hydrogen storage properties of M-BTT metal-organic frameworks. *Journal of the American Chemical Society*, **2013**, 135, 1083-91	16.4	128
179	Characterizing and Understanding the Remarkably Slow Basis Set Convergence of Several Minnesota Density Functionals for Intermolecular Interaction Energies. *Journal of Chemical Theory and Computation*, **2013**, 9, 4453-61	6.4	66
178	A correlated electron view of singlet fission. *Accounts of Chemical Research*, **2013**, 46, 1339-47	24.3	130
177	Association mechanisms of unsaturated C2 hydrocarbons with their cations: acetylene and ethylene. *Physical Chemistry Chemical Physics*, **2013**, 15, 2012-23	3.6	19
176	Insights into the Kinetics of Cracking and Dehydrogenation Reactions of Light Alkanes in H-MFI. *Journal of Physical Chemistry C*, **2013**, 117, 12600-12611	3.8	54
175	Unrestricted absolutely localized molecular orbitals for energy decomposition analysis: theory and applications to intermolecular interactions involving radicals. *Journal of Chemical Physics*, **2013**, 138, 134119	3.9	75
174	The Performance of Density Functionals for Sulfate-Water Clusters. *Journal of Chemical Theory and Computation*, **2013**, 9, 1368-80	6.4	61
173	Useful lower limits to polarization contributions to intermolecular interactions using a minimal basis of localized orthogonal orbitals: theory and analysis of the water dimer. *Journal of Chemical Physics*, **2013**, 138, 084102	3.9	35
172	The role of Rydberg and continuum levels in computing high harmonic generation spectra of the hydrogen atom using time-dependent configuration interaction. *Journal of Chemical Physics*, **2013**, 139, 164121	3.9	28
171	Orbital optimized double-hybrid density functionals. *Journal of Chemical Physics*, **2013**, 139, 024110	3.9	64
170	Accurate Prediction of Hydrocarbon Interactions with Zeolites Utilizing Improved Exchange-Correlation Functionals and QM/MM Methods: Benchmark Calculations of Adsorption Enthalpies and Application to Ethene Methylation by Methanol. *Journal of Physical Chemistry C*, **2012**, 116, 15406-15414	3.8	42
169	Automated Transition State Searches without Evaluating the Hessian. *Journal of Chemical Theory and Computation*, **2012**, 8, 5166-74	6.4	51
168	Attenuating Away the Errors in Inter- and Intramolecular Interactions from Second-Order Møller-Plesset Calculations in the Small Aug-cc-pVDZ Basis Set. *Journal of Physical Chemistry Letters*, **2012**, 3, 3592-8	6.4	31
167	An energy decomposition analysis for intermolecular interactions from an absolutely localized molecular orbital reference at the coupled-cluster singles and doubles level. *Journal of Chemical Physics*, **2012**, 136, 024103	3.9	65
166	Examination of the hydrogen-bonding networks in small water clusters (n = 2-5, 13, 17) using absolutely localized molecular orbital energy decomposition analysis. *Physical Chemistry Chemical Physics*, **2012**, 14, 15328-39	3.6	56
165	Refined energetic ordering for sulphate–water (n = 3–5) clusters using high-level electronic structure calculations. *Molecular Physics*, **2012**, 110, 2513-2521	1.7	21
164	Ab initio simulations reveal that reaction dynamics strongly affect product selectivity for the cracking of alkanes over H-MFI. *Journal of the American Chemical Society*, **2012**, 134, 19468-76	16.4	56

163	Computation of high-harmonic generation spectra of H2 and N2 in intense laser pulses using quantum chemistry methods and time-dependent density functional theory. *Molecular Physics*, **2012**, 110, 909-923	1.7	50
162	A fusion of the closed-shell coupled cluster singles and doubles method and valence-bond theory for bond breaking. *Journal of Chemical Physics*, **2012**, 137, 114103	3.9	46
161	Restricted active space spin-flip configuration interaction: theory and examples for multiple spin flips with odd numbers of electrons. *Journal of Chemical Physics*, **2012**, 137, 164110	3.9	64
160	Iodide solvation in tetrahydrofuran clusters: I(THF) n (1 ≤ n ≤ 30). *Molecular Physics*, **2012**, 110, 1787-1799	1.7	7
