Paul Ayers

List of Publications by Year in Descending Order

328 papers	13,274 citations	60 h-index	100 g-index
335 ext. papers	14,480 ext. citations	3.5 avg, IF	6.98 L-index

#	Paper	IF	Citations
328	Procrustes: A python library to find transformations that maximize the similarity between matrices. *Computer Physics Communications*, **2022**, 276, 108334	4.2	0
327	Charge Transfer and Polarization in Force Fields: An Ab Initio Approach Based on the (Atom-Condensed) Kohn–Sham Equations, Approximated by Second-Order Perturbation Theory About the Reference Atoms (ACKS2) **2022**, 603-629		
326	Basic Formalism **2022**, 47-60		
325	The Hard/Soft Acid/Base Rule: A Perspective from Conceptual Density-Functional Theory **2022**, 263-279		0
324	Bivariational principle for an antisymmetrized product of nonorthogonal geminals appropriate for strong electron correlation. *Computational and Theoretical Chemistry*, **2022**, 1212, 113718	2	1
323	A curated diverse molecular database of blood-brain barrier permeability with chemical descriptors. *Scientific Data*, **2021**, 8, 289	8.2	5
322	Reactivity of Single Transition Metal Atoms on a Hydroxylated Amorphous Silica Surface: A Periodic Conceptual DFT Investigation. *Chemistry - A European Journal*, **2021**, 27, 6050-6063	4.8	4
321	Orbital energies and nuclear forces in DFT: Interpretation and validation. *Journal of Computational Chemistry*, **2021**, 42, 334-343	3.5	4
320	Reactivity and Charge Transfer Beyond the Parabolic Model: the "Big is Good" Principle. *ChemistrySelect*, **2021**, 6, 96-100	1.8	10
319	Flexible ansatz for N-body configuration interaction. *Computational and Theoretical Chemistry*, **2021**, 1202, 113187	2	1
318	Conceptual Density Functional Theory in the Grand Canonical Ensemble **2021**, 191-211		1
317	Well-normalized charge-transfer models: a more general derivation of the hard/soft-acid/base principle. *Theoretical Chemistry Accounts*, **2021**, 140, 1	1.9	3
316	IOData: A python library for reading, writing, and converting computational chemistry file formats and generating input files. *Journal of Computational Chemistry*, **2021**, 42, 458-464	3.5	7
315	Temperature-Dependent Approach to Electronic Charge Transfer. *Journal of Physical Chemistry A*, **2020**, 124, 5465-5473	2.8	2
314	Tribute to Paul Geerlings. *Journal of Physical Chemistry A*, **2020**, 124, 5061-5062	2.8	
313	Study of organic reactions using chemical reactivity descriptors derived through a temperature-dependent approach. *Theoretical Chemistry Accounts*, **2020**, 139, 1	1.9	5
312	Conceptual density functional theory: status, prospects, issues. *Theoretical Chemistry Accounts*, **2020**, 139, 1	1.9	113

311	Understanding Chemical Selectivity through Well Selected Excited States. *Journal of Physical Chemistry A*, **2020**, 124, 633-641	2.8	9
310	CRAHCN-O: A Consistent Reduced Atmospheric Hybrid Chemical Network Oxygen Extension for Hydrogen Cyanide and Formaldehyde Chemistry in CO-, N-, HO-, CH-, and H-Dominated Atmospheres. *Journal of Physical Chemistry A*, **2020**, 124, 8594-8606	2.8	1
309	Richardson-Gaudin mean-field for strong correlation in quantum chemistry. *Journal of Chemical Physics*, **2020**, 153, 104110	3.9	13
308	New Insights and Horizons from the Linear Response Function in Conceptual DFT **2019**,		1
307	On the impossibility of unambiguously selecting the best model for fitting data. *Journal of Mathematical Chemistry*, **2019**, 57, 1755-1769	2.1	8
306	The [illegible]big is good[illegible]rule, the maximum hardness, and minimum electrophilicity principles. *Theoretical Chemistry Accounts*, **2019**, 138, 1	1.9	25
305	A Consistent Reduced Network for HCN Chemistry in Early Earth and Titan Atmospheres: Quantum Calculations of Reaction Rate Coefficients. *Journal of Physical Chemistry A*, **2019**, 123, 1861-1873	2.8	10
