Paul Ayers

List of Publications by Citations

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	Variational Principles for Describing Chemical Reactions:´ The Fukui Function and Chemical Hardness Revisited. *Journal of the American Chemical Society*, **2000**, 122, 2010-2018	16.4	659
327	Critical analysis and extension of the Hirshfeld atoms in molecules. *Journal of Chemical Physics*, **2007**, 126, 144111	3.9	484
326	Perturbative perspectives on the chemical reaction prediction problem. *International Journal of Quantum Chemistry*, **2005**, 101, 520-534	2.1	398
325	Perspective on Density functional approach to the frontier-electron theory of chemical reactivity *Theoretical Chemistry Accounts*, **2000**, 103, 353-360	1.9	374
324	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
323	What is an atom in a molecule?. *Journal of Physical Chemistry A*, **2005**, 109, 3957-9	2.8	329
322	The physical basis of the hard/soft acid/base principle. *Faraday Discussions*, **2007**, 135, 161-90; discussion 237-59, 503-6	3.6	287
321	Elucidating the hard/soft acid/base principle: a perspective based on half-reactions. *Journal of Chemical Physics*, **2006**, 124, 194107	3.9	242
320	The dependence on and continuity of the energy and other molecular properties with respect to the number of electrons. *Journal of Mathematical Chemistry*, **2008**, 43, 285-303	2.1	210
319	Understanding the Woodward-Hoffmann rules by using changes in electron density. *Chemistry - A European Journal*, **2007**, 13, 8240-7	4.8	186
318	Variational principles for describing chemical reactions: Condensed reactivity indices. *Journal of Chemical Physics*, **2002**, 116, 8731-8744	3.9	168
317	An elementary derivation of the hard/soft-acid/base principle. *Journal of Chemical Physics*, **2005**, 122, 141102	3.9	145
316	Variational principles for describing chemical reactions. Reactivity indices based on the external potential. *Journal of the American Chemical Society*, **2001**, 123, 2007-17	16.4	143
315	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
314	Chemical reactivity descriptors for ambiphilic reagents: dual descriptor, local hypersoftness, and electrostatic potential. *Journal of Physical Chemistry A*, **2009**, 113, 8660-7	2.8	133
313	Critical thoughts on computing atom condensed Fukui functions. *Journal of Chemical Physics*, **2007**, 127, 034102	3.9	128
312	Uniqueness and basis set dependence of iterative Hirshfeld charges. *Chemical Physics Letters*, **2007**, 444, 205-208	2.5	125

311	Local kinetic energy and local temperature in the density-functional theory of electronic structure. *International Journal of Quantum Chemistry*, **2002**, 90, 309-326	2.1	125
310	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
309	A high performance grid-based algorithm for computing QTAIM properties. *Chemical Physics Letters* , **2009**, 472, 149-152	2.5	121
308	The Woodward-Hoffmann rules reinterpreted by conceptual density functional theory. *Accounts of Chemical Research*, **2012**, 45, 683-95	24.3	119
307	Conceptual Density-Functional Theory for General Chemical Reactions, Including Those That Are Neither Charge- nor Frontier-Orbital-Controlled. 1. Theory and Derivation of a General-Purpose Reactivity Indicator. *Journal of Chemical Theory and Computation*, **2007**, 3, 358-74	6.4	119
306	Conceptual density functional theory: status, prospects, issues. *Theoretical Chemistry Accounts*, **2020**, 139, 1	1.9	113
305	Indices for predicting the quality of leaving groups. *Physical Chemistry Chemical Physics*, **2005**, 7, 1918-25	3.6	113
304	Density per particle as a descriptor of Coulombic systems. *Proceedings of the National Academy of Sciences of the United States of America*, **2000**, 97, 1959-64	11.5	112
303	How ambiguous is the local kinetic energy?. *Journal of Physical Chemistry A*, **2010**, 114, 8884-95	2.8	111
302	Density-based energy decomposition analysis for intermolecular interactions with variationally determined intermediate state energies. *Journal of Chemical Physics*, **2009**, 131, 164112	3.9	104
301	Atoms in molecules, an axiomatic approach. I. Maximum transferability. *Journal of Chemical Physics*, **2000**, 113, 10886-10898	3.9	104
300	An electron-preceding perspective on the deformation of materials. *Journal of Chemical Physics*, **2009**, 130, 154104	3.9	90
299	Removing electrons can increase the electron density: a computational study of negative Fukui functions. *Journal of Physical Chemistry A*, **2007**, 111, 10017-9	2.8	88
298	The maximum hardness principle implies the hard/soft acid/base rule. *Journal of Chemical Physics*, **2005**, 123, 086101	3.9	88
297	Local hardness equalization: exploiting the ambiguity. *Journal of Chemical Physics*, **2008**, 128, 184108	3.9	87
296	Density-functional theory calculations with correct long-range potentials. *Journal of Chemical Physics*, **2003**, 119, 2978-2990	3.9	87
295	Strategies for computing chemical reactivity indices. *Theoretical Chemistry Accounts*, **2001**, 106, 271-279	1.9	87
294	On the importance of the "density per particle" (shape function) in the density functional theory. *Journal of Chemical Physics*, **2004**, 120, 9969-73	3.9	86

