Jan M L Martin

List of Publications by Year in Descending Order

307 papers	24,002 citations	82 h-index	144 g-index
319 ext. papers	25,926 ext. citations	4.5 avg, IF	7.41 L-index

#	Paper	IF	Citations
307	The MOBH35 Metal-Organic Barrier Heights Reconsidered: Performance of Local-Orbital Coupled Cluster Approaches in Different Static Correlation Regimes.. *Journal of Chemical Theory and Computation*, **2022**,	6.4	5
306	Heavy-Atom Tunneling in the Covalent/Dative Bond Complexation of Cyclo[18]carbon-Piperidine.. *Journal of Physical Chemistry B*, **2022**, 126, 1799-1804	3.4	1
305	Electron Correlation: Nature's Weird and Wonderful Chemical Glue. *Israel Journal of Chemistry*, **2022**, 62,	3.4	4
304	Do Double-Hybrid Functionals Benefit from Regularization in the PT2 Term? Observations from an Extensive Benchmark.. *Journal of Physical Chemistry Letters*, **2022**, 3499-3506	6.4	3
303	Exploring Avenues beyond Revised DSD Functionals: II. Random-Phase Approximation and Scaled MP3 Corrections. *Journal of Physical Chemistry A*, **2021**, 125, 4628-4638	2.8	10
302	Exploring Avenues beyond Revised DSD Functionals: I. Range Separation, with DSD as a Special Case. *Journal of Physical Chemistry A*, **2021**, 125, 4614-4627	2.8	15
301	What Types of Chemical Problems Benefit from Density-Corrected DFT? A Probe Using an Extensive and Chemically Diverse Test Suite. *Journal of Chemical Theory and Computation*, **2021**, 17, 1368-1379	6.4	18
300	Prototypical □□dimers re-examined by means of high-level CCSDT(Q) composite ab initio methods. *Journal of Chemical Physics*, **2021**, 154, 124117	3.9	3
299	Surprisingly Good Performance of XYG3 Family Functionals Using a Scaled KS-MP3 Correlation. *Journal of Physical Chemistry Letters*, **2021**, 12, 9368-9376	6.4	2
298	Coupled Cluster Benchmark of New DFT and Local Correlation Methods: Mechanisms of Hydroarylation and Oxidative Coupling Catalyzed by Ru(II, III) Chloride Carbonyls. *Journal of Physical Chemistry A*, **2021**, 125, 8987-8999	2.8	6
297	Pure and Hybrid SCAN, rSCAN, and rSCAN: Which One Is Preferred in KS- and HF-DFT Calculations, and How Does D4 Dispersion Correction Affect This Ranking?. *Molecules*, **2021**, 27,	4.8	2
296	Canonical and DLPNO-Based Composite Wavefunction Methods Parametrized against Large and Chemically Diverse Training Sets. 2: Correlation-Consistent Basis Sets, Core-Valence Correlation, and F12 Alternatives. *Journal of Chemical Theory and Computation*, **2020**, 16, 7507-7524	6.4	11
295	Canonical and DLPNO-Based G4(MP2)XK-Inspired Composite Wave Function Methods Parametrized against Large and Chemically Diverse Training Sets: Are They More Accurate and/or Robust than Double-Hybrid DFT?. *Journal of Chemical Theory and Computation*, **2020**, 16, 4238-4255	6.4	19
294	Performance of Electronic Structure Methods for the Description of H□kel-M□bius Interconversions in Extended □Systems. *Journal of Physical Chemistry A*, **2020**, 124, 2380-2397	2.8	11
293	Performance of Localized Coupled Cluster Methods in a Moderately Strong Correlation Regime: H□kel-M□bius Interconversions in Expanded Porphyrins. *Journal of Chemical Theory and Computation*, **2020**, 16, 3641-3653	6.4	22
292	Empirical Double-Hybrid Density Functional Theory: A □third Way□ In Between WFT and DFT. *Israel Journal of Chemistry*, **2020**, 60, 787-804	3.4	71
291	The Atomic Partial Charges Arboretum: Trying to See the Forest for the Trees. *ChemPhysChem*, **2020**, 21, 688-696	3.2	23

290	Molecular dynamics simulations of the interaction of Mouse and Torpedo acetylcholinesterase with covalent inhibitors explain their differential reactivity: Implications for drug design. *Chemico-Biological Interactions*, **2019**, 310, 108715	5	7
