Weitao Yang

List of Publications by Year in Descending Order

354 papers	116,358 citations	84 h-index	341 g-index
365 ext. papers	124,707 ext. citations	5.5 avg, IF	8.34 L-index

#	Paper	IF	Citations
354	Multireference Density Functional Theory for Describing Ground and Excited States with Renormalized Singles.. *Journal of Physical Chemistry Letters*, **2022**, 894-903	6.4	1
353	LibSC: Library for Scaling Correction Methods in Density Functional Theory.. *Journal of Chemical Theory and Computation*, **2022**,	6.4	2
352	Combining localized orbital scaling correction and Bethe-Salpeter equation for accurate excitation energies.. *Journal of Chemical Physics*, **2022**, 156, 154101	3.9	1
351	Reformulation of thermally assisted-occupation density functional theory in the Kohn-Sham framework.. *Journal of Chemical Physics*, **2022**, 156, 174108	3.9	0
350	Theoretical studies on triplet-state driven dissociation of formaldehyde by quasi-classical molecular dynamics simulation on machine-learning potential energy surface. *Journal of Chemical Physics*, **2021**, 155, 214105	3.9	2
349	Describing polymer polarizability with localized orbital scaling correction in density functional theory. *Journal of Chemical Physics*, **2021**, 154, 054302	3.9	3
348	Exact Second-Order Corrections and Accurate Quasiparticle Energy Calculations in Density Functional Theory. *Journal of Physical Chemistry Letters*, **2021**, 12, 7236-7244	6.4	4
347	Renormalized Singles Green's Function in the T-Matrix Approximation for Accurate Quasiparticle Energy Calculation. *Journal of Physical Chemistry Letters*, **2021**, 12, 6203-6210	6.4	6
346	Mechanism of Reduction of an Aminyl Radical Intermediate in the Radical SAM GTP 3',8-Cyclase MoaA. *Journal of the American Chemical Society*, **2021**, 143, 13835-13844	16.4	3
345	Cobalt(II)-Catalyzed [4+2] Annulation of Picolinamides with Alkynes via C-H Bond Activation. *Chemistry - A European Journal*, **2020**, 26, 5607-5610	4.8	9
344	Engineering Substrate Interaction To Improve Hydrogen Evolution Catalysis of Monolayer MoS Films beyond Pt. *ACS Nano*, **2020**, 14, 1707-1714	16.7	49
343	Preserving Symmetry and Degeneracy in the Localized Orbital Scaling Correction Approach. *Journal of Physical Chemistry Letters*, **2020**, 11, 1528-1535	6.4	14
342	Mechanism of Rate Acceleration of Radical C-C Bond Formation Reaction by a Radical SAM GTP 3',8-Cyclase. *Journal of the American Chemical Society*, **2020**, 142, 9314-9326	16.4	12
341	Revisiting the Hole Size in Double Helical DNA with Localized Orbital Scaling Corrections. *Journal of Physical Chemistry B*, **2020**, 124, 3428-3435	3.4	4
340	Density Functional Prediction of Quasiparticle, Excitation, and Resonance Energies of Molecules With a Global Scaling Correction Approach. *Frontiers in Chemistry*, **2020**, 8, 588808	5	2
339	Self-Consistent Calculation of the Localized Orbital Scaling Correction for Correct Electron Densities and Energy-Level Alignments in Density Functional Theory. *Journal of Physical Chemistry Letters*, **2020**, 11, 10269-10277	6.4	8
338	Piecewise All-Atom SMD Simulations Reveal Key Secondary Structures in Luciferase Unfolding Pathway. *Biophysical Journal*, **2020**, 119, 2251-2261	2.9	0

337	Arene Substitution Design for Controlled Conformational Changes of Dibenzocycloocta-1,5-dienes. *Journal of the American Chemical Society*, **2020**, 142, 16651-16660	16.4	7
336	Introductory lecture: when the density of the noninteracting reference system is not the density of the physical system in density functional theory. *Faraday Discussions*, **2020**, 224, 9-26	3.6	3
335	Excited-State Potential Energy Surfaces, Conical Intersections, and Analytical Gradients from Ground-State Density Functional Theory. *Journal of Physical Chemistry Letters*, **2019**, 10, 2538-2545	6.4	18
334	Charge transfer excitation energies from ground state density functional theory calculations. *Journal of Chemical Physics*, **2019**, 150, 144109	3.9	7
333	Excitation Energies from the Single-Particle Green's Function with the GW Approximation. *Journal of Physical Chemistry A*, **2019**, 123, 3199-3204	2.8	6
332	1,3-Dipolar cycloaddition of nitrones to oxa(aza)bicyclic alkenes. *Organic Chemistry Frontiers*, **2019**, 6, 3360-3364	5.2	15
331	Solvation Free Energy Calculations with Quantum Mechanics/Molecular Mechanics and Machine Learning Models. *Journal of Physical Chemistry B*, **2019**, 123, 901-908	3.4	15
330	Toward Building Protein Force Fields by Residue-Based Systematic Molecular Fragmentation and Neural Network. *Journal of Chemical Theory and Computation*, **2019**, 15, 1409-1417	6.4	12
329	Approximating Quasiparticle and Excitation Energies from Ground State Generalized Kohn-Sham Calculations. *Journal of Physical Chemistry A*, **2019**, 123, 666-673	2.8	23
328	Renormalized Singles Green's Function for Quasi-Particle Calculations beyond the G W Approximation. *Journal of Physical Chemistry Letters*, **2019**, 10, 447-452	6.4	11
327	Molecular Dynamics Simulations with Quantum Mechanics/Molecular Mechanics and Adaptive Neural Networks. *Journal of Chemical Theory and Computation*, **2018**, 14, 1442-1455	6.4	66
326	Plasmon-Enhanced Catalysis: Distinguishing Thermal and Nonthermal Effects. *Nano Letters*, **2018**, 18, 1714-1723	11.5	165
325	Localized orbital scaling correction for systematic elimination of delocalization error in density functional approximations. *National Science Review*, **2018**, 5, 203-215	10.8	71
324	Accurate density functional prediction of molecular electron affinity with the scaling corrected KohnSham frontier orbital energies. *Molecular Physics*, **2018**, 116, 927-934	1.7	7
323	Accurate Quantum Mechanical/Molecular Mechanical Calculations of Reduction Potentials in Azurin Variants. *Journal of Chemical Theory and Computation*, **2018**, 14, 4948-4957	6.4	11
322	Photocatalytic activity and the radiative lifetimes of excitons via an ab initio approach. *Journal of Materials Chemistry A*, **2018**, 6, 15027-15032	13	9
321	Perspective: Chemical Information Encoded in Electron Density. *Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica*, **2018**, 34, 567-580	3.8	2
320	Spin-state energetics of iron(II) porphyrin from the particle-particle random phase approximation. *European Physical Journal B*, **2018**, 91, 1	1.2	3