159	Exploring the competition between localization and delocalization of the neutral soliton defect in polyenyl chains with the orbital optimized second order opposite spin method. *Journal of Chemical Physics*, **2012**, 136, 054113	3.9	21
158	Selection and Validation of Charge and Lennard-Jones Parameters for QM/MM Simulations of Hydrocarbon Interactions with Zeolites. *Journal of Chemical Theory and Computation*, **2011**, 7, 1695-703	6.4	60
157	Post-modern valence bond theory for strongly correlated electron spins. *Physical Chemistry Chemical Physics*, **2011**, 13, 19285-97	3.6	45
156	Charge-transfer and the hydrogen bond: spectroscopic and structural implications from electronic structure calculations. *Faraday Discussions*, **2011**, 150, 345-62; discussion 391-418	3.6	53
155	On the nature of electron correlation in C60. *Journal of Chemical Physics*, **2011**, 135, 194306	3.9	24
154	Quantum mechanical modeling of catalytic processes. *Annual Review of Chemical and Biomolecular Engineering*, **2011**, 2, 453-77	8.9	58
153	Benchmark results for empirical post-GGA functionals: difficult exchange problems and independent tests. *Physical Chemistry Chemical Physics*, **2011**, 13, 19325-37	3.6	71
152	Fast Sparse Cholesky Decomposition and Inversion using Nested Dissection Matrix Reordering. *Journal of Chemical Theory and Computation*, **2011**, 7, 351-68	6.4	14
151	Initiating molecular growth in the interstellar medium via dimeric complexes of observed ions and molecules. *Astronomy and Astrophysics*, **2011**, 535, A74	5.1	16
150	Approximate spin-projected broken symmetry energies from optimized orbitals that are unrestricted in active pairs. *Chemical Physics Letters*, **2011**, 515, 173-178	2.5	11
149	Efficient exploration of reaction paths via a freezing string method. *Journal of Chemical Physics*, **2011**, 135, 224108	3.9	113
148	Incorporating Linear Synchronous Transit Interpolation into the Growing String Method: Algorithm and Applications. *Journal of Chemical Theory and Computation*, **2011**, 7, 4019-25	6.4	31
147	Ground Electronic State of Peptide Cation Radicals: A Delocalized Unpaired Electron?. *Journal of Physical Chemistry Letters*, **2011**, 2, 1426-1431	6.4	16
146	The formulation and performance of a perturbative correction to the perfect quadruples model. *Journal of Chemical Physics*, **2011**, 134, 154112	3.9	9

145	A tractable and accurate electronic structure method for static correlations: the perfect hextuples model. *Journal of Chemical Physics*, **2010**, 133, 024103	3.9	36
144	A truncation hierarchy of coupled cluster models of strongly correlated systems based on perfect-pairing references: the singles+doubles models. *Journal of Chemical Physics*, **2010**, 133, 124102	3.9	31
143	Introduction to proceedings of Molecular Quantum Mechanics 2010: from methylene to DNA and beyond. *Molecular Physics*, **2010**, 108, 2437-2438	1.7	
142	Ab initio calculations on the electronically excited states of small helium clusters. *Journal of Physical Chemistry A*, **2010**, 114, 8023-32	2.8	28
141	Orbitals that are unrestricted in active pairs for generalized valence bond coupled cluster methods. *Journal of Physical Chemistry A*, **2010**, 114, 2930-8	2.8	24
140	Current status of the AMOEBA polarizable force field. *Journal of Physical Chemistry B*, **2010**, 114, 2549-64	3.4	914
139	A parallel implementation of the analytic nuclear gradient for time-dependent density functional theory within the Tamm□Dancoff approximation. *Molecular Physics*, **2010**, 108, 2791-2800	1.7	49
138	A sparse framework for the derivation and implementation of fermion algebra. *Molecular Physics*, **2010**, 108, 513-522	1.7	18
137	A strategy for obtaining a more accurate transition state estimate using the growing string method. *Chemical Physics Letters*, **2010**, 484, 392-398	2.5	19
136	Dispersion-corrected M□ller-Plesset second-order perturbation theory. *Journal of Chemical Physics*, **2009**, 131, 094106	3.9	172
135	Electron donation in the water-water hydrogen bond. *Chemistry - A European Journal*, **2009**, 15, 851-5	4.8	118
134	A theoretical study of alanine dipeptide and analogs. *International Journal of Quantum Chemistry*, **2009**, 36, 311-322	2.1	5