304	Nine questions on energy decomposition analysis. *Journal of Computational Chemistry*, **2019**, 40, 2248-2283	3.5	70
303	Molecular QTAIM Topology Is Sensitive to Relativistic Corrections. *Chemistry - A European Journal*, **2019**, 25, 2538-2544	4.8	9
302	Temperature-dependent approach to chemical reactivity concepts in density functional theory. *International Journal of Quantum Chemistry*, **2019**, 119, e25797	2.1	26
301	A simple algorithm for the Kohn–Sham inversion problem applicable to general target densities. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	9
300	Reply to the 'Comment on "Revisiting the definition of local hardness and hardness kernel"' by C. Morell, F. Gu[illegible]an, W. Lamine, and H. Chermette, Phys. Chem. Chem. Phys., 2018, 20, DOI. *Physical Chemistry Chemical Physics*, **2018**, 20, 9011-9014	3.6	8
299	Method for making 2-electron response reduced density matrices approximately N-representable. *Journal of Chemical Physics*, **2018**, 148, 084104	3.9	5
298	Thermodynamic Justification for the Parabolic Model for Reactivity Indicators with Respect to Electron Number and a Rigorous Definition for the Electrophilicity: The Essential Role Played by the Electronic Entropy. *Journal of Chemical Theory and Computation*, **2018**, 14, 597-606	6.4	20
297	The general setting for the zero-flux condition: The lagrangian and zero-flux conditions that give the heisenberg equation of motion. *Journal of Computational Chemistry*, **2018**, 39, 1051-1058	3.5	5
296	SCI: a robust and reliable density-based descriptor to determine multiple covalent bond orders. *Journal of Molecular Modeling*, **2018**, 24, 213	2	11
295	Characterizing the sensitivity of bonds to the curvature of carbon nanotubes. *Journal of Molecular Modeling*, **2018**, 24, 249	2	13
294	Grand-Canonical Interpolation Models **2018**, 61-88		5

293	Generalized Hirshfeld Partitioning with Oriented and Promoted Proatoms. *Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica*, **2018**, 34, 514-518	3.8	2
292	Kinetic Energy Density Functionals from Models for the One-Electron Reduced Density Matrix **2018**, 199-208		2
291	A Gradient Corrected Two-Point Weighted Density Approximation for Exchange Energies **2018**, 209-218		
290	A reference-free stockholder partitioning method based on the force on electrons. *Journal of Computational Chemistry*, **2018**, 39, 1044-1050	3.5	9
289	Information-Theoretic Approaches to Atoms-in-Molecules: Hirshfeld Family of Partitioning Schemes. *Journal of Physical Chemistry A*, **2018**, 122, 4219-4245	2.8	69
288	Dipolar cycloadditions and the □big is good□rule: a computational study. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	13
287	Chemical hardness: Temperature dependent definitions and reactivity principles. *Journal of Chemical Physics*, **2018**, 149, 124110	3.9	14
286	Global and local reactivity descriptors based on quadratic and linear energy models for □unsaturated organic compounds. *International Journal of Quantum Chemistry*, **2018**, 118, e25706	2.1	12
285	Time-independent density functional theory for degenerate excited states of Coulomb systems. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	15
284	The axiomatic approach to chemical concepts. *Computational and Theoretical Chemistry*, **2018**, 1142, 83-87	2	12
283	Local and nonlocal counterparts of global descriptors: the cases of chemical softness and hardness. *Journal of Molecular Modeling*, **2018**, 24, 285	2	11
282	Breaking the curse of dimension for the electronic Schr□inger equation with functional analysis. *Computational and Theoretical Chemistry*, **2018**, 1142, 66-77	2	4