319	Role of Conformational Fluctuations of Protein toward Methylation in DNA by Cytosine-5-methyltransferase. *Journal of Chemical Theory and Computation*, **2018**, 14, 6679-6689	6.4	3
318	Field Electron Emission Images Far Away from a Semi-Infinitely Long Emitter: A Multiscale Simulation. *Journal of Physical Chemistry C*, **2018**, 122, 27754-27760	3.8	1
317	Describing strong correlation with fractional-spin correction in density functional theory. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 9678-9683	11.5	41
316	Accurate Treatment of Charge-Transfer Excitations and Thermally Activated Delayed Fluorescence Using the Particle-Particle Random Phase Approximation. *Journal of Chemical Theory and Computation*, **2018**, 14, 3196-3204	6.4	9
315	Force Field for Water Based on Neural Network. *Journal of Physical Chemistry Letters*, **2018**, 9, 3232-3240	6.4	30
314	Single, Double Electronic Excitations and Exciton Effective Conjugation Lengths in Conjugated Systems. *Journal of Physical Chemistry Letters*, **2018**, 9, 4029-4036	6.4	5
313	Product selectivity in plasmonic photocatalysis for carbon dioxide hydrogenation. *Nature Communications*, **2017**, 8, 14542	17.4	247
312	Three Pyrimidine Decarboxylations in the Absence of a Catalyst. *Biochemistry*, **2017**, 56, 1498-1503	3.2	1
311	On the piecewise convex or concave nature of ground state energy as a function of fractional number of electrons for approximate density functionals. *Journal of Chemical Physics*, **2017**, 146, 074107	3.9	10
310	Understanding band gaps of solids in generalized Kohn-Sham theory. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 2801-2806	11.5	280
309	Electron Density, KohnSham Frontier Orbitals, and Fukui Functions **2017**, 303-306		1
308	Competing Pathways and Multiple Folding Nuclei in a Large Multidomain Protein, Luciferase. *Biophysical Journal*, **2017**, 112, 1829-1840	2.9	8
307	On extending Kohn-Sham density functionals to systems with fractional number of electrons. *Journal of Chemical Physics*, **2017**, 146, 214109	3.9	5
306	Charge transfer excitations from particle-particle random phase approximation-Opportunities and challenges arising from two-electron deficient systems. *Journal of Chemical Physics*, **2017**, 146, 124104	3.9	6
305	Activating MoS for pH-Universal Hydrogen Evolution Catalysis. *Journal of the American Chemical Society*, **2017**, 139, 16194-16200	16.4	118
304	Excitation energies from particle-particle random phase approximation with accurate optimized effective potentials. *Journal of Chemical Physics*, **2017**, 147, 134105	3.9	4
303	Multireference Density Functional Theory with Generalized Auxiliary Systems for Ground and Excited States. *Journal of Physical Chemistry Letters*, **2017**, 8, 4479-4485	6.4	14
302	Generalized Optimized Effective Potential for Orbital Functionals and Self-Consistent Calculation of Random Phase Approximations. *Journal of Physical Chemistry Letters*, **2017**, 8, 4746-4751	6.4	16

301	Time-Dependent Coupled Perturbed Hartree-Fock and Density-Functional-Theory Approach for Calculating Frequency-Dependent (Hyper)Polarizabilities with Nonorthogonal Localized Molecular Orbitals. *Journal of Chemical Theory and Computation*, **2017**, 13, 4101-4112	6.4	
300	Internal force corrections with machine learning for quantum mechanics/molecular mechanics simulations. *Journal of Chemical Physics*, **2017**, 147, 161732	3.9	22
299	Accurate Quasiparticle Spectra from the T-Matrix Self-Energy and the Particle-Particle Random Phase Approximation. *Journal of Physical Chemistry Letters*, **2017**, 8, 3223-3227	6.4	9
298	Multiscale Quantum Mechanics/Molecular Mechanics Simulations with Neural Networks. *Journal of Chemical Theory and Computation*, **2016**, 12, 4934-4946	6.4	71
297	Nature of ground and electronic excited states of higher acenes. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, E5098-107	11.5	113
296	Conical Intersections from Particle-Particle Random Phase and Tamm-Dancoff Approximations. *Journal of Physical Chemistry Letters*, **2016**, 7, 2407-11	6.4	17
295	Diverse Optimal Molecular Libraries for Organic Light-Emitting Diodes. *Journal of Chemical Theory and Computation*, **2016**, 12, 1942-52	6.4	14
294	Accurate atomic quantum defects from particle–particle random phase approximation. *Molecular Physics*, **2016**, 114, 1189-1198	1.7	4
293	Single-molecule Force Spectroscopy Reveals the Calcium Dependence of the Alternative Conformations in the Native State of a B-Crystallin Protein. *Journal of Biological Chemistry*, **2016**, 291, 18263-75	5.4	8
292	All The Catalytic Active Sites of MoS for Hydrogen Evolution. *Journal of the American Chemical Society*, **2016**, 138, 16632-16638	16.4	495
291	Determining polarizable force fields with electrostatic potentials from quantum mechanical linear response theory. *Journal of Chemical Physics*, **2016**, 144, 224107	3.9	7
290	Accurate and efficient calculation of excitation energies with the active-space particle-particle random phase approximation. *Journal of Chemical Physics*, **2016**, 145, 144105	3.9	8
289	Quantum Mechanics/Molecular Mechanics Method Combined with Hybrid All-Atom and Coarse-Grained Model: Theory and Application on Redox Potential Calculations. *Journal of Chemical Theory and Computation*, **2016**, 12, 2017-27	6.4	15
288	Strategy to discover diverse optimal molecules in the small molecule universe. *Journal of Chemical Information and Modeling*, **2015**, 55, 529-37	6.1	47
287	Singlet-triplet energy gaps for diradicals from particle-particle random phase approximation. *Journal of Physical Chemistry A*, **2015**, 119, 4923-32	2.8	27
286	Scaling correction approaches for reducing delocalization error in density functional approximations. *Science China Chemistry*, **2015**, 58, 1825-1844	7.9	10
285	Analytic gradients, geometry optimization and excited state potential energy surfaces from the particle-particle random phase approximation. *Physical Chemistry Chemical Physics*, **2015**, 17, 1025-38	3.6	19
284	Gentlest ascent dynamics for calculating first excited state and exploring energy landscape of Kohn-Sham density functionals. *Journal of Chemical Physics*, **2015**, 143, 224110	3.9	5

283	Orbital relaxation effects on Kohn-Sham frontier orbital energies in density functional theory. *Journal of Chemical Physics*, **2015**, 142, 154113	3.9	14
282	Local scaling correction for reducing delocalization error in density functional approximations. *Physical Review Letters*, **2015**, 114, 053001	7.4	59
281	Coupled-Perturbed SCF Approach for Calculating Static Polarizabilities and Hyperpolarizabilities with Nonorthogonal Localized Molecular Orbitals. *Journal of Chemical Theory and Computation*, **2015**, 11, 923-31	6.4	1
280	Direct observation of multimer stabilization in the mechanical unfolding pathway of a protein undergoing oligomerization. *ACS Nano*, **2015**, 9, 1189-97	16.7	13
279	Linear-response time-dependent density-functional theory with pairing fields. *Journal of Chemical Physics*, **2014**, 140, 18A522	3.9	25
278	Characterization of a photoswitching chelator with light-modulated geometric, electronic, and metal-binding properties. *Inorganic Chemistry*, **2014**, 53, 1397-405	5.1	21
277	Layer-dependent electrocatalysis of MoS2 for hydrogen evolution. *Nano Letters*, **2014**, 14, 553-8	11.5	580
276	Shifting Electronic Structure by Inherent Tension in Molecular Bottlebrushes with Polythiophene Backbones.. *ACS Macro Letters*, **2014**, 3, 738-742	6.6	14
275	Revisiting HO Nucleation around Au and Hg: The Peculiar "Pseudo-Soft" Character of the Gold Cation. *Journal of Chemical Theory and Computation*, **2014**, 10, 1900-1909	6.4	6
274	Preface: Special topic on advances in density functional theory. *Journal of Chemical Physics*, **2014**, 140, 18A101	3.9	3
273	Testing exchange□correlation functionals at fractional electron numbers. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	2
272	Fractional charge behavior and band gap predictions with the XYG3 type of doubly hybrid density functionals. *Journal of Physical Chemistry A*, **2014**, 118, 9201-11	2.8	43
271	A tribute to Guosen Yan. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	
270	Restricted second random phase approximations and Tamm-Dancoff approximations for electronic excitation energy calculations. *Journal of Chemical Physics*, **2014**, 141, 214102	3.9	4
269	Exchange-correlation energy from pairing matrix fluctuation and the particle-particle random phase approximation. *Journal of Chemical Physics*, **2014**, 140, 18A511	3.9	31
268	Excitation energies from particle-particle random phase approximation: Davidson algorithm and benchmark studies. *Journal of Chemical Physics*, **2014**, 141, 124104	3.9	33
267	Tensor hypercontracted ppRPA: reducing the cost of the particle-particle random phase approximation from O(r(6)) to O(r(4)). *Journal of Chemical Physics*, **2014**, 141, 024119	3.9	15
266	Chaperones rescue luciferase folding by separating its domains. *Journal of Biological Chemistry*, **2014**, 289, 28607-18	5.4	20