133	An efficient algorithm for the generation of two-electron repulsion integrals over gaussian basis functions. *International Journal of Quantum Chemistry*, **2009**, 36, 269-280	2.1	21
132	Quadratically convergent simultaneous optimization of wavefunction and geometry. *International Journal of Quantum Chemistry*, **2009**, 36, 291-303	2.1	4
131	Tractable spin-pure methods for bond breaking: Local many-electron spin-vector sets and an approximate valence bond model. *Journal of Chemical Physics*, **2009**, 130, 084103	3.9	42
130	Transition state-finding strategies for use with the growing string method. *Journal of Chemical Physics*, **2009**, 130, 244108	3.9	45
129	Violations of N-representability from spin-unrestricted orbitals in M□ller□Plesset perturbation theory and related double-hybrid density functional theory. *Molecular Physics*, **2009**, 107, 1223-1232	1.7	61
128	Long-range corrected double-hybrid density functionals. *Journal of Chemical Physics*, **2009**, 131, 174105	3.9	271

127	Hartree-Fock solutions as a quasidiabatic basis for nonorthogonal configuration interaction. *Journal of Chemical Physics*, **2009**, 131, 124113	3.9	67
126	Restricted active space spin-flip configuration interaction approach: theory, implementation and examples. *Physical Chemistry Chemical Physics*, **2009**, 11, 9779-90	3.6	187
125	Quartic-Scaling Analytical Gradient of Quasidegenerate Scaled Opposite Spin Second-Order Perturbation Corrections to Single Excitation Configuration Interaction. *Journal of Chemical Theory and Computation*, **2009**, 5, 1224-36	6.4	23
124	Non-Covalent Interactions with Dual-Basis Methods: Pairings for Augmented Basis Sets. *Journal of Chemical Theory and Computation*, **2009**, 5, 1560-72	6.4	38
123	The perfect quadruples model for electron correlation in a valence active space. *Journal of Chemical Physics*, **2009**, 130, 084101	3.9	58
122	LOBA: a localized orbital bonding analysis to calculate oxidation states, with application to a model water oxidation catalyst. *Physical Chemistry Chemical Physics*, **2009**, 11, 11297-304	3.6	81
121	Analysis of multi-configuration density functional theory methods: theory and model application to bond-breaking. *Molecular Physics*, **2009**, 107, 2103-2110	1.7	28
120	Systematic optimization of long-range corrected hybrid density functionals. *Journal of Chemical Physics*, **2008**, 128, 084106	3.9	2290
119	Penalty functions for combining coupled-cluster and perturbation amplitudes in local correlation methods with optimized orbitals. *Molecular Physics*, **2008**, 106, 2309-2324	1.7	27
118	Locating multiple self-consistent field solutions: an approach inspired by metadynamics. *Physical Review Letters*, **2008**, 101, 193001	7.4	65
117	Analysis of charge transfer effects in molecular complexes based on absolutely localized molecular orbitals. *Journal of Chemical Physics*, **2008**, 128, 184112	3.9	156
116	Hartree-Fock exchange computed using the atomic resolution of the identity approximation. *Journal of Chemical Physics*, **2008**, 128, 104106	3.9	55
115	The limits of local correlation theory: electronic delocalization and chemically smooth potential energy surfaces. *Journal of Chemical Physics*, **2008**, 128, 034103	3.9	54
114	Central moments in quantum chemistry. *International Journal of Quantum Chemistry*, **2008**, 108, 1220-1231	2.1	
113	Long-range corrected hybrid density functionals with damped atom-atom dispersion corrections. *Physical Chemistry Chemical Physics*, **2008**, 10, 6615-20	3.6	7709
112	Localized orbital theory and ammonia triborane. *Physical Chemistry Chemical Physics*, **2007**, 9, 5522-30	3.6	27
111	Quartic-Scaling Analytical Energy Gradient of Scaled Opposite-Spin Second-Order Møller-Plesset Perturbation Theory. *Journal of Chemical Theory and Computation*, **2007**, 3, 988-1003	6.4	42
110	Unravelling the origin of intermolecular interactions using absolutely localized molecular orbitals. *Journal of Physical Chemistry A*, **2007**, 111, 8753-65	2.8	433