281	Note: Maximum hardness and minimum electrophilicity principles. *Journal of Chemical Physics*, **2018**, 148, 196101	3.9	19
280	Elementary Derivation of the "□Big Is Good" Rule. *Journal of Physical Chemistry Letters*, **2018**, 9, 4344-4348	6.4	30
279	On the multi-reference nature of plutonium oxides: PuO, PuO, PuO and PuO(OH). *Physical Chemistry Chemical Physics*, **2017**, 19, 4317-4329	3.6	21
278	The exact Fermi potential yielding the Hartree□ock electron density from orbital-free density functional theory. *International Journal of Quantum Chemistry*, **2017**, 117, e25364	2.1	11
277	Local chemical potential, local hardness, and dual descriptors in temperature dependent chemical reactivity theory. *Physical Chemistry Chemical Physics*, **2017**, 19, 13687-13695	3.6	19
276	Strategies for extending geminal-based wavefunctions: Open shells and beyond. *Computational and Theoretical Chemistry*, **2017**, 1116, 207-219	2	11

275	New Fukui, dual and hyper-dual kernels as bond reactivity descriptors. *Physical Chemistry Chemical Physics*, **2017**, 19, 16095-16104	3.6	11
274	Exploring the substrate selectivity of human sEH and M. tuberculosis EHB using QM/MM. *Structural Chemistry*, **2017**, 28, 1501-1511	1.8	6
273	Negative Condensed-to-Atom Fukui Functions: A Signature of Oxidation-Induced Reduction of Functional Groups **2017**, 269-278		3
272	Going beyond the three-state ensemble model: the electronic chemical potential and Fukui function for the general case. *Physical Chemistry Chemical Physics*, **2017**, 19, 11588-11602	3.6	23
271	Revisiting the definition of local hardness and hardness kernel. *Physical Chemistry Chemical Physics*, **2017**, 19, 12355-12364	3.6	23
270	Interpolating Hamiltonians in chemical compound space. *International Journal of Quantum Chemistry*, **2017**, 117, e25384	2.1	3
269	Hirshfeld partitioning from non-extensive entropies. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	8
268	Benchmarking pK prediction methods for Lys115 in acetoacetate decarboxylase. *Journal of Molecular Modeling*, **2017**, 23, 155	2	2
267	The local response of global descriptors. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	8
266	Bonding reactivity descriptor from conceptual density functional theory and its applications to elucidate bonding formation. *Journal of Chemical Physics*, **2017**, 147, 134303	3.9	6
265	Two-point weighted density approximations for the kinetic energy density functional. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	3
264	Chemical transferability of functional groups follows from the nearsightedness of electronic matter. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 11633-11638	11.5	29
263	Thermodynamic hardness and the maximum hardness principle. *Journal of Chemical Physics*, **2017**, 147, 074113	3.9	19
262	Thermodynamic responses of electronic systems. *Journal of Chemical Physics*, **2017**, 147, 094105	3.9	20
261	Robert G. Parr (1921–2017). *Angewandte Chemie*, **2017**, 129, 10775-10775	3.6	
260	Conceptual DFT analysis of the regioselectivity of 1,3-dipolar cycloadditions: nitrones as a case of study. *Journal of Molecular Modeling*, **2017**, 23, 236	2	10
259	Fuzzy atoms in molecules from Bregman divergences. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	6
258	Robert G. Parr (1921-2017). *Angewandte Chemie - International Edition*, **2017**, 56, 10639	16.4	

257	Finite temperature grand canonical ensemble study of the minimum electrophilicity principle. *Journal of Chemical Physics*, **2017**, 147, 124103	3.9	23
256	Fractional nuclear charge approach to isolated anion densities for Hirshfeld partitioning methods. *Journal of Molecular Modeling*, **2017**, 23, 348	2	4