289	Minimally Empirical Double-Hybrid Functionals Trained against the GMTKN55 Database: revDSD-PBEP86-D4, revDOD-PBE-D4, and DOD-SCAN-D4. *Journal of Physical Chemistry A*, **2019**, 123, 5129-5143	2.8	128
288	Probing the basis set limit for thermochemical contributions of inner-shell correlation: balance of core-core and core-valence contributions** In memory of Dieter Cremer (1944–2017)View all notes. *Molecular Physics*, **2019**, 117, 1078-1087	1.7	11
287	A simple model for scalar relativistic corrections to molecular total atomisation energies. *Molecular Physics*, **2019**, 117, 2225-2232	1.7	4
286	Some observations on the performance of the most recent exchange-correlation functionals for the large and chemically diverse GMTKN55 benchmark **2019**,		8
285	Coupled cluster benchmark of new density functionals and of domain pair natural orbital methods: Mechanisms of hydroarylation and oxidative coupling catalyzed by Ru(II) chloride carbonyls **2019**,		9
284	The kinetics and mechanism of oxidation of reduced phosphovanadomolybdates by molecular oxygen: theory and experiment in concert. *Physical Chemistry Chemical Physics*, **2018**, 20, 7579-7587	3.6	6
283	The X40□10 Halogen Bonding Benchmark Revisited: Surprising Importance of (n-1)d Subvalence Correlation. *Journal of Physical Chemistry A*, **2018**, 122, 2184-2197	2.8	23
282	The S66 Non-Covalent Interactions Benchmark Reconsidered Using Explicitly Correlated Methods Near the Basis Set Limit. *Australian Journal of Chemistry*, **2018**, 71, 238	1.2	30
281	A simple □ange extender□For basis set extrapolation methods for MP2 and coupled cluster correlation energies **2018**,		9
280	Do CCSD and approximate CCSD-F12 variants converge to the same basis set limits? The case of atomization energies. *Journal of Chemical Physics*, **2018**, 149, 154109	3.9	27
279	A Thiourea Tether in the Second Coordination Sphere as a Binding Site for CO and a Proton Donor Promotes the Electrochemical Reduction of CO to CO Catalyzed by a Rhenium Bipyridine-Type Complex. *Journal of the American Chemical Society*, **2018**, 140, 12451-12456	16.4	83
278	Prediction of electronic couplings for molecular charge transfer using optimally tuned range-separated hybrid functionals. *Molecular Physics*, **2018**, 116, 2497-2505	1.7	12
277	Chirality-induced spin polarization places symmetry constraints on biomolecular interactions. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 2474-2478	11.5	110
276	Conventional and Explicitly Correlated ab Initio Benchmark Study on Water Clusters: Revision of the BEGDB and WATER27 Data Sets. *Journal of Chemical Theory and Computation*, **2017**, 13, 3136-3152	6.4	65
275	The aug-cc-pVnZ-F12 basis set family: Correlation consistent basis sets for explicitly correlated benchmark calculations on anions and noncovalent complexes. *Journal of Chemical Physics*, **2017**, 147, 134106	3.9	34
274	W4-17: A diverse and high-confidence dataset of atomization energies for benchmarking high-level electronic structure methods. *Journal of Computational Chemistry*, **2017**, 38, 2063-2075	3.5	85
273	Surprising performance for vibrational frequencies of the distinguishable clusters with singles and doubles (DCSD) and MP2.5 approximations **2017**,		6

272	MP2-F12 basis set convergence for the S66 noncovalent interactions benchmark: Transferability of the complementary auxiliary basis set (CABS) **2017**,		2
271	Electron Transfer Oxidation of Benzene and Aerobic Oxidation to Phenol. *ACS Catalysis*, **2016**, 6, 6403-6407	10.1	41