293	Conceptual Density-Functional Theory for General Chemical Reactions, Including Those That Are Neither Charge- nor Frontier-Orbital-Controlled. 2. Application to Molecules Where Frontier Molecular Orbital Theory Fails. *Journal of Chemical Theory and Computation*, **2007**, 3, 375-89	6.4	85
292	Information Theory, the Shape Function, and the Hirshfeld Atom. *Theoretical Chemistry Accounts*, **2006**, 115, 370-378	1.9	85
291	On the applicability of local softness and hardness. *Physical Chemistry Chemical Physics*, **2010**, 12, 1072-80	3.6	84
290	An example where orbital relaxation is an important contribution to the Fukui function. *Journal of Physical Chemistry A*, **2005**, 109, 1146-51	2.8	84
289	Potential functionals: dual to density functionals and solution to the v-representability problem. *Physical Review Letters*, **2004**, 92, 146404	7.4	84
288	Rationalization of Diels-Alder reactions through the use of the dual reactivity descriptor Deltaf(r). *Physical Chemistry Chemical Physics*, **2008**, 10, 7239-46	3.6	83
287	Are the Hirshfeld and Mulliken population analysis schemes consistent with chemical intuition?. *International Journal of Quantum Chemistry*, **2009**, 109, 1790-1806	2.1	81
286	Minimal Basis Iterative Stockholder: Atoms in Molecules for Force-Field Development. *Journal of Chemical Theory and Computation*, **2016**, 12, 3894-912	6.4	81
285	Efficient description of strongly correlated electrons with mean-field cost. *Physical Review B*, **2014**, 89,	3.3	80
284	Further links between the maximum hardness principle and the hard/soft acid/base principle: insights from hard/soft exchange reactions. *Physical Chemistry Chemical Physics*, **2007**, 9, 3853-6	3.6	77
283	Generalized density functional theories using the k-electron densities: Development of kinetic energy functionals. *Journal of Mathematical Physics*, **2005**, 46, 062107	1.2	73
282	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
281	Generalizations of the Hohenberg-Kohn theorem: I. Legendre transform constructions of variational principles for density matrices and electron distribution functions. *Journal of Chemical Physics*, **2006**, 124, 054101	3.9	71
280	Nine questions on energy decomposition analysis. *Journal of Computational Chemistry*, **2019**, 40, 2248-2283	3.3	70
279	Generalized density-functional theory: Conquering theN-representability problem with exact functionals for the electron pair density and the second-order reduced density matrix. *Journal of Chemical Sciences*, **2005**, 117, 507-514	1.8	70
278	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
277	Information-Theoretic Approaches to Atoms-in-Molecules: Hirshfeld Family of Partitioning Schemes. *Journal of Physical Chemistry A*, **2018**, 122, 4219-4245	2.8	69
276	Do the local softness and hardness indicate the softest and hardest regions of a molecule?. *Chemistry - A European Journal*, **2008**, 14, 8652-60	4.8	67