265	Stochastic voyages into uncharted chemical space produce a representative library of all possible drug-like compounds. *Journal of the American Chemical Society*, **2013**, 135, 7296-303	16.4	166
264	Effective preconditioning for ab initio ground state energy minimization with non-orthogonal localized molecular orbitals. *Physical Chemistry Chemical Physics*, **2013**, 15, 15518-27	3.6	12
263	Concerted proton transfer mechanism of Clostridium thermocellum ribose-5-phosphate isomerase. *Journal of Physical Chemistry B*, **2013**, 117, 9354-61	3.4	8
262	Exchange-correlation energy from pairing matrix fluctuation and the particle-particle random-phase approximation. *Physical Review A*, **2013**, 88,	2.6	68
261	A nonempirical scaling correction approach for density functional methods involving substantial amount of Hartree-Fock exchange. *Journal of Chemical Physics*, **2013**, 138, 174105	3.9	19
260	The tensor hypercontracted parametric reduced density matrix algorithm: coupled-cluster accuracy with O(r(4)) scaling. *Journal of Chemical Physics*, **2013**, 139, 054110	3.9	17
259	Wave function methods for fractional electrons. *Journal of Chemical Physics*, **2013**, 139, 074107	3.9	17
258	Equivalence of particle-particle random phase approximation correlation energy and ladder-coupled-cluster doubles. *Journal of Chemical Physics*, **2013**, 139, 104112	3.9	44
257	Extension of many-body theory and approximate density functionals to fractional charges and fractional spins. *Journal of Chemical Physics*, **2013**, 139, 104114	3.9	26
256	Noncovalent Interaction Analysis in Fluctuating Environments. *Journal of Chemical Theory and Computation*, **2013**, 9, 2226-2234	6.4	102
255	Pushing the boundaries of intrinsically stable radicals: inverse design using the thiadiazinyl radical as a template. *Journal of Organic Chemistry*, **2013**, 78, 3151-8	4.2	15
254	Fukui function and response function for nonlocal and fractional systems. *Journal of Chemical Physics*, **2013**, 138, 184108	3.9	16
253	Dynamical second-order Bethe-Salpeter equation kernel: a method for electronic excitation beyond the adiabatic approximation. *Journal of Chemical Physics*, **2013**, 139, 154109	3.9	20
252	Accurate Computation of the Non-Interacting Kinetic Energy from Electron Densities. *Recent Advances in Computational*, **2013**, 13-29		
251	Double, Rydberg and charge transfer excitations from pairing matrix fluctuation and particle-particle random phase approximation. *Journal of Chemical Physics*, **2013**, 139, 224105	3.9	43
250	Pseudobond parameters for QM/MM studies involving nucleosides, nucleotides, and their analogs. *Journal of Chemical Physics*, **2013**, 138, 045102	3.9	5
249	Contributions of Pauli repulsions to the energetics and physical properties computed in QM/MM methods. *Journal of Computational Chemistry*, **2013**, 34, 2380-8	3.5	7
248	Benchmark tests and spin adaptation for the particle-particle random phase approximation. *Journal of Chemical Physics*, **2013**, 139, 174110	3.9	33

247	Sulfur-doped zinc oxide (ZnO) Nanostars: Synthesis and simulation of growth mechanism. *Nano Research*, **2012**, 5, 20-26	10	35
246	Fragment-based Quantum Mechanical/Molecular Mechanical Simulations of Thermodynamic and Kinetic Process of the Ru-Ru Self-Exchange Electron Transfer. *Journal of Chemical Theory and Computation*, **2012**, 8, 4960-4967	6.4	17
245	Variational fractional-spin density-functional theory for diradicals. *Journal of Chemical Physics*, **2012** , 137, 114112	3.9	23
244	Higher-order split operator schemes for solving the Schr□dinger equation in the time-dependent wave packet method: applications to triatomic reactive scattering calculations. *Physical Chemistry Chemical Physics*, **2012**, 14, 1827-45	3.6	31
243	Liquid water simulations with the density fragment interaction approach. *Physical Chemistry Chemical Physics*, **2012**, 14, 7700-9	3.6	14
242	Design of Coupled Porphyrin Chromophores with Unusually Large Hyperpolarizabilities. *Journal of Physical Chemistry C*, **2012**, 116, 9724-9733	3.8	31
241	Catalytic mechanism of 4-oxalocrotonate tautomerase: significances of protein-protein interactions on proton transfer pathways. *Journal of Physical Chemistry B*, **2012**, 116, 6889-97	3.4	7
240	Density-Functional Errors in Alkanes: A Real-Space Perspective. *Journal of Chemical Theory and Computation*, **2012**, 8, 2676-81	6.4	15
239	Coupling quantum interpretative techniques: another look at chemical mechanisms in organic reactions. *Journal of Chemical Theory and Computation*, **2012**, 8, 3993-3997	6.4	90
238	Analytical evaluation of Fukui functions and real-space linear response function. *Journal of Chemical Physics*, **2012**, 136, 144110	3.9	53
237	Derivative discontinuity, bandgap and lowest unoccupied molecular orbital in density functional theory. *Journal of Chemical Physics*, **2012**, 136, 204111	3.9	129
236	Mechanical anisotropy of ankyrin repeats. *Biophysical Journal*, **2012**, 102, 1118-26	2.9	20
235	Highly tunable spin-dependent electron transport through carbon atomic chains connecting two zigzag graphene nanoribbons. *Journal of Chemical Physics*, **2012**, 137, 104107	3.9	17
234	Inverse design of molecules with optimal reactivity properties: acidity of 2-naphthol derivatives. *Physical Chemistry Chemical Physics*, **2012**, 14, 16002-13	3.6	22
233	Challenges for density functional theory. *Chemical Reviews*, **2012**, 112, 289-320	68.1	1521
232	Failure of the random-phase-approximation correlation energy. *Physical Review A*, **2012**, 85,	2.6	49
231	Achieving partial decoherence in surface hopping through phase correction. *Journal of Chemical Physics*, **2012**, 137, 22A528	3.9	40
230	Delocalization error of density-functional approximations: a distinct manifestation in hydrogen molecular chains. *Journal of Chemical Physics*, **2012**, 137, 214106	3.9	60

