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The dependence on and continuity of the energy and other molecular properties with respect to the number of electrons

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223	Predicting the reactivity of ambidentate nucleophiles and electrophiles using a single, general-purpose, reactivity indicator. 2007 , 9, 2371-8		34
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221	On the electronegativity nonlocality paradox. <i>Theoretical Chemistry Accounts</i> , 2007 , 118, 371-381	1.9	57
220	Universal mathematical identities in density functional theory: results from three different spin-resolved representations. <i>Journal of Chemical Physics</i> , 2008 , 128, 204108	3.9	61
219	Calculation of Fukui Functions Without Differentiating to the Number of Electrons. 3. Local Fukui Function and Dual Descriptor. 2008 , 4, 1065-72		38
218	Beyond electronegativity and local hardness: Higher-order equalization criteria for determination of a ground-state electron density. <i>Journal of Chemical Physics</i> , 2008 , 129, 054111	3.9	55
217	Local hardness equalization: exploiting the ambiguity. <i>Journal of Chemical Physics</i> , 2008 , 128, 184108	3.9	87
216	Orbital energies and negative electron affinities from density functional theory: Insight from the integer discontinuity. <i>Journal of Chemical Physics</i> , 2008 , 129, 044110	3.9	104
215	N-dependence problem of local hardness parameter. 2008 , 10, 5591-8		24
214	Regioselectivity in azahydro[60]fullerene derivatives: application of general-purpose reactivity indicators. 2008 , 112, 8154-63		4
213	Optimized effective potentials from arbitrary basis sets. <i>Journal of Chemical Physics</i> , 2008 , 129, 194102	3.9	38
212	A KohnBham system at zero temperature. 2008 , 41, 385304		
211	Density-functional theory with additional basic variables: Extended Legendre transform. 2009 , 80,		28
210	Nonuniqueness of magnetic fields and energy derivatives in spin-polarized density functional theory. <i>Journal of Chemical Physics</i> , 2009 , 131, 154114	3.9	14
209	Relationships between the third-order reactivity indicators in chemical density-functional theory. <i>Journal of Chemical Physics</i> , 2009 , 130, 244105	3.9	31
208	Conceptual DFT properties-based 3D QSAR: analysis of inhibitors of the nicotine metabolizing CYP2A6 enzyme. 2009 , 30, 1749-57		17
207	Are the Hirshfeld and Mulliken population analysis schemes consistent with chemical intuition?. 2009 , 109, 1790-1806		81

(2010-2009)

206	functions. 2009 , 109, 2356-2364	2
205	A comparison between theoretical and experimental models of electrophilicity and nucleophilicity. 2009 , 896, 73-79	49
204	Ab initio studies of BN-acenes and cyclo BN-acenes electronic properties and their dependence on the molecular size and the number of electrons. 2009 , 905, 1-7	2
203	Linear regression analysis of molecular energy properties for poly heterocyclic compounds. 2009 , 906, 35-40	O
202	Is size-consistency possible with density functional approximations?. 2009 , 356, 91-97	39
201	Electrophilicity index within a conceptual DFT framework. 2009 , 105, 13	143
200	Cyclopolymerization reactions of diallyl monomers: exploring electronic and steric effects using DFT reactivity indices. 2009 , 113, 8704-11	30
199	Molecular Orbital-Averaged Fukui Function for the Reactivity Description of Alkaline Earth Metal Oxide Clusters. 2009 , 5, 1245-53	21
198	Potentialphilicity and potentialphobicity: Reactivity indicators for external potential changes from density functional reactivity theory. <i>Journal of Chemical Physics</i> , 2009 , 131, 114106	44
197	Chemical reactivity descriptors for ambiphilic reagents: dual descriptor, local hypersoftness, and electrostatic potential. 2009 , 113, 8660-7	133
196	Comparison of the Hirshfeld-I and iterated stockholder atoms in molecules schemes. 2009 , 11, 3424-9	50
195	Physical signatures of discontinuities of the time-dependent exchange-correlation potential. 2009 , 11, 4647-54	19
194	Predicting the quality of leaving groups in organic chemistry: Tests against experimental data. 2010 , 943, 168-177	18
193	The linear response kernel of conceptual DFT as a measure of electron delocalisation. 2010 , 498, 192-197	39
192	Energy surface, chemical potentials, Kohn-Sham energies in spin-polarized density functional theory. <i>Journal of Chemical Physics</i> , 2010 , 133, 144105	10
191	Computing Second-Order Functional Derivatives with Respect to the External Potential. 2010 , 6, 3671-3680	30
190	Simple charge-transfer model for metallic complexes. 2010 , 114, 7945-51	16
189	Derivative of the Lieb definition for the energy functional of density-functional theory with respect to the particle number and the spin number. 2010 , 81,	13