109	Fast evaluation of scaled opposite spin second-order Møller-Plesset correlation energies using auxiliary basis expansions and exploiting sparsity. *Journal of Computational Chemistry*, **2007**, 28, 1953-64	3.5	53
108	An improved algorithm for analytical gradient evaluation in resolution-of-the-identity second-order Møller-Plesset perturbation theory: application to alanine tetrapeptide conformational analysis. *Journal of Computational Chemistry*, **2007**, 28, 839-56	3.5	120
107	Charged polycyclic aromatic hydrocarbon clusters and the galactic extended red emission. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 5274-8	11.5	97
106	The analytical gradient of dual-basis resolution-of-the-identity second-order Møller–Plesset perturbation theory. *Molecular Physics*, **2007**, 105, 2731-2742	1.7	31
105	Optimized spin-component scaled second-order Møller-Plesset perturbation theory for intermolecular interaction energies. *Molecular Physics*, **2007**, 105, 1073-1083	1.7	213
104	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
103	Linear scaling density fitting. *Journal of Chemical Physics*, **2006**, 125, 194109	3.9	132
102	An efficient self-consistent field method for large systems of weakly interacting components. *Journal of Chemical Physics*, **2006**, 124, 204105	3.9	166
101	Second-order correction to perfect pairing: an inexpensive electronic structure method for the treatment of strong electron-electron correlations. *Journal of Chemical Physics*, **2006**, 124, 114107	3.9	32
100	A Fast Implementation of Perfect Pairing and Imperfect Pairing Using the Resolution of the Identity Approximation. *Journal of Chemical Theory and Computation*, **2006**, 2, 300-5	6.4	18
99	The localizability of valence space electron–electron correlations in pair-based coupled cluster models. *Molecular Physics*, **2006**, 104, 1191-1206	1.7	10
98	Self-interaction error of local density functionals for alkali–halide dissociation. *Chemical Physics Letters*, **2006**, 422, 230-233	2.5	95
97	Analytical gradient of restricted second-order Møller–Plesset correlation energy with the resolution of the identity approximation, applied to the TCNE dimer anion complex. *Chemical Physics Letters*, **2006**, 426, 197-203	2.5	26
96	Advances in methods and algorithms in a modern quantum chemistry program package. *Physical Chemistry Chemical Physics*, **2006**, 8, 3172-91	3.6	2371
95	Accurate local approximations to the triples correlation energy: formulation, implementation and tests of 5th-order scaling models. *Molecular Physics*, **2005**, 103, 425-437	1.7	50
94	Electronic transitions in the IR: Matrix isolation spectroscopy and electronic structure theory calculations on polyacenes and dibenzopolyacenes. *Physical Chemistry Chemical Physics*, **2005**, 7, 109	3.6	32
93	Unrestricted perfect pairing: the simplest wave-function-based model chemistry beyond mean field. *Journal of Physical Chemistry A*, **2005**, 109, 9183-92	2.8	39
92	Characterizing the dimerizations of phenalenyl radicals by ab initio calculations and spectroscopy: sigma-bond formation versus resonance pi-stabilization. *Journal of Physical Chemistry A*, **2005**, 109, 11261-7	2.8	82

91	A Resolution-Of-The-Identity Implementation of the Local Triatomics-In-Molecules Model for Second-Order Møller-Plesset Perturbation Theory with Application to Alanine Tetrapeptide Conformational Energies. *Journal of Chemical Theory and Computation*, **2005**, 1, 862-76	6.4	82
90	Scaled opposite spin second order Møller-Plesset theory with improved physical description of long-range dispersion interactions. *Journal of Physical Chemistry A*, **2005**, 109, 7598-605	2.8	78
89	Single-reference ab initio methods for the calculation of excited states of large molecules. *Chemical Reviews*, **2005**, 105, 4009-37	68.1	2042
88	Simulated quantum computation of molecular energies. *Science*, **2005**, 309, 1704-7	33.3	555
87	Fast localized orthonormal virtual orbitals which depend smoothly on nuclear coordinates. *Journal of Chemical Physics*, **2005**, 123, 114108	3.9	76
86	What is the nature of the long bond in the TCNE22− dimer?. *Physical Chemistry Chemical Physics*, **2004**, 6, 2008-2011	3.6	83