229	Theoretical study of catalytic mechanism for single-site water oxidation process. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 15669-72	11.5	49
228	Optimized effective potential for calculations with orbital-free potential functionals. *Molecular Physics*, **2012**, 110, 925-934	1.7	2
227	Insight and progress in density functional theory **2012**,		3
226	Analysis of hydrogen-bond interaction potentials from the electron density: integration of noncovalent interaction regions. *Journal of Physical Chemistry A*, **2011**, 115, 12983-90	2.8	271
225	Conical intersections in solution: formulation, algorithm, and implementation with combined quantum mechanics/molecular mechanics method. *Journal of Chemical Physics*, **2011**, 134, 204115	3.9	12
224	Singlet-triplet energy gaps for diradicals from fractional-spin density-functional theory. *Journal of Physical Chemistry A*, **2011**, 115, 76-83	2.8	97
223	NCIPLOT: a program for plotting non-covalent interaction regions. *Journal of Chemical Theory and Computation*, **2011**, 7, 625-632	6.4	2067
222	Single-molecule conductance of pyridine-terminated dithienylethene switch molecules. *ACS Nano*, **2011**, 5, 5115-23	16.7	84
221	Autocatalytic intramolecular isopeptide bond formation in gram-positive bacterial pili: a QM/MM simulation. *Journal of the American Chemical Society*, **2011**, 133, 478-85	16.4	31
220	Improving band gap prediction in density functional theory from molecules to solids. *Physical Review Letters*, **2011**, 107, 026403	7.4	139
219	-Meta Dynamics Approach To Compute Absolute Solvation Free Energy. *Journal of Physical Chemistry Letters*, **2011**, 2, 2099-2103	6.4	20
218	Phase-corrected surface hopping: correcting the phase evolution of the electronic wavefunction. *Journal of Chemical Physics*, **2011**, 135, 024101	3.9	81
217	Simultaneous-trajectory surface hopping: a parameter-free algorithm for implementing decoherence in nonadiabatic dynamics. *Journal of Chemical Physics*, **2011**, 134, 144102	3.9	109
216	Communication: An exact short-time solver for the time-dependent Schr□dinger equation. *Journal of Chemical Physics*, **2011**, 134, 041101	3.9	13
215	An algebraic operator approach to electronic structure. *Journal of Chemical Physics*, **2011**, 135, 244111	3.9	
214	Concerted O atom-proton transfer in the O-O bond forming step in water oxidation. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 7225-9	11.5	263
213	Full reconstruction of a vectorial protein folding pathway by atomic force microscopy and molecular dynamics simulations. *Journal of Biological Chemistry*, **2010**, 285, 38167-72	5.4	34
212	Spin-state splittings, highest-occupied-molecular-orbital and lowest-unoccupied-molecular-orbital energies, and chemical hardness. *Journal of Chemical Physics*, **2010**, 133, 164107	3.9	12

211	Efficient construction of nonorthogonal localized molecular orbitals in large systems. *Journal of Physical Chemistry A*, **2010**, 114, 8878-83	2.8	9
210	Conductive junctions with parallel graphene sheets. *Journal of Chemical Physics*, **2010**, 132, 114703	3.9	10
209	Equilibrium sampling for biomolecules under mechanical tension. *Biophysical Journal*, **2010**, 98, 733-40	2.9	5
208	Predicting the Frequency Dispersion of Electronic Hyperpolarizabilities on the Basis of Absorption Data and Thomas–Kuhn Sum Rules. *Journal of Physical Chemistry C*, **2010**, 114, 2349-2359	3.8	46
207	Challenges with range-separated exchange-correlation functionals in time-dependent density functional theory calculations. *Molecular Physics*, **2010**, 108, 2745-2750	1.7	16
206	Elucidating solvent contributions to solution reactions with ab initio QM/MM methods. *Journal of Physical Chemistry B*, **2010**, 114, 2755-9	3.4	16
205	Time-dependent transport through molecular junctions. *Journal of Chemical Physics*, **2010**, 132, 234105	3.9	39
204	Structural manifestation of the delocalization error of density functional approximations: C(4N+2) rings and C(20) bowl, cage, and ring isomers. *Journal of Chemical Physics*, **2010**, 132, 234113	3.9	60
203	Reformulating time-dependent density functional theory with non-orthogonal localized molecular orbitals. *Physical Chemistry Chemical Physics*, **2010**, 12, 416-21	3.6	24
202	Accelerating self-consistent field convergence with the augmented Roothaan-Hall energy function. *Journal of Chemical Physics*, **2010**, 132, 054109	3.9	55
201	Revealing noncovalent interactions. *Journal of the American Chemical Society*, **2010**, 132, 6498-506	16.4	4471
200	Synthesis and chemical diversity analysis of bicyclo[3.3.1]non-3-en-2-ones. *Tetrahedron*, **2010**, 66, 5852-5862	2.9	10
199	A gradient-directed Monte Carlo approach for protein design. *Journal of Computational Chemistry*, **2010**, 31, 2164-8	3.5	12
198	Coarse-grained modeling of allosteric regulation in protein receptors. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 14253-8	11.5	42
197	A gradient-directed Monte Carlo method for global optimization in a discrete space: application to protein sequence design and folding. *Journal of Chemical Physics*, **2009**, 131, 154117	3.9	15
196	Development and application of ab initio QM/MM methods for mechanistic simulation of reactions in solution and in enzymes. *Computational and Theoretical Chemistry*, **2009**, 898, 17-30		70
195	Emergent strategies for inverse molecular design. *Science in China Series B: Chemistry*, **2009**, 52, 1769-1776		9
194	Analysis of HIF-1 inhibition by manassantin A and analogues with modified tetrahydrofuran configurations. *Bioorganic and Medicinal Chemistry Letters*, **2009**, 19, 3783-6	2.9	23

193	Discrete Optimization of Electronic Hyperpolarizabilities in a Chemical Subspace. *Journal of Chemical Theory and Computation*, **2009**, 5, 3321-9	6.4	19
192	Discontinuous nature of the exchange-correlation functional in strongly correlated systems. *Physical Review Letters*, **2009**, 102, 066403	7.4	178
191	Mechanism of Cdc25B phosphatase with the small molecule substrate p-nitrophenyl phosphate from QM/MM-MFEP calculations. *Journal of Physical Chemistry B*, **2009**, 113, 5217-24	3.4	21
190	Thermopower of molecular junctions: an ab initio study. *Nano Letters*, **2009**, 9, 1011-4	11.5	86
189	Contact geometry and conductance of crossed nanotube junctions under pressure. *Nano Letters*, **2009**, 9, 1759-63	11.5	9
188	Second-Order Perturbation Theory with Fractional Charges and Fractional Spins. *Journal of Chemical Theory and Computation*, **2009**, 5, 786-92	6.4	57
187	Calculating solution redox free energies with ab initio quantum mechanical/molecular mechanical minimum free energy path method. *Journal of Chemical Physics*, **2009**, 130, 164111	3.9	33
186	Fukui Function **2009**,		31
185	Comparison Of Reaction Barriers In Energy And Free Energy For Enzyme Catalysis. *Challenges and Advances in Computational Chemistry and Physics*, **2009**, 57-78	0.7	1
184	Transport properties of an armchair carbon nanotube with a double vacancy under stretching. *Journal of Physics Condensed Matter*, **2008**, 20, 345225	1.8	2
183	Ab initio quantum mechanical/molecular mechanical simulation of electron transfer process: fractional electron approach. *Journal of Chemical Physics*, **2008**, 128, 124510	3.9	57
182	Localization and delocalization errors in density functional theory and implications for band-gap prediction. *Physical Review Letters*, **2008**, 100, 146401	7.4	859
181	A donor-nanotube paradigm for nonlinear optical materials. *Nano Letters*, **2008**, 8, 2814-8	11.5	93
180	Fractional charge perspective on the band gap in density-functional theory. *Physical Review B*, **2008**, 77,	3.3	415
179	Quantum-interference-controlled molecular electronics. *Nano Letters*, **2008**, 8, 3257-61	11.5	213
178	Computational design, synthesis and biological evaluation of para-quinone-based inhibitors for redox regulation of the dual-specificity phosphatase Cdc25B. *Organic and Biomolecular Chemistry*, **2008**, 6, 3256-63	3.9	34
177	Molecular design of porphyrin-based nonlinear optical materials. *Journal of Physical Chemistry A*, **2008**, 112, 12203-7	2.8	89
176	Insights into current limitations of density functional theory. *Science*, **2008**, 321, 792-4	33.3	1749