188	Studies of regioselectivity of large molecular systems using DFT based reactivity descriptors. 2010 , 106, 118	73
187	DFT Study of Interaction of Azoles with Cu(111) and Al(111) Surfaces: Role of Azole Nitrogen Atoms and DipoleDipole Interactions. 2011 , 115, 24189-24197	126
186	Quantum Mechanical Origins of the Iczkowski-Margrave Model of Chemical Potential. 2011 , 7, 2253-61	19
185	Reactivity indicators for degenerate states in the density-functional theoretic chemical reactivity theory. <i>Journal of Chemical Physics</i> , 2011 , 134, 174103	62
184	The Fukui matrix: a simple approach to the analysis of the Fukui function and its positive character. 2011 , 13, 6110-5	44
183	Charge Density and Chemical Reactions: A Unified View from Conceptual DFT. 2011 , 715-764	37
182	Stability conditions for density functional reactivity theory: an interpretation of the total local hardness. 2011 , 13, 4427-33	11
181	Assembling Small Silicon Clusters Using Criteria of Maximum Matching of the Fukui Functions. 2011 , 7, 3995-4001	13
180	Should negative electron affinities be used for evaluating the chemical hardness?. 2011 , 13, 2285-93	58
179	The unconstrained local hardness: an intriguing quantity, beset by problems. 2011 , 13, 19594-600	20
178	Interplay between molecular conformation and intermolecular interactions in conformational polymorphism: a molecular perspective from electronic calculations of tolfenamic acid. 2011 , 418, 179-86	22
177	Update 2 of: electrophilicity index. 2011 , 111, PR43-75	233
176	The Fukui potential and the capacity of charge and the global hardness of atoms. 2011 , 115, 2325-31	44
175	Calculations of ionization energies and electron affinities for atoms and molecules: A comparative study with different methods. 2011 , 6, 269-279	17
174	Triazole, benzotriazole, and naphthotriazole as copper corrosion inhibitors: I. Molecular electronic and adsorption properties. 2011 , 12, 3547-55	35
173	A self-consistent Hirshfeld method for the atom in the molecule based on minimization of information loss. 2011 , 32, 1561-7	20
172	Fast density matrix-based partitioning of the energy over the atoms in a molecule consistent with the Hirshfeld-I partitioning of the electron density. 2011 , 32, 3485-96	6
171	The dual descriptor: Working equations applied on electronic open-shell molecular systems. 2011 , 506, 104-111	15

(2012-2011)