85	An exact reformulation of the diagonalization step in electronic structure calculations as a set of second order nonlinear equations. *Journal of Chemical Physics*, **2004**, 120, 10379-84	3.9	18
84	Density Functional Theory Investigations of the Direct Oxidation of Methane on an Fe-Exchanged Zeolite. *Journal of Physical Chemistry B*, **2004**, 108, 4362-4368	3.4	38
83	An efficient method for calculating maxima of homogeneous functions of orthogonal matrices: applications to localized occupied orbitals. *Journal of Chemical Physics*, **2004**, 121, 9220-9	3.9	53
82	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
81	Intermolecular pi-to-pi bonding between stacked aromatic dyads. Experimental and theoretical binding energies and near-IR optical transitions for phenalenyl radical/radical versus radical/cation dimerizations. *Journal of the American Chemical Society*, **2004**, 126, 13850-8	16.4	249
80	Initiation of Electro-Oxidation of CO on Pt Based Electrodes at Full Coverage Conditions Simulated by Ab Initio Electronic Structure Calculations. *Journal of Physical Chemistry B*, **2004**, 108, 9888-9892	3.4	16
79	Scaled opposite-spin second order Møller-Plesset correlation energy: an economical electronic structure method. *Journal of Chemical Physics*, **2004**, 121, 9793-802	3.9	440
78	Approaching the Basis Set Limit in Density Functional Theory Calculations Using Dual Basis Sets without Diagonalization *Journal of Physical Chemistry A*, **2004**, 108, 3206-3210	2.8	73
77	How diradicaloid is a stable diradical?. *ChemPhysChem*, **2003**, 4, 522-5	3.2	95
76	Sparse matrix multiplications for linear scaling electronic structure calculations in an atom-centered basis set using multiatom blocks. *Journal of Computational Chemistry*, **2003**, 24, 618-22	3.5	49
75	Characterizing unpaired electrons from the one-particle density matrix. *Chemical Physics Letters*, **2003**, 372, 508-511	2.5	238
74	Chlorophyll fluorescence quenching by xanthophylls. *Physical Chemistry Chemical Physics*, **2003**, 5, 3247	3.6	115

73	Approaching closed-shell accuracy for radicals using coupled cluster theory with perturbative triple substitutions. *Physical Chemistry Chemical Physics*, **2003**, 5, 2488	3.6	51
72	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
71	Exact solution (within a triple-zeta, double polarization basis set) of the electronic Schrödinger equation for water. *Journal of Chemical Physics*, **2003**, 118, 8551-8554	3.9	106
70	Curvy steps for density matrix based energy minimization: tensor formulation and toy applications. *Molecular Physics*, **2003**, 101, 37-43	1.7	22
69	Time-Dependent Density Functional Study of the Electronic Excited States of Polycyclic Aromatic Hydrocarbon Radical Ions. *Journal of Physical Chemistry A*, **2003**, 107, 4940-4951	2.8	86
68	Electronic Absorption Spectra of Neutral Perylene (C20H12), Terrylene (C30H16), and Quaterrylene (C40H20) and Their Positive and Negative Ions: Ne Matrix-Isolation Spectroscopy and Time-Dependent Density Functional Theory Calculations. *Journal of Physical Chemistry A*, **2003**, 107, 3660-3669	2.8	134
67	Charge-Transfer State as a Possible Signature of a Zeaxanthin–Chlorophyll Dimer in the Non-photochemical Quenching Process in Green Plants. *Journal of Physical Chemistry B*, **2003**, 107, 6500-6503	3.4	129
66	Vibrational and Electronic Spectroscopy of Acenaphthylene and Its Cation. *Journal of Physical Chemistry A*, **2003**, 107, 782-793	2.8	42
65	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
64	Controlling the Extent of Diradical Character by Utilizing Neighboring Group Interactions. *Journal of Physical Chemistry A*, **2003**, 107, 7475-7481	2.8	50
63	Improved Fermi operator expansion methods for fast electronic structure calculations. *Journal of Chemical Physics*, **2003**, 119, 4117-4125	3.9	76
62	A perturbative correction to the quadratic coupled-cluster doubles method for higher excitations. *Chemical Physics Letters*, **2002**, 353, 359-367	2.5	78
61	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