175	Mechanism of OMP decarboxylation in orotidine 5'-monophosphate decarboxylase. *Journal of the American Chemical Society*, **2008**, 130, 14493-503	16.4	39
174	Hepatitis C virus NS5B polymerase: QM/MM calculations show the important role of the internal energy in ligand binding. *Journal of Physical Chemistry B*, **2008**, 112, 3168-76	3.4	13
173	Exploring chemical space with discrete, gradient, and hybrid optimization methods. *Journal of Chemical Physics*, **2008**, 129, 174105	3.9	33
172	Inverse molecular design in a tight-binding framework. *Journal of Chemical Physics*, **2008**, 129, 044106	3.9	34
171	A gradient-directed Monte Carlo approach to molecular design. *Journal of Chemical Physics*, **2008**, 129, 064102	3.9	36
170	Density-fragment interaction approach for quantum-mechanical/molecular-mechanical calculations with application to the excited states of a Mg(2+)-sensitive dye. *Journal of Chemical Physics*, **2008**, 129, 054102	3.9	41
169	Optimized effective potentials from arbitrary basis sets. *Journal of Chemical Physics*, **2008**, 129, 194102	3.9	38
168	Delocalization errors in density functionals and implications for main-group thermochemistry. *Journal of Chemical Physics*, **2008**, 129, 204112	3.9	139
167	Fractional spins and static correlation error in density functional theory. *Journal of Chemical Physics*, **2008**, 129, 121104	3.9	183
166	Size extensivity of the direct optimized effective potential method. *Journal of Chemical Physics*, **2008**, 128, 114702	3.9	5
165	A pseudobond parametrization for improved electrostatics in quantum mechanical/molecular mechanical simulations of enzymes. *Journal of Chemical Physics*, **2008**, 129, 154106	3.9	30
164	Linear-scaling quantum calculations using non-orthogonal localized molecular orbitals. *Journal of Physics Condensed Matter*, **2008**, 20, 294209	1.8	9
163	First-principles study for transport properties of armchair carbon nanotubes with a double vacancy under strain. *Journal of Applied Physics*, **2008**, 103, 113714	2.5	5
162	Lead-molecule coupling effects on the distortion-dependent conductance of carbon nanotubes. *Physical Review B*, **2008**, 77,	3.3	3
161	Quantum mechanics/molecular mechanics minimum free-energy path for accurate reaction energetics in solution and enzymes: sequential sampling and optimization on the potential of mean force surface. *Journal of Chemical Physics*, **2008**, 128, 034105	3.9	103
160	Free energies of chemical reactions in solution and in enzymes with ab initio quantum mechanics/molecular mechanics methods. *Annual Review of Physical Chemistry*, **2008**, 59, 573-601	15.7	364
159	Designing molecules with optimal properties using the linear combination of atomic potentials approach in an AM1 semiempirical framework. *Journal of Physical Chemistry A*, **2007**, 111, 176-81	2.8	45
158	Simulating water with the self-consistent-charge density functional tight binding method: from molecular clusters to the liquid state. *Journal of Physical Chemistry A*, **2007**, 111, 5685-91	2.8	74

157	Computational study on the relative acidity of acetic acid by the QM/MM method combined with the theory of energy representation. *Journal of Physical Chemistry B*, **2007**, 111, 581-8	3.4	24
156	Development of exchange-correlation functionals with minimal many-electron self-interaction error. *Journal of Chemical Physics*, **2007**, 126, 191109	3.9	268
155	Role of the exchange-correlation potential in ab initio electron transport calculations. *Journal of Chemical Physics*, **2007**, 126, 201102	3.9	99
154	Electron transport through single conjugated organic molecules: basis set effects in ab initio calculations. *Journal of Chemical Physics*, **2007**, 127, 144107	3.9	40
153	Sequential quadratic programming method for determining the minimum energy path. *Journal of Chemical Physics*, **2007**, 127, 164107	3.9	28
152	Assessment and formal properties of exchange-correlation functionals constructed from the adiabatic connection. *Journal of Chemical Physics*, **2007**, 127, 034101	3.9	52
151	Spin-potential functional formalism for current-carrying noncollinear magnetic systems. *Physical Review Letters*, **2007**, 98, 036403	7.4	20
150	Optimized effective potentials in finite basis sets. *Physical Review Letters*, **2007**, 98, 256401	7.4	109
149	QM/MM Minimum Free Energy Path: Methodology and Application to Triosephosphate Isomerase. *Journal of Chemical Theory and Computation*, **2007**, 3, 390-406	6.4	127
148	Contact transparency of nanotube-molecule-nanotube junctions. *Physical Review Letters*, **2007**, 99, 146802	7.4	47
147	Synthesis, structures, and optical properties of cadmium iodide/phenethylamine hybrid materials with controlled structures and emissions. *Inorganic Chemistry*, **2007**, 46, 10252-60	5.1	17
146	Cobaltocene as a spin filter. *Journal of Chemical Physics*, **2007**, 127, 141104	3.9	46
145	Fitting Molecular Electrostatic Potentials from Quantum Mechanical Calculations. *Journal of Chemical Theory and Computation*, **2007**, 3, 1004-13	6.4	103
144	Optimized effective potentials from electron densities in finite basis sets. *Journal of Chemical Physics*, **2007**, 127, 174101	3.9	46
143	Quadratic string method for determining the minimum-energy path based on multiobjective optimization. *Journal of Chemical Physics*, **2006**, 124, 054109	3.9	84
142	A combined explicit-implicit method for high accuracy reaction path integration. *Journal of Chemical Physics*, **2006**, 124, 224102	3.9	8
141	Organometallic molecular rectification. *Journal of Chemical Physics*, **2006**, 124, 024718	3.9	67
140	Legendre-transform functionals for spin-density-functional theory. *Journal of Chemical Physics*, **2006**, 124, 224108	3.9	55