170	On the consistent use of electrophilicity index and HSAB-based electron transfer and its associated change of energy parameters. 2011 , 507, 181-184	36
169	Stockholder projector analysis: a Hilbert-space partitioning of the molecular one-electron density matrix with orthogonal projectors. <i>Journal of Chemical Physics</i> , 2012 , 136, 014107) 12
168	Mapping Kohn-Sham eigenenergies onto vertical ionization energies and electron affinities. 2012 , 85,	1
167	Time-independent density-functional theory for excited states of Coulomb systems. 2012, 85,	41
166	Constraint on the second functional derivative of the exchange-correlation energy. 2012 , 110, 2275-2279	
165	Revisiting caffeate's capabilities as a complexation agent to silver cation in mining processes by means of the dual descriptora conceptual DFT approach. 2012 , 18, 4299-307	35
164	Influence of electron correlation and degeneracy on the Fukui matrix and extension of frontier molecular orbital theory to correlated quantum chemical methods. 2012 , 14, 2408-16	23
163	Energy Densities in the Strong-Interaction Limit of Density Functional Theory. 2012 , 8, 3097-107	36
162	A relation between different scales of electrophilicity: are the scales consistent along a chemical reaction?. 2012 , 116, 7074-81	9
161	Symmetric Nonlocal Weighted Density Approximations from the Exchange-Correlation Hole of the Uniform Electron Gas. 2012 , 8, 4081-93	19
160	Improved electronic excitation energies from shape-corrected semilocal Kohn-Sham potentials. 2012 , 108, 253005	32
159	Analytical evaluation of Fukui functions and real-space linear response function. <i>Journal of Chemical Physics</i> , 2012 , 136, 144110	53
158	Derivative discontinuity, bandgap and lowest unoccupied molecular orbital in density functional theory. <i>Journal of Chemical Physics</i> , 2012 , 136, 204111) 129
157	Protonfloupled electron transfer versus hydrogen atom transfer: A density functional reactivity theory characterization. 2012 , 988, 13-18	4
156	Ground and excited state similarity studies by means of Fukui and dual-descriptor matrices. 2012 , 549, 103-107	4
155	Surface Reactivity for Chlorination on Chlorinated (5,5) Armchair SWCNT: A Computational Approach. 2012 , 116, 22399-22410	56
154	Insights into the mechanism of an S(N)2 reaction from the reaction force and the reaction electronic flux. 2012 , 116, 10015-26	29
153	Density-functional derivative discontinuities at the maximum number of bound electrons. 2012 , 85,	3

152	Exact expressions for ensemble functionals from particle number dependence. <i>Journal of Chemical Physics</i> , 2012 , 136, 174113	1
151	Challenges for density functional theory. 2012 , 112, 289-320	1521
150	Natural orbital Fukui function and application in understanding cycloaddition reaction mechanisms. 2012 , 14, 9890-6	24
149	On the HSAB based estimate of charge transfer between adsorbates and metal surfaces. 2012 , 393, 1-12	206
148	Condensed descriptors for reactivity: A methodological study. 2012 , 527, 67-72	54
147	Fukui and dual-descriptor matrices in the basis-set representation: A spin-free approach. 2012 , 533, 114-117	8
146	A variational principle for the electron density using the exchange hole & its implications for N-representability. 2012 , 376, 839-844	6
145	Some formal properties of ensemble density functionals. 2013 , 113, 1076-1085	2
144	Fukui and dual-descriptor matrices within the framework of spin-polarized density functional theory. 2013 , 15, 9594-604	12
143	In pursuit of negative Fukui functions: examples where the highest occupied molecular orbital fails to dominate the chemical reactivity. 2013 , 19, 2779-83	35
142	An approximate approach to calculate the potential acting on an electron in a molecule and construct the molecular face. 2013 , 1019, 61-70	2
141	A theoretical study on the gas-phase protonation of pyridine and phosphinine derivatives. 2013 , 19, 4049-58	8
140	How reliable is the hard-soft acid-base principle? An assessment from numerical simulations of electron transfer energies. 2013 , 15, 13959-68	35
139	Bond Fukui indices: comparison of frozen molecular orbital and finite differences through Mulliken populations. 2013 , 34, 2421-9	12
138	An intermediate level of approximation for computing the dual descriptor. 2013 , 19, 2811-20	2
137	On the exponential model for energy with respect to number of electrons. 2013 , 19, 2849-53	24
136	Shape entropy's response to molecular ionization. 2013 , 19, 1677-83	5
135	Derivative discontinuity in the strong-interaction limit of density-functional theory. 2013 , 111, 126402	24