270	Heats of formation of platonic hydrocarbon cages by means of high-level thermochemical procedures. *Journal of Computational Chemistry*, **2016**, 37, 49-58	3.5	47
269	The S66x8 benchmark for noncovalent interactions revisited: explicitly correlated ab initio methods and density functional theory. *Physical Chemistry Chemical Physics*, **2016**, 18, 20905-25	3.6	127
268	What Are the Ground State Structures of C20 and C24? An Explicitly Correlated Ab Initio Approach. *Journal of Physical Chemistry A*, **2016**, 120, 153-60	2.8	32
267	Benchmark ab Initio Conformational Energies for the Proteinogenic Amino Acids through Explicitly Correlated Methods. Assessment of Density Functional Methods. *Journal of Chemical Theory and Computation*, **2016**, 12, 444-54	6.4	75
266	Toward a W4-F12 approach: Can explicitly correlated and orbital-based ab initio CCSD(T) limits be reconciled?. *Journal of Chemical Physics*, **2016**, 144, 214101	3.9	69
265	Exploring the Accuracy Limits of Local Pair Natural Orbital Coupled-Cluster Theory. *Journal of Chemical Theory and Computation*, **2015**, 11, 1525-39	6.4	389
264	Explicitly correlated coupled cluster benchmarks with realistic-sized ligands for some late-transition metal reactions: basis sets convergence and performance of more approximate methods. *Highlights in Theoretical Chemistry*, **2015**, 233-246		1
263	The cc-pV5Z-F12 basis set: reaching the basis set limit in explicitly correlated calculations. *Molecular Physics*, **2015**, 113, 1551-1558	1.7	43
262	Frequency and zero-point vibrational energy scale factors for double-hybrid density functionals (and other selected methods): can anharmonic force fields be avoided?. *Journal of Physical Chemistry A*, **2015**, 119, 1701-14	2.8	315
261	Comment on "Doubly hybrid density functional xDH-PBE0 from a parameter-free global hybrid model PBE0" [J. Chem. Phys. 136, 174103 (2012)]. *Journal of Chemical Physics*, **2015**, 143, 187101; discussion 187102	3.9	11
260	New ruthenium nitrosyl pincer complexes bearing an O2 ligand. Mono-oxygen transfer. *Inorganic Chemistry*, **2015**, 54, 2253-63	5.1	10
259	Explicitly correlated coupled cluster benchmarks with realistic-sized ligands for some late-transition metal reactions: basis sets convergence and performance of more approximate methods. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	33
258	Conformational equilibria in butane-1,4-diol: a benchmark of a prototypical system with strong intramolecular H-bonds. *Journal of Physical Chemistry A*, **2014**, 118, 293-303	2.8	45
257	Equilibrium gas-phase structures of sodium fluoride, bromide, and iodide monomers and dimers. *Journal of Physical Chemistry A*, **2014**, 118, 1927-35	2.8	5
256	Some Observations on Counterpoise Corrections for Explicitly Correlated Calculations on Noncovalent Interactions. *Journal of Chemical Theory and Computation*, **2014**, 10, 3791-9	6.4	84
255	Assessment of CCSD(T)-F12 Approximations and Basis Sets for Harmonic Vibrational Frequencies. *Journal of Chemical Theory and Computation*, **2014**, 10, 2085-90	6.4	34

254	The eight-valence-electron systems re-examined: convergence of the coupled-cluster series and performance of quasiperturbative methods for quadruple excitations. *Molecular Physics*, **2014**, 112, 785-793	1.7	21
253	Heats of formation of the amino acids re-examined by means of W1-F12 and W2-F12 theories. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	63
252	A simple DFT-based diagnostic for nondynamical correlation. *Highlights in Theoretical Chemistry*, **2014**, 251-259		