139	Nuclear quantum effects on an enzyme-catalyzed reaction with reaction path potential: proton transfer in triosephosphate isomerase. *Journal of Chemical Physics*, **2006**, 124, 124516	3.9	46
138	Negative differential resistance and hysteresis through an organometallic molecule from molecular-level crossing. *Journal of the American Chemical Society*, **2006**, 128, 6274-5	16.4	66
137	Many-electron self-interaction error in approximate density functionals. *Journal of Chemical Physics* , **2006**, 125, 201102	3.9	547
136	Nanotube-metal junctions: 2- and 3-terminal electrical transport. *Journal of Chemical Physics*, **2006**, 124, 181102	3.9	19
135	Direct detection of the formation of V-amylose helix by single molecule force spectroscopy. *Journal of the American Chemical Society*, **2006**, 128, 9387-93	16.4	43
134	Simulating force-induced conformational transitions in polysaccharides with the SMD replica exchange method. *Biophysical Journal*, **2006**, 91, L57-9	2.9	6
133	Density functional theory investigation of the polarizability and second hyperpolarizability of polydiacetylene and polybutatriene chains: treatment of exact exchange and role of correlation. *Journal of Chemical Physics*, **2006**, 125, 194114	3.9	55
132	Designing molecules by optimizing potentials. *Journal of the American Chemical Society*, **2006**, 128, 3228-32	16.4	121
131	Theoretical and experimental determination on two substrates turned over by 4-oxalocrotonate tautomerase. *Journal of Physical Chemistry A*, **2006**, 110, 700-8	2.8	21
130	Self-interaction-free exchange-correlation functional for thermochemistry and kinetics. *Journal of Chemical Physics*, **2006**, 124, 91102	3.9	168
129	Automatic integration of the reaction path using diagonally implicit Runge-Kutta methods. *Journal of Chemical Physics*, **2006**, 125, 244108	3.9	9
128	Searching for the minimum energy path in the sulfuryl transfer reaction catalyzed by human estrogen sulfotransferase: Role of enzyme dynamics. *International Journal of Quantum Chemistry*, **2006**, 106, 2981-2998	2.1	12
127	A QM/MM study combined with the theory of energy representation: Solvation free energies for anti/syn acetic acids in aqueous solution. *Chemical Physics Letters*, **2006**, 419, 240-244	2.5	25
126	Development of Ab Initio Calculation for Electron Transport and the Effects of Lead and Contact Structures in Molecular Electronics. *Journal of Computational and Theoretical Nanoscience*, **2006**, 3, 819-823	0.3	4
125	Dual-topology/dual-coordinate free-energy simulation using QM/MM force field. *Journal of Chemical Physics*, **2005**, 123, 041102	3.9	28
124	Excitation energies from time-dependent density functional theory with accurate exchange-correlation potentials. *Molecular Physics*, **2005**, 103, 711-717	1.7	19
123	Experimental validation of the docking orientation of Cdc25 with its Cdk2-CycA protein substrate. *Biochemistry*, **2005**, 44, 16563-73	3.2	40
122	Intermolecular effect in molecular electronics. *Journal of Chemical Physics*, **2005**, 122, 44703	3.9	49

121	Models of electrodes and contacts in molecular electronics. *Journal of Chemical Physics*, **2005**, 123, 114701	3.9	78
120	Near-perfect conduction through a ferrocene-based molecular wire. *Physical Review B*, **2005**, 71,	3.3	107
119	Organometallic spintronics: dicobaltocene switch. *Nano Letters*, **2005**, 5, 1959-62	11.5	104
118	Density-functional theory (hyper)polarizabilities of push-pull pi-conjugated systems: treatment of exact exchange and role of correlation. *Journal of Chemical Physics*, **2005**, 123, 014319	3.9	113
117	Orbital-dependent correlation energy in density-functional theory based on a second-order perturbation approach: success and failure. *Journal of Chemical Physics*, **2005**, 123, 62204	3.9	94
116	Electron transport through molecules: Gate-induced polarization and potential shift. *Physical Review B*, **2005**, 71,	3.3	44
115	Interactions and broken time-reversal symmetry in chaotic quantum dots. *Physical Review B*, **2005**, 71,	3.3	2
114	Reaction path determination for quantum mechanical/molecular mechanical modeling of enzyme reactions by combining first order and second order "chain-of-replicas" methods. *Journal of Chemical Physics*, **2005**, 122, 114502	3.9	35
113	Contact atomic structure and electron transport through molecules. *Journal of Chemical Physics*, **2005**, 122, 074704	3.9	118
112	Scrambling and gate-induced fluctuations in realistic quantum dots. *Physical Review B*, **2005**, 71,	3.3	4
111	Analytic energy gradients of the optimized effective potential method. *Journal of Chemical Physics*, **2005**, 123, 134111	3.9	12
110	Conjugate-gradient optimization method for orbital-free density functional calculations. *Journal of Chemical Physics*, **2004**, 121, 2030-6	3.9	27
109	Electron transport through molecules: Self-consistent and non-self-consistent approaches. *Physical Review B*, **2004**, 70,	3.3	195
108	Parallel iterative reaction path optimization in ab initio quantum mechanical/molecular mechanical modeling of enzyme reactions. *Journal of Chemical Physics*, **2004**, 121, 697-706	3.9	43
107	Adapting the nudged elastic band method for determining minimum-energy paths of chemical reactions in enzymes. *Journal of Chemical Physics*, **2004**, 120, 8039-52	3.9	65
106	An efficient method for constructing nonorthogonal localized molecular orbitals. *Journal of Chemical Physics*, **2004**, 120, 9458-66	3.9	22
105	Electron-electron interactions in isolated and realistic quantum dots: A density functional theory study. *Physical Review B*, **2004**, 69,	3.3	13
104	Transmission coefficient calculation for proton transfer in triosephosphate isomerase based on the reaction path potential method. *Journal of Chemical Physics*, **2004**, 121, 101-7	3.9	17

103	Landau Fermi-liquid picture of spin density functional theory: Strutinsky approach to quantum dots. *Physical Review B*, **2004**, 70,	3.3	12
102	Reaction path potential for complex systems derived from combined ab initio quantum mechanical and molecular mechanical calculations. *Journal of Chemical Physics*, **2004**, 121, 89-100	3.9	57
101	Calculation of nuclear magnetic resonance shielding constants using potential-based methods. *Chemical Physics Letters*, **2004**, 399, 84-88	2.5	24
100	Elastic properties of single amylose chains in water: a quantum mechanical and AFM study. *Journal of the American Chemical Society*, **2004**, 126, 9033-41	16.4	40
99	The protein backbone makes important contributions to 4-oxalocrotonate tautomerase enzyme catalysis: understanding from theory and experiment. *Biochemistry*, **2004**, 43, 6885-92	3.2	64
98	Molecular conductance: chemical trends of anchoring groups. *Journal of the American Chemical Society*, **2004**, 126, 15897-904	16.4	84
97	Potential functionals: dual to density functionals and solution to the v-representability problem. *Physical Review Letters*, **2004**, 92, 146404	7.4	84
96	Accurate polymer polarizabilities with exact exchange density-functional theory. *Journal of Chemical Physics*, **2003**, 119, 11001-11004	3.9	130
95	ALGEBRAIC EQUATION AND ITERATIVE OPTIMIZATION FOR THE OPTIMIZED EFFECTIVE POTENTIAL IN DENSITY FUNCTIONAL THEORY. *Journal of Theoretical and Computational Chemistry*, **2003**, 02, 627-638	1.8	79
94	Dramatic effect of homoallylic substitution on the rate of palladium-catalyzed diene cycloisomerization. *Journal of Organometallic Chemistry*, **2003**, 687, 498-507	2.3	15
93	Energetics of the Electron Transfer from Bacteriopheophytin to Ubiquinone in the Photosynthetic Reaction Center of Rhodopseudomonas Viridis: Theoretical Study. *Journal of Physical Chemistry B*, **2003**, 107, 838-847	3.4	17
92	Ab initio QM/MM study shows there is no general acid in the reaction catalyzed by 4-oxalocrotonate tautomerase. *Journal of the American Chemical Society*, **2003**, 125, 10384-93	16.4	89
91	Density-functional theory calculations with correct long-range potentials. *Journal of Chemical Physics*, **2003**, 119, 2978-2990	3.9	87
90	A direct optimization method for calculating density functionals and exchange□correlation potentials from electron densities. *Journal of Chemical Physics*, **2003**, 118, 2498	3.9	232
89	Addition energies of fullerenes and carbon nanotubes as quantum dots: the role of symmetry. *Physical Review Letters*, **2003**, 91, 116803	7.4	22
88	Spin and conductance-peak-spacing distributions in large quantum dots: a density-functional theory study. *Physical Review Letters*, **2003**, 90, 026806	7.4	26
87	Density-functional theory simulation of large quantum dots. *Physical Review B*, **2003**, 68,	3.3	26
86	Density-Functional Theory **2003**,		8