134	ACKS2: atom-condensed Kohn-Sham DFT approximated to second order. <i>Journal of Chemical Physics</i> , 2013 , 138, 074108	60
133	Evaluation of absolute hardness: a new approach. 2013 , 117, 939-46	16
132	The relation between adsorption bonding and corrosion inhibition of azole molecules on copper. 2013 , 73, 7-17	71
131	Topological analysis of tetraphosphorus oxides (P4O 6+n (n = 0-4)). 2013 , 19, 2057-67	3
130	Computational nanochemistry report on the oxicamsconceptual DFT indices and chemical reactivity. 2013 , 117, 6339-51	27
129	Fukui function and response function for nonlocal and fractional systems. <i>Journal of Chemical Physics</i> , 2013 , 138, 184108	16
128	Electrophilicity kernel and its hierarchy through softness in conceptual density functional theory. 2013 , 113, 2163-2171	13
127	Computational Nutraceutics: Chemical Reactivity Properties of the Flavonoid Naringin by Means of Conceptual DFT. 2013 , 2013, 1-8	13
126	Relevance of coordinate and particle-number scaling in density-functional theory. 2013, 87,	34
125	. 2014,	7
125	. 2014, Kinetic and electron-electron energies for convex sums of ground state densities with degeneracies and fractional electron number. <i>Journal of Chemical Physics</i> , 2014, 140, 18A538	
	Kinetic and electron-electron energies for convex sums of ground state densities with	
124	Kinetic and electron-electron energies for convex sums of ground state densities with degeneracies and fractional electron number. <i>Journal of Chemical Physics</i> , 2014 , 140, 18A538 Reactivity of low-oxidation state tin compounds: an overview of the benefits of combining DFT	9
124	Kinetic and electron-electron energies for convex sums of ground state densities with degeneracies and fractional electron number. <i>Journal of Chemical Physics</i> , 2014 , 140, 18A538 Reactivity of low-oxidation state tin compounds: an overview of the benefits of combining DFT Theory and experimental NMR spectroscopy. 2014 , 92, 447-461	9
124 123	Kinetic and electron-electron energies for convex sums of ground state densities with degeneracies and fractional electron number. <i>Journal of Chemical Physics</i> , 2014 , 140, 18A538 Reactivity of low-oxidation state tin compounds: an overview of the benefits of combining DFT Theory and experimental NMR spectroscopy. 2014 , 92, 447-461 On energetic prerequisites of attracting electrons. <i>Journal of Chemical Physics</i> , 2014 , 140, 234111 3.9	9 0
124 123 122	Kinetic and electron-electron energies for convex sums of ground state densities with degeneracies and fractional electron number. <i>Journal of Chemical Physics</i> , 2014 , 140, 18A538 Reactivity of low-oxidation state tin compounds: an overview of the benefits of combining DFT Theory and experimental NMR spectroscopy. 2014 , 92, 447-461 On energetic prerequisites of attracting electrons. <i>Journal of Chemical Physics</i> , 2014 , 140, 234111 3.9 Density functional theory of chemical reactivity. 2014 , 151-174	9
124 123 122 121	Kinetic and electron-electron energies for convex sums of ground state densities with degeneracies and fractional electron number. <i>Journal of Chemical Physics</i> , 2014 , 140, 18A538 Reactivity of low-oxidation state tin compounds: an overview of the benefits of combining DFT Theory and experimental NMR spectroscopy. 2014 , 92, 447-461 On energetic prerequisites of attracting electrons. <i>Journal of Chemical Physics</i> , 2014 , 140, 234111 3.9 Density functional theory of chemical reactivity. 2014 , 151-174 Deriving the Hirshfeld partitioning using distance metrics. <i>Journal of Chemical Physics</i> , 2014 , 141, 094103.9	9 0
124 123 122 121 120	Kinetic and electron-electron energies for convex sums of ground state densities with degeneracies and fractional electron number. <i>Journal of Chemical Physics</i> , 2014 , 140, 18A538 Reactivity of low-oxidation state tin compounds: an overview of the benefits of combining DFT Theory and experimental NMR spectroscopy. 2014 , 92, 447-461 On energetic prerequisites of attracting electrons. <i>Journal of Chemical Physics</i> , 2014 , 140, 234111 3.9 Density functional theory of chemical reactivity. 2014 , 151-174 Deriving the Hirshfeld partitioning using distance metrics. <i>Journal of Chemical Physics</i> , 2014 , 141, 094103.9 In pursuit of negative Fukui functions: molecules with very small band gaps. 2014 , 20, 2162 QSAR study of the DPPHDradical scavenging activity of coumarin derivatives and xanthine oxidase	9 0 22 13