255	The HSAB principle from a finite-temperature grand-canonical perspective. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	19
254	Finite Field Method for Nonlinear Optical Property Prediction Using Rational Function Approximants. *Journal of Physical Chemistry A*, **2017**, 121, 5313-5323	2.8	6
253	Relativistic (SR-ZORA) quantum theory of atoms in molecules properties. *Journal of Computational Chemistry*, **2017**, 38, 81-86	3.5	11
252	A Diagonally Updated Limited-Memory Quasi-Newton Method for the Weighted Density Approximation. *Computation*, **2017**, 5, 42	2.2	2
251	Benchmark values of chemical potential and chemical hardness for atoms and atomic ions (including unstable anions) from the energies of isoelectronic series. *Physical Chemistry Chemical Physics*, **2016**, 18, 25721-25734	3.6	42
250	Systematic treatment of spin-reactivity indicators in conceptual density functional theory. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	10
249	Electronegativity and redox reactions. *Physical Chemistry Chemical Physics*, **2016**, 18, 22235-43	3.6	29
248	An explicit approach to conceptual density functional theory descriptors of arbitrary order. *Chemical Physics Letters*, **2016**, 660, 307-312	2.5	34
247	When is the Fukui Function Not Normalized? The Danger of Inconsistent Energy Interpolation Models in Density Functional Theory. *Journal of Chemical Theory and Computation*, **2016**, 12, 5777-5787	6.4	29
246	Smooth models for the Coulomb potential. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	6
245	Functional constructions with specified functional derivatives. *Theoretical Chemistry Accounts*, **2016** , 135, 1	1.9	3
244	Charge transfer and chemical potential in 1,3-dipolar cycloadditions. *Theoretical Chemistry Accounts* , **2016**, 135, 1	1.9	24
243	Communication: Two types of flat-planes conditions in density functional theory. *Journal of Chemical Physics*, **2016**, 145, 031102	3.9	10
242	Using the general-purpose reactivity indicator: challenging examples. *Journal of Molecular Modeling* , **2016**, 22, 57	2	2
241	Alternative Ornstein‐Zernike models from the homogeneous electron liquid for density functional theory calculations. *International Journal of Quantum Chemistry*, **2016**, 116, 852-861	2.1	3
240	Minimal Basis Iterative Stockholder: Atoms in Molecules for Force-Field Development. *Journal of Chemical Theory and Computation*, **2016**, 12, 3894-912	6.4	81

239	Response to "Comment on 'Kohn-Sham exchange-correlation potentials from second-order reduced density matrices'" [J. Chem. Phys. 145, 037101 (2016)]. *Journal of Chemical Physics*, **2016**, 145, 037102	3.9	14
238	Interpolation of property-values between electron numbers is inconsistent with ensemble averaging. *Journal of Chemical Physics*, **2016**, 144, 244112	3.9	31
237	Performance of Shannon-entropy compacted N-electron wave functions for configuration interaction methods. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	13
236	Fractional electron number, temperature, and perturbations in chemical reactions. *Physical Chemistry Chemical Physics*, **2016**, 18, 15070-80	3.6	58
235	Average electronic energy is the central quantity in conceptual chemical reactivity theory. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	21
234	Scaling properties of information-theoretic quantities in density functional reactivity theory. *Physical Chemistry Chemical Physics*, **2015**, 17, 4977-88	3.6	59
233	CheMPS2 : Improved DMRG-SCF routine and correlation functions. *Computer Physics Communications*, **2015**, 191, 235-237	4.2	13
232	Singlet ground state actinide chemistry with geminals. *Physical Chemistry Chemical Physics*, **2015**, 17, 14427-36	3.6	27
231	Density functional reactivity theory study of SN2 reactions from the information-theoretic perspective. *Physical Chemistry Chemical Physics*, **2015**, 17, 27052-61	3.6	28