275	The influence of orbital rotation on the energy of closed-shell wavefunctions. *Molecular Physics*, **2014**, 112, 853-862	1.7	65
274	Can one oxidize an atom by reducing the molecule that contains it?. *Physical Chemistry Chemical Physics*, **2006**, 8, 3387-90	3.6	63
273	Assessing the accuracy of new geminal-based approaches. *Journal of Physical Chemistry A*, **2014**, 118, 9058-68	2.8	62
272	Reactivity indicators for degenerate states in the density-functional theoretic chemical reactivity theory. *Journal of Chemical Physics*, **2011**, 134, 174103	3.9	62
271	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
270	An efficient grid-based scheme to compute QTAIM atomic properties without explicit calculation of zero-flux surfaces. *Journal of Computational Chemistry*, **2009**, 30, 1082-92	3.5	61
269	Universal mathematical identities in density functional theory: results from three different spin-resolved representations. *Journal of Chemical Physics*, **2008**, 128, 204108	3.9	61
268	ACKS2: atom-condensed Kohn-Sham DFT approximated to second order. *Journal of Chemical Physics*, **2013**, 138, 074108	3.9	60
267	Scaling properties of information-theoretic quantities in density functional reactivity theory. *Physical Chemistry Chemical Physics*, **2015**, 17, 4977-88	3.6	59
266	Projected seniority-two orbital optimization of the antisymmetric product of one-reference orbital geminal. *Journal of Chemical Physics*, **2014**, 140, 214114	3.9	59
265	Should negative electron affinities be used for evaluating the chemical hardness?. *Physical Chemistry Chemical Physics*, **2011**, 13, 2285-93	3.6	58
264	Fractional electron number, temperature, and perturbations in chemical reactions. *Physical Chemistry Chemical Physics*, **2016**, 18, 15070-80	3.6	58
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262	Woodward-Hoffmann rules in density functional theory: initial hardness response. *Journal of Chemical Physics*, **2006**, 125, 214101	3.9	56
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260	Legendre-transform functionals for spin-density-functional theory. *Journal of Chemical Physics*, **2006**, 124, 224108	3.9	55
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258	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

257	Computing Fukui functions without differentiating with respect to electron number. I. Fundamentals. *Journal of Chemical Physics*, **2007**, 126, 224107	3.9	53
256	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
255	Fermi-Amaldi model for exchange-correlation: atomic excitation energies from orbital energy differences. *Molecular Physics*, **2005**, 103, 2061-2072	1.7	51
254	Necessary and sufficient conditions for the N-representability of density functionals. *Physical Review A*, **2007**, 75,	2.6	50
253	Electron localization functions and local measures of the covariance. *Journal of Chemical Sciences*, **2005**, 117, 441-454	1.8	49
252	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
251	Computing Fukui functions without differentiating with respect to electron number. II. Calculation of condensed molecular Fukui functions. *Journal of Chemical Physics*, **2007**, 126, 224108	3.9	46
250	Necessary conditions for the N-representability of pair distribution functions. *International Journal of Quantum Chemistry*, **2006**, 106, 1487-1498	2.1	46
249	Nonvariational Orbital Optimization Techniques for the AP1roG Wave Function. *Journal of Chemical Theory and Computation*, **2014**, 10, 4873-82	6.4	44
248	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
247	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
246	Potentialphilicity and potentialphobicity: Reactivity indicators for external potential changes from density functional reactivity theory. *Journal of Chemical Physics*, **2009**, 131, 114106	3.9	44
245	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
244	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
243	Local and linear chemical reactivity response functions at finite temperature in density functional theory. *Journal of Chemical Physics*, **2015**, 143, 244117	3.9	42
242	Using classical many-body structure to determine electronic structure: An approach using k-electron distribution functions. *Physical Review A*, **2006**, 74,	2.6	42
241	Axiomatic formulations of the Hohenberg-Kohn functional. *Physical Review A*, **2006**, 73,	2.6	42
240	Bond metallicity of materials from real space charge density distributions. *Chemical Physics Letters*, **2009**, 471, 174-177	2.5	41