116	How to Compute the Fukui Matrix and Function for Systems with (Quasi-)Degenerate States. 2014 , 10, 202-10		43
115	An information-theoretic resolution of the ambiguity in the local hardness. 2014 , 16, 6019-26		26
114	Morphology directing synthesis of 1-pyrene carboxaldehyde microstructures and their photo physical properties. 2014 , 4, 10903		16
113	Introducing "UCA-FUKUI" software: reactivity-index calculations. 2014 , 20, 2492		74
112	Testing exchangeBorrelation functionals at fractional electron numbers. <i>Theoretical Chemistry Accounts</i> , 2014 , 133, 1	9	2
111	Fractional charge behavior and band gap predictions with the XYG3 type of doubly hybrid density functionals. 2014 , 118, 9201-11		43
110	Computational chemistry of natural products: a comparison of the chemical reactivity of isonaringin calculated with the M06 family of density functionals. 2014 , 20, 2316		15
109	Aggregation induced emission enhancement from Bathophenanthroline microstructures and its potential use as sensor of mercury ions in water. 2014 , 16, 6283-93		37
108	Computational Nanochemistry Study of the Molecular Structure, Spectra and Chemical Reactivity Properties of the BFPF Green Fluorescent Protein Chromophore. 2014 , 199-238		
107	Electronic chemical response indexes at finite temperature in the canonical ensemble. <i>Journal of Chemical Physics</i> , 2015 , 143, 024112	9	15
106	Revisiting the definition of the electronic chemical potential, chemical hardness, and softness at finite temperatures. <i>Journal of Chemical Physics</i> , 2015 , 143, 154103	9	53
105	Local and linear chemical reactivity response functions at finite temperature in density functional theory. <i>Journal of Chemical Physics</i> , 2015 , 143, 244117	9	42
104	Morphology directing synthesis of benzo[a]pyrene microstructures and their photo physical properties. 2015 , 206, 47-55		18
103	Computational study of the structure, bonding and reactivity of selected helical metallocenes. 2015 , 438, 203-207		4
102	On the non-integer number of particles in molecular system domains: treatment and description. Theoretical Chemistry Accounts, 2015, 134, 1	9	8
101	Integration approach at the second-order perturbation theory: applications to ionization potential and electron affinity calculations. 2015 , 11, 4677-88		13
100	Aggregation induced emission enhancement of 4,4'-bis(diethylamino)benzophenone with an exceptionally large blue shift and its potential use as glucose sensor. 2015 , 17, 3343-54		46
99	DFT study of nucleophilicity of organometallic (2,2?-bipyridine)platinum(II) complexes. 2015 , 776, 77-82		6

(2016-2016)