230	The effect of nitrido, azide, and nitrosyl ligands on magnetization densities and magnetic properties of iridium PNP pincer-type complexes. *RSC Advances*, **2015**, 5, 84311-84320	3.7	
229	Linearized Coupled Cluster Correction on the Antisymmetric Product of 1-Reference Orbital Geminals. *Journal of Chemical Theory and Computation*, **2015**, 11, 5252-61	6.4	40
228	Bond metallicity measures. *Computational and Theoretical Chemistry*, **2015**, 1053, 112-122	2	31
227	Revisiting the definition of the electronic chemical potential, chemical hardness, and softness at finite temperatures. *Journal of Chemical Physics*, **2015**, 143, 154103	3.9	53
226	Local and linear chemical reactivity response functions at finite temperature in density functional theory. *Journal of Chemical Physics*, **2015**, 143, 244117	3.9	42
225	Communication: Kohn-Sham theory for excited states of Coulomb systems. *Journal of Chemical Physics*, **2015**, 143, 191101	3.9	24
224	Kohn-Sham exchange-correlation potentials from second-order reduced density matrices. *Journal of Chemical Physics*, **2015**, 143, 244116	3.9	35
223	How pervasive is the Hirshfeld partitioning?. *Journal of Chemical Physics*, **2015**, 142, 044107	3.9	13
222	Dissecting the bond-formation process of d 10-metal-ethene complexes with multireference approaches. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	13

221	A quantum informational approach for dissecting chemical reactions. *Chemical Physics Letters*, **2015**, 621, 160-164	2.5	26
220	In pursuit of negative Fukui functions: molecules with very small band gaps. *Journal of Molecular Modeling*, **2014**, 20, 2162	2	19
219	Efficient parameterization of torsional terms for force fields. *Journal of Computational Chemistry*, **2014**, 35, 1438-45	3.5	12
218	Efficient description of strongly correlated electrons with mean-field cost. *Physical Review B*, **2014**, 89,	3.3	80
217	The Conceptual Density Functional Theory Perspective of Bonding **2014**, 233-270		21
216	How to Compute the Fukui Matrix and Function for Systems with (Quasi-)Degenerate States. *Journal of Chemical Theory and Computation*, **2014**, 10, 202-10	6.4	43
215	The influence of orbital rotation on the energy of closed-shell wavefunctions. *Molecular Physics*, **2014**, 112, 853-862	1.7	65
214	An information-theoretic resolution of the ambiguity in the local hardness. *Physical Chemistry Chemical Physics*, **2014**, 16, 6019-26	3.6	26
213	The influence of Ser-154, Cys-113, and the phosphorylated threonine residue on the catalytic reaction mechanism of Pin1. *Journal of Physical Chemistry B*, **2014**, 118, 9871-80	3.4	14
212	Electron localization-delocalization matrices in the prediction of pKa's and UV-wavelengths of maximum absorbance of p-benzoic acids and the definition of super-atoms in molecules. *Chemical Physics Letters*, **2014**, 612, 190-197	2.5	16
211	Simple and inexpensive perturbative correction schemes for antisymmetric products of nonorthogonal geminals. *Physical Chemistry Chemical Physics*, **2014**, 16, 5061-5	3.6	39
210	Nonvariational Orbital Optimization Techniques for the AP1roG Wave Function. *Journal of Chemical Theory and Computation*, **2014**, 10, 4873-82	6.4	44
209	CheMPS2: A free open-source spin-adapted implementation of the density matrix renormalization group for ab initio quantum chemistry. *Computer Physics Communications*, **2014**, 185, 1501-1514	4.2	122
208	Drug release by pH-responsive molecular tweezers: atomistic details from molecular modeling. *Journal of Computational Chemistry*, **2014**, 35, 1545-51	3.5	2
207	Assessing the accuracy of new geminal-based approaches. *Journal of Physical Chemistry A*, **2014**, 118, 9058-68	2.8	62