60	Can coupled cluster singles and doubles be approximated by a valence active space model?. *Journal of Chemical Physics*, **2002**, 117, 3040-3048	3.9	14
59	GEOMETRIC DIRECT MINIMIZATION OF HARTREE–FOCK CALCULATIONS INVOLVING OPEN SHELL WAVEFUNCTIONS WITH SPIN RESTRICTED ORBITALS. *Journal of Theoretical and Computational Chemistry*, **2002**, 01, 255-261	1.8	8
58	Quadratic Coupled-Cluster Doubles: Implementation and Assessment of Perfect Pairing Optimized Geometries. *Journal of Physical Chemistry B*, **2002**, 106, 8070-8077	3.4	22
57	Implementation of generalized valence bond-inspired coupled cluster theories. *Journal of Chemical Physics*, **2002**, 117, 9190-9201	3.9	48
56	A geometric approach to direct minimization. *Molecular Physics*, **2002**, 100, 1713-1721	1.7	116

55	Parallelization of analytical Hartree–Fock and density functional theory Hessian calculations. Part I: parallelization of coupled-perturbed Hartree–Fock equations. *Molecular Physics*, **2002**, 100, 1755-1761	1.7	19
54	Two-body coupled cluster expansions. *Journal of Chemical Physics*, **2001**, 115, 5033-5040	3.9	46
53	Efficient evaluation of the Coulomb force in density-functional theory calculations. *Journal of Chemical Physics*, **2001**, 114, 6572-6577	3.9	105
52	The Theoretical Prediction of Molecular Radical Species: a Systematic Study of Equilibrium Geometries and Harmonic Vibrational Frequencies. *Journal of Physical Chemistry A*, **2001**, 105, 9736-9747	2.8	133
51	Calculating the equilibrium structure of the BNB molecule: Real s. artifactual symmetry breaking. *Physical Chemistry Chemical Physics*, **2001**, 3, 4495-4500	3.6	26
50	A second-order perturbative correction to the coupled-cluster singles and doubles method: CCSD(2). *Journal of Chemical Physics*, **2001**, 115, 2014-2021	3.9	144
49	Connections between coupled cluster and generalized valence bond theories. *Journal of Chemical Physics*, **2001**, 115, 7814-7821	3.9	51
48	Extracting polarized atomic orbitals from molecular orbital calculations. *International Journal of Quantum Chemistry*, **2000**, 76, 169-184	2.1	34
47	Q-Chem 2.0: a high-performance ab initio electronic structure program package. *Journal of Computational Chemistry*, **2000**, 21, 1532-1548	3.5	588
46	The quadratic coupled cluster doubles model. *Chemical Physics Letters*, **2000**, 330, 585-594	2.5	70
45	A second-order correction to singles and doubles coupled-cluster methods based on a perturbative expansion of a similarity-transformed Hamiltonian. *Chemical Physics Letters*, **2000**, 323, 21-28	2.5	132
44	Benchmark variational coupled cluster doubles results. *Journal of Chemical Physics*, **2000**, 113, 8873-8879	3.9	102
43	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
42	Closely approximating second-order Mo/ller–Plesset perturbation theory with a local triatomics in molecules model. *Journal of Chemical Physics*, **2000**, 112, 3592-3601	3.9	158
41	Complete basis set extrapolations for low-lying triplet electronic states of acetylene and vinylidene. *Journal of Chemical Physics*, **2000**, 113, 1447-1454	3.9	23
40	A nonorthogonal approach to perfect pairing. *Journal of Chemical Physics*, **2000**, 112, 5633-5638	3.9	40
39	Excited states theory for optimized orbitals and valence optimized orbitals coupled-cluster doubles models. *Journal of Chemical Physics*, **2000**, 113, 6509-6527	3.9	122
38	On the performance of density functional theory for symmetry-breaking problems. *Chemical Physics Letters*, **1999**, 302, 425-430	2.5	119

37	Time-dependent density functional theory within the Tamm–Dancoff approximation. *Chemical Physics Letters*, **1999**, 314, 291-299	2.5	1363
36	Quasidegenerate second-order perturbation corrections to single-excitation configuration interaction. *Molecular Physics*, **1999**, 96, 593-602	1.7	40
35	Analytical second derivatives for excited electronic states using the single excitation configuration interaction method: theory and application to benzo[a]pyrene and chalcone. *Molecular Physics*, **1999**, 96, 1533-1541	1.7	49
34	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
33	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