98	Alternative Ornstein dernike models from the homogeneous electron liquid for density functional theory calculations. 2016 , 116, 852-861		3	
97	Interpolation of property-values between electron numbers is inconsistent with ensemble averaging. <i>Journal of Chemical Physics</i> , 2016 , 144, 244112	3.9	31	
96	Topological Analysis of the Fukui Function. 2016 , 227-241		16	
95	Fractional electron number, temperature, and perturbations in chemical reactions. 2016 , 18, 15070-80		58	
94	Intramolecular charge transfer model in fluorescence processes. <i>Theoretical Chemistry Accounts</i> , 2016 , 135, 1	1.9	4	
93	Atom and Bond Fukui Functions and Matrices: A Hirshfeld-I Atoms-in-Molecule Approach. 2016 , 17, 288	1-9	7	
92	Average electronic energy is the central quantity in conceptual chemical reactivity theory. <i>Theoretical Chemistry Accounts</i> , 2016 , 135, 1	1.9	21	
91	Benchmark values of chemical potential and chemical hardness for atoms and atomic ions (including unstable anions) from the energies of isoelectronic series. 2016 , 18, 25721-25734		42	
90	Range-Separation Parameter in Tuned Exchange-Correlation Functionals: Successive Ionizations and the Fukui Function. 2016 , 12, 4879-4884		6	
89	Systematic treatment of spin-reactivity indicators in conceptual density functional theory. <i>Theoretical Chemistry Accounts</i> , 2016 , 135, 1	1.9	10	
88	Electronegativity and redox reactions. 2016 , 18, 22235-43		29	
87	A generalized operational formula based on total electronic densities to obtain 3D pictures of the dual descriptor to reveal nucleophilic and electrophilic sites accurately on closed-shell molecules. 2016 , 37, 2279-303		12	
86	An explicit approach to conceptual density functional theory descriptors of arbitrary order. 2016 , 660, 307-312		34	
85	A Fractionally Ionic Approach to Polarizability and van der Waals Many-Body Dispersion Calculations. 2016 , 12, 5920-5930		62	
84	Role of Defects on Regioselectivity of Nano Pristine Graphene. 2016 , 120, 9101-9108		16	
83	When is the Fukui Function Not Normalized? The Danger of Inconsistent Energy Interpolation Models in Density Functional Theory. 2016 , 12, 5777-5787		29	
82	Charge transfer and chemical potential in 1,3-dipolar cycloadditions. <i>Theoretical Chemistry Accounts</i> , 2016 , 135, 1	1.9	24	
81	Using the general-purpose reactivity indicator: challenging examples. 2016 , 22, 57		2	

80 Comparison of reactivity of Pt(II) center in the mononuclear and binuclear organometallic diimineplatinum complexes toward oxidative addition of methyl iodide. **2016**, 1103, 132-139

79	Global and Local Partitioning of the Charge Transferred in the Parr-Pearson Model. 2017 , 121, 4019-402	29	13
78	Local chemical potential, local hardness, and dual descriptors in temperature dependent chemical reactivity theory. 2017 , 19, 13687-13695		19
77	Perturbed reactivity descriptors: the chemical hardness. <i>Theoretical Chemistry Accounts</i> , 2017 , 136, 1	1.9	22
76	Strategies for extending geminal-based wavefunctions: Open shells and beyond. 2017 , 1116, 207-219		11
75	Donation and back-donation analyzed through a charge transfer model based on density functional theory. 2017 , 23, 207		13
74	Thermodynamic electrophilicity. <i>Journal of Chemical Physics</i> , 2017 , 146, 214113	3.9	24
73	New Fukui, dual and hyper-dual kernels as bond reactivity descriptors. 2017 , 19, 16095-16104		11
72	Negative Condensed-to-Atom Fukui Functions: A Signature of Oxidation-Induced Reduction of Functional Groups. 2017 , 269-278		3
71	Going beyond the three-state ensemble model: the electronic chemical potential and Fukui function for the general case. 2017 , 19, 11588-11602		23
70	Revisiting the definition of local hardness and hardness kernel. 2017 , 19, 12355-12364		23
69	Interpolating Hamiltonians in chemical compound space. 2017 , 117, e25384		3
68	The local response of global descriptors. <i>Theoretical Chemistry Accounts</i> , 2017 , 136, 1	1.9	8
67	Thermodynamic hardness and the maximum hardness principle. <i>Journal of Chemical Physics</i> , 2017 , 147, 074113	3.9	19
66	Thermodynamic responses of electronic systems. <i>Journal of Chemical Physics</i> , 2017 , 147, 094105	3.9	20
65	Quantum chemical study of Triton X-100 modified graphene surface. 2017 , 248, 225-231		22
64	Conceptual DFT analysis of the regioselectivity of 1,3-dipolar cycloadditions: nitrones as a case of study. 2017 , 23, 236		10
63	Geometrical distortions and charge transfer in munchnfle regio-selectivity: A conceptual density functional study. 2017 , 117, e25444		3