206	Resolving the nature of the reactive sites of phenylsulfinate (PhSO2-) with a single general-purpose reactivity indicator. *Computational and Theoretical Chemistry*, **2014**, 1043, 1-4	2	4
205	Kinetic and electron-electron energies for convex sums of ground state densities with degeneracies and fractional electron number. *Journal of Chemical Physics*, **2014**, 140, 18A538	3.9	9
204	Projected seniority-two orbital optimization of the antisymmetric product of one-reference orbital geminal. *Journal of Chemical Physics*, **2014**, 140, 214114	3.9	59

203	Deriving the Hirshfeld partitioning using distance metrics. *Journal of Chemical Physics*, **2014**, 141, 094103	3.9	13
202	Tight constraints on the exchange-correlation potentials of degenerate states. *Journal of Chemical Physics*, **2014**, 140, 18A537	3.9	5
201	Direct computation of parameters for accurate polarizable force fields. *Journal of Chemical Physics*, **2014**, 141, 194114	3.9	19
200	Electronic stress as a guiding force for chemical bonding. *Topics in Current Chemistry*, **2014**, 351, 103-24		10
199	Molecular alignment as a penalized permutation Procrustes problem. *Journal of Mathematical Chemistry*, **2013**, 51, 927-936	2.1	4
198	In pursuit of negative Fukui functions: examples where the highest occupied molecular orbital fails to dominate the chemical reactivity. *Journal of Molecular Modeling*, **2013**, 19, 2779-83	2	35
197	A proposal for an extended dual descriptor: a possible solution when Frontier Molecular Orbital Theory fails. *Physical Chemistry Chemical Physics*, **2013**, 15, 14465-75	3.6	61
196	How reliable is the hard-soft acid-base principle? An assessment from numerical simulations of electron transfer energies. *Physical Chemistry Chemical Physics*, **2013**, 15, 13959-68	3.6	35
195	The density per particle can be used as the fundamental descriptor for systems with rapidly decaying external potentials. *Journal of Molecular Modeling*, **2013**, 19, 2767-71	2	
194	Quantum mechanics/molecular mechanics restrained electrostatic potential fitting. *Journal of Physical Chemistry B*, **2013**, 117, 14960-6	3.4	9
193	The Ehrenfest force topology: a physically intuitive approach for analyzing chemical interactions. *Physical Chemistry Chemical Physics*, **2013**, 15, 17823-36	3.6	31
192	Communication: a case where the hard/soft acid/base principle holds regardless of acid/base strength. *Journal of Chemical Physics*, **2013**, 138, 181106	3.9	25
191	Atomic Charges and the Electrostatic Potential Are Ill-Defined in Degenerate Ground States. *Journal of Chemical Theory and Computation*, **2013**, 9, 4779-88	6.4	40
190	The sharp-G N-representability condition. *Computational and Theoretical Chemistry*, **2013**, 1003, 32-36	2	0
189	Extended random phase approximation method for atomic excitation energies from correlated and variationally optimized second-order density matrices. *Computational and Theoretical Chemistry*, **2013**, 1003, 50-54	2	14
188	ACKS2: atom-condensed Kohn-Sham DFT approximated to second order. *Journal of Chemical Physics*, **2013**, 138, 074108	3.9	60
187	□□aromaticity and anti-aromaticity as retrieved by the linear response kernel. *Physical Chemistry Chemical Physics*, **2013**, 15, 2882-9	3.6	34
186	Hirshfeld-E Partitioning: AIM Charges with an Improved Trade-off between Robustness and Accurate Electrostatics. *Journal of Chemical Theory and Computation*, **2013**, 9, 2221-5	6.4	72

185	A size-consistent approach to strongly correlated systems using a generalized antisymmetrized product of nonorthogonal geminals. *Computational and Theoretical Chemistry*, **2013**, 1003, 101-113	2	69