32	An improved semidirect MP2 gradient method. *Molecular Physics*, **1999**, 96, 673-679	1.7	34
31	A hierarchy of local electron correlation models based on atomic truncations **1999**,		2
30	Electronic reaction field cavity optimization: Extension to solvation of molecules **1999**,		1
29	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
28	Linear and sublinear scaling formation of Hartree–Fock-type exchange matrices. *Journal of Chemical Physics*, **1998**, 109, 1663-1669	3.9	277
27	A multipole acceptability criterion for electronic structure theory. *Journal of Chemical Physics*, **1998**, 109, 8764-8769	3.9	23
26	A tensor formulation of many-electron theory in a nonorthogonal single-particle basis. *Journal of Chemical Physics*, **1998**, 108, 616-625	3.9	130
25	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
24	Periodic boundary conditions and the fast multipole method. *Journal of Chemical Physics*, **1997**, 107, 10131-10140	3.9	66
23	Polarized atomic orbitals for self-consistent field electronic structure calculations. *Journal of Chemical Physics*, **1997**, 107, 9085-9095	3.9	41
22	A coupled-cluster ab initio study of triplet C3H2 and the neutral–neutral reaction to interstellar C3H. *Journal of Chemical Physics*, **1997**, 106, 4141-4151	3.9	102
21	SINGLE REFERENCE COUPLED CLUSTER AND PERTURBATION THEORIES OF ELECTRONIC EXCITATION ENERGIES. *Recent Advances in Computational*, **1997**, 221-253		15
20	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

19	On the Nature of Electronic Transitions in Radicals: An Extended Single Excitation Configuration Interaction Method. *The Journal of Physical Chemistry*, **1996**, 100, 6131-6137		66
18	Quantum Chemistry and Molecular Processes. *The Journal of Physical Chemistry*, **1996**, 100, 13213-13225		210
17	Linear scaling density functional calculations via the continuous fast multipole method. *Chemical Physics Letters*, **1996**, 253, 268-278	2.5	285
16	The first solvation shell of magnesium ion in a model protein environment with formate, water, and X-NH3, H2S, imidazole, formaldehyde, and chloride as ligands: an Ab initio study. *Proteins: Structure, Function and Bioinformatics*, **1995**, 21, 244-55	4.2	17
15	Configuration interaction with single substitutions for excited states of open-shell molecules. *International Journal of Quantum Chemistry*, **1995**, 56, 361-370	2.1	51
14	Analytical gradient of the CIS(D) perturbative correction to single-excitation configuration interaction excited states. *International Journal of Quantum Chemistry*, **1995**, 56, 421-427	2.1	6
13	Analysis of Electronic Transitions as the Difference of Electron Attachment and Detachment Densities. *The Journal of Physical Chemistry*, **1995**, 99, 14261-14270		254
12	A perturbative correction to restricted open shell configuration interaction with single substitutions for excited states of radicals. *Chemical Physics Letters*, **1995**, 246, 114-121	2.5	147
11	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
10	The continuous fast multipole method. *Chemical Physics Letters*, **1994**, 230, 8-16	2.5	342
9	Simulations of femtosecond laser-induced desorption of CO from Cu(100). *Surface Science*, **1994**, 320, L57-L62	1.8	70
8	Toward a systematic molecular orbital theory for excited states. *The Journal of Physical Chemistry*, **1992**, 96, 135-149		2142
7	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
6	Size-consistent Brueckner theory limited to double substitutions. *Chemical Physics Letters*, **1989**, 164, 185-192	2.5	440
5	A fifth-order perturbation comparison of electron correlation theories. *Chemical Physics Letters*, **1989**, 157, 479-483	2.5	6685
4	An improved semidirect MP2 gradient method		3
3	Pathways for the Formation of C2+ Products under Alkaline Conditions during the Electrochemical Reduction of CO2. *ACS Energy Letters*,1679-1686	20.1	8
2	NewtonNet: a Newtonian message passing network for deep learning of interatomic potentials and forces		5

List of Publications

1	Computing X-Ray Absorption Spectra from Linear-Response Particles atop Optimized Holes. *Journal of Chemical Physics*,	3.9	2