251	Spin-component-scaled double hybrids: An extensive search for the best fifth-rung functionals blending DFT and perturbation theory. *Journal of Computational Chemistry*, **2013**, 34, 2327-44	3.5	200
250	CO-Induced Methyl Migration in a Rhodium Thiophosphoryl Pincer Complex and Its Comparison with Phosphine-Based Complexes: The Divergent Effects of S and P Donor Ligands. *Organometallics* , **2013**, 32, 7163-7180	3.8	16
249	Benzyl Cation Stabilized by Metal Complexation. Relative Stability of Coordinated Methylene Arenium, Benzylic, and Benzylic Structures. *Organometallics*, **2013**, 32, 4813-4819	3.8	6
248	Halogen Bonds: Benchmarks and Theoretical Analysis. *Journal of Chemical Theory and Computation*, **2013**, 9, 1918-31	6.4	357
247	Accurate quantum chemical energies for tetrapeptide conformations: why MP2 data with an insufficient basis set should be handled with caution. *Physical Chemistry Chemical Physics*, **2013**, 15, 7028-31	3.6	57
246	What can we learn about dispersion from the conformer surface of n-pentane?. *Journal of Physical Chemistry A*, **2013**, 117, 3118-32	2.8	51
245	The melatonin conformer space: benchmark and assessment of wave function and DFT methods for a paradigmatic biological and pharmacological molecule. *Journal of Physical Chemistry A*, **2013**, 117, 2269-77	2.8	77
244	A simple DFT-based diagnostic for nondynamical correlation. *Theoretical Chemistry Accounts*, **2013**, 132, 1	1.9	88
243	Polyoxometalate-catalyzed insertion of oxygen from O(2) into tin-alkyl bonds. *Journal of the American Chemical Society*, **2013**, 135, 19304-10	16.4	38
242	Turning Over Definitions in Catalytic Cycles. *ACS Catalysis*, **2012**, 2, 2787-2794	13.1	282
241	O(3P) + CO2 collisions at hyperthermal energies: dynamics of nonreactive scattering, oxygen isotope exchange, and oxygen-atom abstraction. *Journal of Physical Chemistry A*, **2012**, 116, 64-84	2.8	15
240	Exclusive C Oxidative Addition in a Rhodium Thiophosphoryl Pincer Complex and Computational Evidence for an -C H Agostic Intermediate. *Organometallics*, **2012**, 31, 505-512	3.8	30
239	Explicitly correlated Wn theory: W1-F12 and W2-F12. *Journal of Chemical Physics*, **2012**, 136, 124114	3.9	176
238	Explicitly correlated benchmark calculations on C8H8 isomer energy separations: how accurate are DFT, double-hybrid, and composite ab initio procedures?. *Molecular Physics*, **2012**, 110, 2477-2491	1.7	47
237	Comment on "Revised electron affinity of SF6 from kinetic data" [J. Chem. Phys. 136, 121102 (2012)]. *Journal of Chemical Physics*, **2012**, 136, 197101	3.9	12

236	DSD-PBEP86: in search of the best double-hybrid DFT with spin-component scaled MP2 and dispersion corrections. *Physical Chemistry Chemical Physics*, **2011**, 13, 20104-7	3.6	304
235	What makes for a good catalytic cycle? A theoretical study of the SPhos ligand in the Suzuki-Miyaura reaction. *Chemical Communications*, **2011**, 47, 4935-7	5.8	32
234	What Makes for a Bad Catalytic Cycle? A Theoretical Study on the Suzuki−Miyaura Reaction within the Energetic Span Model. *ACS Catalysis*, **2011**, 1, 246-253	13.1	106
233	Basis set convergence of explicitly correlated double-hybrid density functional theory calculations. *Journal of Chemical Physics*, **2011**, 135, 144119	3.9	23
232	The rate-determining step is dead. Long live the rate-determining state!. *ChemPhysChem*, **2011**, 12, 1413-8	3.2	99
231	W4-11: A high-confidence benchmark dataset for computational thermochemistry derived from first-principles W4 data. *Chemical Physics Letters*, **2011**, 510, 165-178	2.5	285
230	Performance of W4 theory for spectroscopic constants and electrical properties of small molecules. *Journal of Chemical Physics*, **2010**, 133, 144102	3.9	56