184	A New Mean-Field Method Suitable for Strongly Correlated Electrons: Computationally Facile Antisymmetric Products of Nonorthogonal Geminals. *Journal of Chemical Theory and Computation*, **2013**, 9, 1394-401	6.4	138
183	Using the spin-resolved electronic direct correlation function to estimate the correlation energy of the spin-polarized uniform electron gas. *Journal of Physics and Chemistry of Solids*, **2012**, 73, 670-673	3.9	6
182	A variational principle for the electron density using the exchange hole & its implications for N-representability. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2012**, 376, 839-844	2.3	6
181	Src homology 2 domain proteomimetics: developing phosphopeptide selective receptors. *MedChemComm*, **2012**, 3, 763	5	9
180	Influence of electron correlation and degeneracy on the Fukui matrix and extension of frontier molecular orbital theory to correlated quantum chemical methods. *Physical Chemistry Chemical Physics*, **2012**, 14, 2408-16	3.6	23
179	Symmetric Nonlocal Weighted Density Approximations from the Exchange-Correlation Hole of the Uniform Electron Gas. *Journal of Chemical Theory and Computation*, **2012**, 8, 4081-93	6.4	19
178	Addressing the Coulomb potential singularity in exchange-correlation energy integrals with one-electron and two-electron basis sets. *Chemical Physics Letters*, **2012**, 539-540, 163-167	2.5	6
177	Understanding chemical binding using the Berlin function and the reaction force. *Chemical Physics Letters*, **2012**, 539-540, 168-171	2.5	9
176	Insights into the mechanism of an S(N)2 reaction from the reaction force and the reaction electronic flux. *Journal of Physical Chemistry A*, **2012**, 116, 10015-26	2.8	29
175	Phosphopeptide selective coordination complexes as promising SRC homology 2 domain mimetics. *Inorganic Chemistry*, **2012**, 51, 8284-91	5.1	10
174	Automated Parametrization of AMBER Force Field Terms from Vibrational Analysis with a Focus on Functionalizing Dinuclear Zinc(II) Scaffolds. *Journal of Chemical Theory and Computation*, **2012**, 8, 554-62	6.4	39
173	The Woodward-Hoffmann rules reinterpreted by conceptual density functional theory. *Accounts of Chemical Research*, **2012**, 45, 683-95	24.3	119
172	Richard Bader (1931–2012). *Angewandte Chemie*, **2012**, 124, 4599-4600	3.6	
171	Natural orbital Fukui function and application in understanding cycloaddition reaction mechanisms. *Physical Chemistry Chemical Physics*, **2012**, 14, 9890-6	3.6	24
170	Considerations on describing non-singlet spin states in variational second order density matrix methods. *Journal of Chemical Physics*, **2012**, 136, 014110	3.9	7
169	Longitudinal static optical properties of hydrogen chains: finite field extrapolations of matrix product state calculations. *Journal of Chemical Physics*, **2012**, 136, 134110	3.9	51
168	Stockholder projector analysis: a Hilbert-space partitioning of the molecular one-electron density matrix with orthogonal projectors. *Journal of Chemical Physics*, **2012**, 136, 014107	3.9	12

167	Symmetric two-point weighted density approximation for exchange energies. *Physical Review A*, **2012**, 85,	2.6	11
166	Time-independent density-functional theory for excited states of Coulomb systems. *Physical Review A*, **2012**, 85,	2.6	41
165	Application of the electron density force to chemical reactivity. *Physical Chemistry Chemical Physics*, **2011**, 13, 9601-8	3.6	14
164	Computational study of the binding modes of caffeine to the adenosine A2A receptor. *Journal of Physical Chemistry B*, **2011**, 115, 13880-90	3.4	15
163	The Significance of Parameters in Charge Equilibration Models. *Journal of Chemical Theory and Computation*, **2011**, 7, 1750-64	6.4	39
162	Reactivity indicators for degenerate states in the density-functional theoretic chemical reactivity theory. *Journal of Chemical Physics*, **2011**, 134, 174103	3.9	62