85	Empirical correction to density functional theory for van der Waals interactions. *Journal of Chemical Physics*, **2002**, 116, 515-524	3.9	708
84	Direct method for optimized effective potentials in density-functional theory. *Physical Review Letters*, **2002**, 89, 143002	7.4	227
83	PARAMETERIZATION OF COSMO SOLVENT MODEL FOR SELF-CONSISTENT CHARGE DENSITY-FUNCTIONAL BASED TIGHT-BINDING CALCULATIONS **2002**, 1606-1614		3
82	Ab Initio QM/MM and Free Energy Calculations of Enzyme Reactions. *Lecture Notes in Computational Science and Engineering*, **2002**, 333-355	0.3	5
81	Quantum mechanics simulation of protein dynamics on long timescale. *Proteins: Structure, Function and Bioinformatics*, **2001**, 44, 484-9	4.2	127
80	Using Density Functional Theory To Design DNA Base Analogues with Low Oxidation Potentials. *Journal of Physical Chemistry B*, **2001**, 105, 6437-6444	3.4	69
79	Density functional study of a weakly hydrogen-bonded benzene□ammonia complex: The importance of the exchange functional. *International Journal of Quantum Chemistry*, **2000**, 79, 325-329	2.1	14
78	Perspective on □Density-functional theory for fractional particle number: derivative discontinuities of the energy□*Theoretical Chemistry Accounts*, **2000**, 103, 346-348	1.9	112
77	Degenerate ground states and a fractional number of electrons in density and reduced density matrix functional theory. *Physical Review Letters*, **2000**, 84, 5172-5	7.4	345
76	Free energy calculation on enzyme reactions with an efficient iterative procedure to determine minimum energy paths on a combined ab initio QM/MM potential energy surface. *Journal of Chemical Physics*, **2000**, 112, 3483-3492	3.9	398
75	Perspective on □Density-functional theory for fractional particle number: derivative discontinuities of the energy□**2000**, 346-348		8
74	Nonorthogonal localized molecular orbitals in electronic structure theory. *Journal of Chemical Physics*, **2000**, 112, 1634-1644	3.9	92
73	How Is the Active Site of Enolase Organized To Catalyze Two Different Reaction Steps?. *Journal of the American Chemical Society*, **2000**, 122, 6560-6570	16.4	98
72	A Comparison of Calculated and Experimental Geometries for Crowded polycyclic Aromatic Hydrocarbons and their Metabolites. *Polycyclic Aromatic Compounds*, **1999**, 14, 53-61	1.3	5
71	A Linear-Scaling Quantum Mechanical Investigation of Cytidine Deaminase. *Journal of Computational Physics*, **1999**, 151, 242-263	4.1	18
70	A pseudobond approach to combining quantum mechanical and molecular mechanical methods. *Journal of Chemical Physics*, **1999**, 110, 46-54	3.9	421
69	On the scaling of multipole methods for particle□particle interactions. *Chemical Physics Letters*, **1998**, 282, 71-78	2.5	6
68	Comment on □Generalized Gradient Approximation Made Simple□*Physical Review Letters*, **1998**, 80, 890-890	7.4	1910

67	Parallel implementation of divide-and-conquer semiempirical quantum chemistry calculations. *Journal of Computational Chemistry*, **1998**, 19, 1101-1109	3.5	17
66	Frozen density matrix approach for electronic structure calculations. *International Journal of Quantum Chemistry*, **1998**, 69, 397-404	2.1	18
65	Linear-scaling quantum mechanical calculations of biological molecules: The divide-and-conquer approach. *Computational Materials Science*, **1998**, 12, 259-277	3.2	41
64	Active Species for the Ground-State Complex of Cytidine Deaminase: A Linear-Scaling Quantum Mechanical Investigation. *Journal of the American Chemical Society*, **1998**, 120, 5407-5410	16.4	37
63	Generalized adiabatic connection in density functional theory. *Journal of Chemical Physics*, **1998**, 109, 10107-10110	3.9	66
62	A challenge for density functionals: Self-interaction error increases for systems with a noninteger number of electrons. *Journal of Chemical Physics*, **1998**, 109, 2604-2608	3.9	470
61	Quantum Mechanical Treatment of Biological Macromolecules in Solution Using Linear-Scaling Electronic Structure Methods. *Physical Review Letters*, **1998**, 80, 5011-5014	7.4	63
60	Fast evaluation of the Coulomb energy for electron densities. *Journal of Chemical Physics*, **1997**, 107, 1218-1226	3.9	44
59	First-principles study of the structural and electronic properties of ethylene adsorption on Si(100)-(2×1) surface. *Journal of Chemical Physics*, **1997**, 107, 3981-3985	3.9	74
58	Absolute-energy-minimum principles for linear-scaling electronic-structure calculations. *Physical Review B*, **1997**, 56, 9294-9297	3.3	85
57	Describing van der Waals Interaction in diatomic molecules with generalized gradient approximations: The role of the exchange functional. *Journal of Chemical Physics*, **1997**, 107, 7921-7925	3.9	262
56	Divide-and-conquer calculations for clean surfaces and surface adsorption. *Theoretical Chemistry Accounts*, **1997**, 96, 2-6	1.9	4
55	Quantum Mechanical Study of Aqueous Polarization Effects on Biological Macromolecules. *Journal of the American Chemical Society*, **1996**, 118, 10940-10941	16.4	54
54	Density-Functional Study of the Geometries, Stabilities, and Bond Energies of Group IIIV (13×15) Four-Membered-Ring Compounds. *Journal of the American Chemical Society*, **1996**, 118, 5732-5736	16.4	16
53	Parameterization and efficient implementation of a solvent model for linear-scaling semiempirical quantum mechanical calculations of biological macromolecules. *Chemical Physics Letters*, **1996**, 263, 297-304	2.5	45
52	A concise redefinition of the solid spherical harmonics and its use in fast multipole methods. *Journal of Chemical Physics*, **1996**, 104, 8003-8006	3.9	39
51	A chemical potential equalization method for molecular simulations. *Journal of Chemical Physics*, **1996**, 104, 159-172	3.9	201
50	Linear-scaling semiempirical quantum calculations for macromolecules. *Journal of Chemical Physics*, **1996**, 105, 2744-2750	3.9	155