229	DSD-BLYP: A General Purpose Double Hybrid Density Functional Including Spin Component Scaling and Dispersion Correction *Journal of Physical Chemistry C*, **2010**, 114, 20801-20808	3.8	261
228	DFT study of the structure and reactivity of the terminal Pt(IV)-oxo complex bearing no electron-withdrawing ligands. *Journal of the American Chemical Society*, **2010**, 132, 14886-900	16.4	46
227	Can DFT methods correctly and efficiently predict the coordination number of copper(I) complexes? A case study. *Journal of Computational Chemistry*, **2010**, 31, 75-83	3.5	16
226	Effect of CO on the oxidative addition of arene C-H bonds by cationic rhodium complexes. *Chemistry - A European Journal*, **2010**, 16, 328-53	4.8	45
225	Photochemical reduction of carbon dioxide catalyzed by a ruthenium-substituted polyoxometalate. *Chemistry - A European Journal*, **2010**, 16, 1356-64	4.8	123
224	Borane-lewis base complexes as homolytic hydrogen atom donors. *Chemistry - A European Journal*, **2010**, 16, 6861-5	4.8	64
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222	A coordination controlled aryl-halide oxidative addition to platinum. *Chemistry - A European Journal* , **2009**, 15, 10025-8	4.8	12
221	Performance of ab initio and density functional methods for conformational equilibria of C(n)H(2n+2) alkane isomers (n = 4-8). *Journal of Physical Chemistry A*, **2009**, 113, 11974-83	2.8	134
220	Economical post-CCSD(T) computational thermochemistry protocol and applications to some aromatic compounds. *Journal of Physical Chemistry A*, **2009**, 113, 7610-20	2.8	55
219	Unrestricted Coupled Cluster and Brueckner Doubles Variations of W1 Theory. *Journal of Chemical Theory and Computation*, **2009**, 5, 2687-93	6.4	184

218	Benchmark thermochemistry of the C(n)H(2n+2) alkane isomers (n = 2-8) and performance of DFT and composite ab initio methods for dispersion-driven isomeric equilibria. *Journal of Physical Chemistry A*, **2009**, 113, 8434-47	2.8	110
217	Atomization energies of the carbon clusters C n (n = 2□10) revisited by means of W4 theory as well as density functional, Gn, and CBS methods. *Molecular Physics*, **2009**, 107, 977-990	1.7	37
216	A DFT study on the mechanism of a novel, regioselective, intramolecular N-pi rearrangement of cis and trans-eta1-N-Cp*Rh-hydroxytamoxifen complexes to their eta6 derivatives; potential breast cancer pharmaceuticals, and fluorescent probes. *Dalton Transactions*, **2009**, 4334-43	4.3	7
215	Evidence for a terminal Pt(iv)-oxo complex exhibiting diverse reactivity. *Nature*, **2008**, 455, 1093-1096	50.4	176
214	Highly accurate first-principles benchmark data sets for the parametrization and validation of density functional and other approximate methods. Derivation of a robust, generally applicable, double-hybrid functional for thermochemistry and thermochemical kinetics. *Journal of Physical Chemistry A*, **2008**, 112, 12868-86	2.8	578
213	Halogen-Bonded Supramolecular Assemblies Based on Phenylethynyl Pyridine Derivatives: Driving Crystal Packing through Systematic Chemical Modifications. *Crystal Growth and Design*, **2008**, 8, 3066-3072	3.5	25
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211	Directing aryl-I versus Aryl-Br bond activation by nickel via a ring walking process. *Inorganic Chemistry*, **2008**, 47, 5114-21	5.1	60
210	The impact of weak C-H...Rh interactions on the structure and reactivity of trans-[Rh(CO)2(phosphine)2]+: an experimental and theoretical examination. *Chemistry - A European Journal*, **2008**, 14, 8183-94	4.8	11