161	The Fukui matrix: a simple approach to the analysis of the Fukui function and its positive character. *Physical Chemistry Chemical Physics*, **2011**, 13, 6110-5	3.6	44
160	Practical calculation of molecular acidity with the aid of a reference molecule. *Journal of Physical Chemistry A*, **2011**, 115, 1293-304	2.8	22
159	Charge Density and Chemical Reactions: A Unified View from Conceptual DFT **2011**, 715-764		37
158	Stability conditions for density functional reactivity theory: an interpretation of the total local hardness. *Physical Chemistry Chemical Physics*, **2011**, 13, 4427-33	3.6	11
157	Quantum mechanics/molecular mechanics strategies for docking pose refinement: distinguishing between binders and decoys in cytochrome C peroxidase. *Journal of Chemical Information and Modeling*, **2011**, 51, 93-101	6.1	30
156	Pointing the way to the products? Comparison of the stress tensor and the second-derivative tensor of the electron density. *Journal of Chemical Physics*, **2011**, 134, 234106	3.9	46
155	Should negative electron affinities be used for evaluating the chemical hardness?. *Physical Chemistry Chemical Physics*, **2011**, 13, 2285-93	3.6	58
154	The unconstrained local hardness: an intriguing quantity, beset by problems. *Physical Chemistry Chemical Physics*, **2011**, 13, 19594-600	3.6	20
153	Information theoretic properties from the quantum theory of atoms in molecules. *Chemical Physics Letters*, **2011**, 514, 379-383	2.5	31
152	The Fukui potential and the capacity of charge and the global hardness of atoms. *Journal of Physical Chemistry A*, **2011**, 115, 2325-31	2.8	44
151	The relationship between the eigenvalues and eigenvectors of a similarity matrix and its associated Carb□ndex matrix. *Journal of Mathematical Chemistry*, **2011**, 49, 6-11	2.1	2
150	Finding minimum energy reaction paths on ab initio potential energy surfaces using the fast marching method. *Journal of Mathematical Chemistry*, **2011**, 49, 1291-1301	2.1	3

149	Failure of the Weizsäcker kinetic energy functional for one-, two-, and three-electron distribution functions. *Journal of Mathematical Chemistry*, **2011**, 49, 1810-1821	2.1	24
148	Assessment of the March-Santamaria kinetic energy pair-density functional. *Journal of Mathematical Chemistry*, **2011**, 49, 1822-1830	2.1	4
147	Newton trajectories for finding stationary points on molecular potential energy surfaces. *Journal of Mathematical Chemistry*, **2011**, 49, 1915-1927	2.1	10
146	The mechanics of charge-shift bonds: A perspective from the electronic stress tensor. *Chemical Physics Letters*, **2011**, 510, 18-20	2.5	26
145	A parameterized, continuum electrostatic model for predicting protein pKa values. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 2044-52	4.2	6
144	A self-consistent Hirshfeld method for the atom in the molecule based on minimization of information loss. *Journal of Computational Chemistry*, **2011**, 32, 1561-7	3.5	20
143	Empirical prediction of protein pKa values with residue mutation. *Journal of Computational Chemistry*, **2011**, 32, 2140-8	3.5	2
142	Fast density matrix-based partitioning of the energy over the atoms in a molecule consistent with the Hirshfeld-I partitioning of the electron density. *Journal of Computational Chemistry*, **2011**, 32, 3485-96	3.5	6
141	Use of the dual potential to rationalize the occurrence of some DNA lesions (pyrimidic dimers). *Journal of Physical Chemistry A*, **2011**, 115, 8032-40	2.8	11
140	Quantum theory of atoms in molecules: results for the SR-ZORA Hamiltonian. *Journal of Physical Chemistry A*, **2011**, 115, 13001-6	2.8	23
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