49	Structure of solid-state systems from embedded-cluster calculations: A divide-and-conquer approach. *Physical Review B*, **1996**, 53, 12713-12724	3.3	21
48	Electronic Structure of Solid-State Systems via the Divide-and-Conquer Method **1996**, 177-188		
47	A simple O(N log N) algorithm for the rapid evaluation of particle-particle interactions. *Chemical Physics Letters*, **1995**, 247, 484-490	2.5	20
46	Density-functional theory of the electronic structure of molecules. *Annual Review of Physical Chemistry*, **1995**, 46, 701-28	15.7	732
45	Structure and stability of molybdenum carbide clusters (MoC4)n (n=1 to 4) and their anions. *Physical Review B*, **1995**, 51, 7224-7230	3.3	4
44	A density-matrix divide-and-conquer approach for electronic structure calculations of large molecules. *Journal of Chemical Physics*, **1995**, 103, 5674-5678	3.9	457
43	A new definition of atomic charges based on a variational principle for the electrostatic potential energy. *Journal of Chemical Physics*, **1995**, 102, 7549-7556	3.9	13
42	Toward the Accurate Modeling of DNA: The Importance of Long-Range Electrostatics. *Journal of the American Chemical Society*, **1995**, 117, 5001-5002	16.4	162
41	Analytical energy gradients and geometry optimization in the divide-and-conquer method for large molecules. *Journal of Chemical Physics*, **1995**, 102, 9598-9603	3.9	63
40	An algorithm for 3D numerical integration that scales linearly with the size of the molecule. *Chemical Physics Letters*, **1995**, 241, 469-476	2.5	41
39	Density-functional calculations of the structure and stability of C240. *Physical Review B*, **1994**, 49, 8526-8528	3.3	50
38	The fast Fourier Poisson method for calculating Ewald sums. *Journal of Chemical Physics*, **1994**, 101, 3298-3300	3.9	98
37	Structure of the ammonia dimer studied by density functional theory. *International Journal of Quantum Chemistry*, **1994**, 49, 613-623	2.1	21
36	Shape of large single- and multiple-shell fullerenes. *Physical Review B*, **1994**, 49, 11421-11424	3.3	98
35	Examination of several exchange-correlation energy functionals by accurate self-consistent atomic calculations. *Journal of Chemical Physics*, **1993**, 98, 4814-4821	3.9	20
34	Nonlocal density functional calculations: Comparison of two implementation schemes. *Journal of Chemical Physics*, **1993**, 98, 2971-2974	3.9	18
33	The Ar□2H2 intermolecular potential from high resolution spectroscopy and ab initio theory: A case for multicenter interactions. *Journal of Chemical Physics*, **1993**, 99, 8585-8598	3.9	87
32	Density-Functional Theory of Large Systems: A Divide-and-Conquer Approach **1993**, 367-372		

31	The divide-and-conquer density-functional approach: Molecular internal rotation and density of states. *Journal of Chemical Physics*, **1992**, 96, 2408-2411	3.9	53
30	Electron density as the basic variable: a divide-and-conquer approach to the ab initio computation of large molecules. *Computational and Theoretical Chemistry*, **1992**, 255, 461-479		56
29	The Hartley basis functions and transform: alternatives to plane waves and the Fourier transform. *Chemical Physics Letters*, **1992**, 192, 45-48	2.5	3
28	A local projection method for the linear combination of atomic orbital implementation of density-functional theory. *Journal of Chemical Physics*, **1991**, 94, 1208-1214	3.9	38
27	Direct calculation of electron density in density-functional theory: Implementation for benzene and a tetrapeptide. *Physical Review A*, **1991**, 44, 7823-7826	2.6	131
26	Direct calculation of electron density in density-functional theory. *Physical Review Letters*, **1991**, 66, 1438-1441	7.4	836
25	Integral Formulation of Density-Functional Theory. *Advances in Quantum Chemistry*, **1990**, 21, 293-302	1.4	4
24	Approximate density matrices and wigner distribution functions from density, kinetic energy density, and idempotency constraints. *International Journal of Quantum Chemistry*, **1990**, 38, 819-830	2.1	9
23	A method for calculating vibrational bound states: Iterative solution of the collocation equations constructed from localized basis sets. *Journal of Chemical Physics*, **1990**, 92, 522-526	3.9	41
22	The collocation method for calculating vibrational bound states of molecular systems with application to Ar–HCl. *Journal of Chemical Physics*, **1989**, 90, 1746-1751	3.9	60
21	An adapted form of the collocation method for calculating energy levels of rotating atom–diatom complexes. *Journal of Chemical Physics*, **1989**, 91, 6598-6603	3.9	48
20	A collocation approach for quantum scattering based on the S-matrix version of the Kohn variational principle. *Journal of Chemical Physics*, **1989**, 91, 7537-7542	3.9	18
19	Block Lanczos approach combined with matrix continued fraction for the S-matrix Kohn variational principle in quantum scattering. *Journal of Chemical Physics*, **1989**, 91, 3504-3508	3.9	16
18	The collocation method for bound solutions of the Schrödinger equation. *Chemical Physics Letters*, **1988**, 153, 98-104	2.5	118
17	Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. *Physical Review B*, **1988**, 37, 785-789	3.3	76833
16	Local softness and chemical reactivity in the molecules CO, SCN and H2CO. *Computational and Theoretical Chemistry*, **1988**, 163, 305-313		198
15	Ab initio approach for many-electron systems without invoking orbitals: An integral formulation of density-functional theory. *Physical Review A*, **1988**, 38, 5494-5503	2.6	16
14	Thermal properties of many-electron systems: An integral formulation of density-functional theory. *Physical Review A*, **1988**, 38, 5504-5511	2.6	15

13	Dynamic linear response of many-electron systems: An integral formulation of density-functional theory. *Physical Review A*, **1988**, 38, 5512-5519	2.6	17
12	Ab initio approach for many-electron systems without invoking orbitals: An integral formulation of density-functional theory. *Physical Review Letters*, **1987**, 59, 1569-1572	7.4	30
11	New relation between hardness and compressibility of minerals. *Physics and Chemistry of Minerals*, **1987**, 15, 191-195	1.6	36
10	Some Remarks on Scaling Relations in Density Functional Theory **1987**, 499-506		9
9	The use of global and local molecular parameters for the analysis of the gas-phase basicity of amines. *Journal of the American Chemical Society*, **1986**, 108, 5708-11	16.4	1330
8	Various functionals for the kinetic energy density of an atom or molecule. *Physical Review A*, **1986**, 34, 4586-4590	2.6	84
7	Gradient correction in Thomas-Fermi theory. *Physical Review A*, **1986**, 34, 4575-4585	2.6	118
6	Analysis of the kinetic energy functional in density functional theory. *Journal of Chemical Physics*, **1986**, 84, 3320-3323	3.9	8
5	Hardness, softness, and the fukui function in the electronic theory of metals and catalysis. *Proceedings of the National Academy of Sciences of the United States of America*, **1985**, 82, 6723-6	11.5	1186
4	A new functional with homogeneous coordinate scaling in density functional theory: F [*Journal of Chemical Physics*, **1985**, 83, 2334-2336	3.9	44
3	Molecular softness as the average of atomic softnesses: companion principle to the geometric mean principle for electronegativity equalization. *The Journal of Physical Chemistry*, **1985**, 89, 5412-5414		103
2	Density functional approach to the frontier-electron theory of chemical reactivity. *Journal of the American Chemical Society*, **1984**, 106, 4049-4050	16.4	2356
1	Electron density, KohnSham frontier orbitals, and Fukui functions. *Journal of Chemical Physics*, **1984**, 81, 2862-2863	3.9	372