209	Fundamental vibrational frequencies and dominant resonances in methylamine isotopologues by ab initio and density functional theory methods. *Journal of Computational Chemistry*, **2008**, 29, 1268-76	3.5	15
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207	Polarizability of small carbon cluster anions from first principles. *Journal of Physical Chemistry A*, **2007**, 111, 2028-32	2.8	13
206	Basis set limit coupled cluster study of h-bonded systems and assessment of more approximate methods. *Journal of Physical Chemistry A*, **2007**, 111, 11122-33	2.8	85
205	Co-Crystallization of Sym-Triiodo-Trifluorobenzene with Bipyridyl Donors: Consistent Formation of Two Instead of Anticipated Three N▩ Halogen Bonds. *Crystal Growth and Design*, **2007**, 7, 386-392	3.5	81
204	Heats of formation of beryllium, boron, aluminum, and silicon re-examined by means of W4 theory. *Journal of Physical Chemistry A*, **2007**, 111, 5936-44	2.8	82
203	Gd3+ complexes as potential spin labels for high field pulsed EPR distance measurements. *Journal of the American Chemical Society*, **2007**, 129, 14138-9	16.4	129
202	Proton walk in the aqueous platinum complex [TpPtMeCO] via a sticky sigma-methane ligand. *Chemistry - A European Journal*, **2007**, 13, 2812-23	4.8	13
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200	Benchmark atomization energy of ethane: Importance of accurate zero-point vibrational energies and diagonal Born–Oppenheimer corrections for a simple organic molecule. *Computational and Theoretical Chemistry*, **2007**, 811, 345-353		57
199	Basis set convergence of post-CCSD contributions to molecular atomization energies. *Journal of Chemical Physics*, **2007**, 127, 064104	3.9	127
198	The Protonation Site of Aniline Revisited: A 'Torture Test' for Electron Correlation Methods. *ACS Symposium Series*, **2007**, 183-192	0.4	3
197	Charge Transport in Conjugated Aromatic Molecular Junctions: Molecular Conjugation and Molecule–Electrode Coupling. *Journal of Physical Chemistry C*, **2007**, 111, 14893-14902	3.8	89
196	Comment on: Estimating the Hartree–Fock limit from finite basis set calculations [Jensen F (2005) Theor Chem Acc 113:267]. *Theoretical Chemistry Accounts*, **2006**, 115, 330-333	1.9	318
195	Selective sp3 C-H activation of ketones at the beta position by Ir(I). Origin of regioselectivity and water effect. *Journal of the American Chemical Society*, **2006**, 128, 12400-1	16.4	63
194	The lowest singlet-triplet excitation energy of BN: A converged coupled cluster perspective. *Journal of Chemical Physics*, **2006**, 125, 144313	3.9	39
193	Benchmark study of DFT functionals for late-transition-metal reactions. *Journal of Physical Chemistry A*, **2006**, 110, 709-16	2.8	193
192	W4 theory for computational thermochemistry: In pursuit of confident sub-kJ/mol predictions. *Journal of Chemical Physics*, **2006**, 125, 144108	3.9	561
191	Rozen's epoxidation reagent, CH3CN.HOF: a theoretical study of its structure, vibrational spectroscopy, and reaction mechanism. *Journal of Physical Chemistry A*, **2006**, 110, 8275-81	2.8	8
190	ortho C–H Activation of Haloarenes and Anisole by an Electron-Rich Iridium(I) Complex: Mechanism and Origin of Regio- and Chemoselectivity. An Experimental and Theoretical Study. *Organometallics*, **2006**, 25, 3190-3210	3.8	98
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188	Heats of formation of perchloric acid, HClO4, and perchloric anhydride, Cl2O7. Probing the limits of W1 and W2 theory. *Computational and Theoretical Chemistry*, **2006**, 771, 19-26		40
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182	IUPAC Critical Evaluation of Thermochemical Properties of Selected Radicals. Part I. *Journal of Physical and Chemical Reference Data*, **2005**, 34, 573-656	4.3	275