239	Time-independent density-functional theory for excited states of Coulomb systems. *Physical Review A*, **2012**, 85,	2.6	41
238	Exact ionization potentials from wavefunction asymptotics: the extended Koopmans' theorem, revisited. *Journal of Chemical Physics*, **2009**, 130, 194104	3.9	41
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233	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	39
232	Simple and inexpensive perturbative correction schemes for antisymmetric products of nonorthogonal geminals. *Physical Chemistry Chemical Physics*, **2014**, 16, 5061-5	3.6	39
231	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
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227	Charge Density and Chemical Reactions: A Unified View from Conceptual DFT **2011**, 715-764		37
226	Subsystem constraints in variational second order density matrix optimization: curing the dissociative behavior. *Journal of Chemical Physics*, **2010**, 132, 114113	3.9	37
225	Virial theorem in the Kohn-Sham density-functional theory formalism: accurate calculation of the atomic quantum theory of atoms in molecules energies. *Journal of Chemical Physics*, **2009**, 131, 021101	3.9	37
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215	aromaticity and anti-aromaticity as retrieved by the linear response kernel. *Physical Chemistry Chemical Physics*, **2013**, 15, 2882-9	3.6	34
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210	Information theoretic properties from the quantum theory of atoms in molecules. *Chemical Physics Letters*, **2011**, 514, 379-383	2.5	31
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201	Elementary Derivation of the "Big Is Good" Rule. *Journal of Physical Chemistry Letters*, **2018**, 9, 4344-4348	6.4	30
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199	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
198	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
197	Chemical verification of variational second-order density matrix based potential energy surfaces for the N2 isoelectronic series. *Journal of Chemical Physics*, **2010**, 132, 114112	3.9	29
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195	Density functional reactivity theory study of SN2 reactions from the information-theoretic perspective. *Physical Chemistry Chemical Physics*, **2015**, 17, 27052-61	3.6	28
194	Density-functional theory with additional basic variables: Extended Legendre transform. *Physical Review A*, **2009**, 80,	2.6	28
193	The electron-propagator approach to conceptual density-functional theory. *Journal of Chemical Sciences*, **2005**, 117, 387-400	1.8	28
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188	Numerical integration of exchange-correlation energies and potentials using transformed sparse grids. *Journal of Chemical Physics*, **2008**, 128, 224103	3.9	26
187	Temperature-dependent approach to chemical reactivity concepts in density functional theory. *International Journal of Quantum Chemistry*, **2019**, 119, e25797	2.1	26
186	The big is good rule, the maximum hardness, and minimum electrophilicity principles. *Theoretical Chemistry Accounts*, **2019**, 138, 1	1.9	25

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181	Natural orbital Fukui function and application in understanding cycloaddition reaction mechanisms. *Physical Chemistry Chemical Physics*, **2012**, 14, 9890-6	3.6	24
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178	Revisiting the definition of local hardness and hardness kernel. *Physical Chemistry Chemical Physics*, **2017**, 19, 12355-12364	3.6	23
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176	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
175	Methods for finding transition states on reduced potential energy surfaces. *Journal of Chemical Physics*, **2010**, 132, 234110	3.9	23
174	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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166	Average electronic energy is the central quantity in conceptual chemical reactivity theory. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	21
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158	Thermodynamic hardness and the maximum hardness principle. *Journal of Chemical Physics*, **2017**, 147, 074113	3.9	19
157	The HSAB principle from a finite-temperature grand-canonical perspective. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	19
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