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175	Vibrational Spectra of the Azabenzenes Revisited: Anharmonic Force Fields *Journal of Physical Chemistry A*, **2004**, 108, 3085-3096	2.8	145
174	Mechanism of the Methylene Transfer Reaction. C Activation and Reductive Elimination in One System. A DFT Study. *Organometallics*, **2004**, 23, 2336-2342	3.8	21
173	Thermodynamic Properties of C1and C2Bromo Compounds and Radicals. A Relativistic ab Initio Study. *Journal of Physical Chemistry A*, **2004**, 108, 7752-7761	2.8	29
172	Arene Hapticity in (C6H6)Cr(CO)n (n = 1 3) Complexes: A DFT Study of Singlet and Triplet Energy Surfaces. *Organometallics*, **2004**, 23, 2315-2325	3.8	23
171	A computational foray into the formation and reactivity of metallabenzenes. *Journal of the American Chemical Society*, **2004**, 126, 11699-710	16.4	131
170	Development of density functionals for thermochemical kinetics. *Journal of Chemical Physics*, **2004**, 121, 3405-16	3.9	1213
169	The mechanism of aluminum-catalyzed Meerwein-Schmidt-Ponndorf-Verley reduction of carbonyls to alcohols. *Journal of the American Chemical Society*, **2004**, 126, 14796-803	16.4	120
168	Cycloaddition reactions of metalloaromatic complexes of iridium and rhodium: a mechanistic DFT investigation. *Journal of the American Chemical Society*, **2003**, 125, 11702-9	16.4	51
167	Novel azine reactivity: facile N-N bond cleavage, C-H activation, and N-N coupling mediated by RhI. *Angewandte Chemie - International Edition*, **2003**, 42, 1949-52	16.4	35
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165	Active site electronic structure and dynamics during metalloenzyme catalysis. *Nature Structural Biology*, **2003**, 10, 98-103		89

164	Metallabenzene versus Cp complex formation: a DFT investigation. *Journal of the American Chemical Society*, **2003**, 125, 13020-1	16.4	65
163	Metallacarbenes from diazoalkanes: an experimental and computational study of the reaction mechanism. *Journal of the American Chemical Society*, **2003**, 125, 6532-46	16.4	102
162	The role of the basis set: Assessing density functional theory. *Journal of Chemical Physics*, **2003**, 119, 3005-3014	3.9	159
161	Catalytic reduction of acetone by [(bpy)Rh]+: a theoretical mechanistic investigation and insight into cooperativity effects in this system. *Journal of the American Chemical Society*, **2003**, 125, 11430-41	16.4	19
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159	Aromatic vs aliphatic C-H bond activation by rhodium(I) as a function of agostic interactions: catalytic H/D exchange between olefins and methanol or water. *Journal of the American Chemical Society*, **2003**, 125, 11041-50	16.4	104
158	Alkali and alkaline earth metal compounds: core–valence basis sets and importance of subvalence correlation. *Molecular Physics*, **2003**, 101, 1345-1361	1.7	99
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156	From ab initio quantum chemistry to molecular dynamics: The delicate case of hydrogen bonding in ammonia. *Journal of Chemical Physics*, **2003**, 119, 5965-5980	3.9	145
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154	The heats of formation of the haloacetylenes XCCY [X, Y = H, F, Cl]: basis set limit ab initio results and thermochemical analysis. *Molecular Physics*, **2002**, 100, 453-464	1.7	19
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List of Publications

2	Benchmark Studies on Small Molecules	2
1	Benchmark ab initio thermochemistry of the isomers of diimide, N2H2, using accurate computed structures and anharmonic force fields	4