62	DFT and conceptual-DFT assessment on selective tertiary amine functionalized calix[4]arene-anion interaction. 2017 , 1117, 292-298		1	
61	Finite temperature grand canonical ensemble study of the minimum electrophilicity principle. <i>Journal of Chemical Physics</i> , 2017 , 147, 124103	3.9	23	
60	Analytical Fukui and cyclic voltammetric studies on ferrocene modified carbon electrodes and effect of Triton X-100 by immobilization method. 2017 , 258, 1025-1034		28	
59	Insights into the Mechanism of Ground and Excited State Double Proton Transfer Reaction in Formic Acid Dimer. 2017 , 121, 9531-9543		12	
58	Fractional nuclear charge approach to isolated anion densities for Hirshfeld partitioning methods. 2017 , 23, 348		4	
57	The HSAB principle from a finite-temperature grand-canonical perspective. <i>Theoretical Chemistry Accounts</i> , 2017 , 136, 1	1.9	19	
56	Dissociation energy for the P2S2 ring in a family of thionation reagents and the corresponding chemical reactivity of separated species: a density functional theory analysis. <i>Journal of Physical Organic Chemistry</i> , 2017 , 30, e3624	2.1	3	
55	Aggregation induced emission of 9-Anthraldehyde microstructures and its selective sensing behavior towards picric acid. 2018 , 261, 446-455		5	
54	Role of Reaction Conditions in the Global and Local Two Parabolas Charge Transfer Model. 2018 , 122, 1796-1806		9	
53	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. 2018 , 14, 597-606		20	
52	Information-Theoretic Approaches to Atoms-in-Molecules: Hirshfeld Family of Partitioning Schemes. 2018 , 122, 4219-4245		69	
51	New insights in conceptual DFT: New model for the calculation of local reactivity indices based on the Sanderson's principle. 2018 , 119, e25844		3	
50	Chemical hardness: Temperature dependent definitions and reactivity principles. <i>Journal of Chemical Physics</i> , 2018 , 149, 124110	3.9	14	
49	Global and local reactivity descriptors based on quadratic and linear energy models for <code>Hunsaturated</code> organic compounds. 2018 , 118, e25706		12	
48	Delocalization Errors in Density Functional Theory Are Essentially Quadratic in Fractional Occupation Number. 2018 , 9, 6280-6288		45	
47	Intermolecular Interactions and Computational Modeling. 2018, 123-167		2	
46	Local electrophilicity. 2018 , 24, 245		12	
45	Global and local charge transfer in electron donor-acceptor complexes. 2018 , 24, 250		6	

44	An electronic temperature definition for the reactive electronic species: Conciliating practical approaches in conceptual chemical reactivity theory with a rigorous ensemble formulation. <i>Journal of Chemical Physics</i> , 2019 , 151, 074105	3.9	5
43	Electronegativities of Pauling and Mulliken in Density Functional Theory. 2019 , 123, 10065-10071		12
42	The density response kernel, the Fukui function, and other response functions from the KohnBham orbitals. <i>Theoretical Chemistry Accounts</i> , 2019 , 138, 1	1.9	4
41	New advances in conceptual-DFT: an alternative way to calculate the Fukui function and dual descriptor. 2019 , 25, 123		10
40	Temperature-dependent approach to chemical reactivity concepts in density functional theory. 2019 , 119, e25797		26
39	On derivatives of the energy with respect to total electron number and orbital occupation numbers. A critique of Janak's theorem ** This paper honours the memory of Dieter Cremer and his penetrating analysis of fundamentals of DFT.View all notes. 2020 , 118, e1612955		7
38	Temperature-Dependent Approach to Electronic Charge Transfer. 2020, 124, 5465-5473		2
37	Negative Electron Affinities and Derivative Discontinuity Contribution from a Generalized Gradient Approximation Exchange Functional. 2020 , 124, 1334-1342		1
36	Conceptual density functional theory: status, prospects, issues. <i>Theoretical Chemistry Accounts</i> , 2020 , 139, 1	1.9	113
35	What do we learn from the classical turning surface of the Kohn-Sham potential as electron number is varied continuously?. <i>Journal of Chemical Physics</i> , 2020 , 152, 054105	3.9	O
34	Reactivity and Charge Transfer Beyond the Parabolic Model: the IPBig is GoodIPrinciple. 2021 , 6, 96-100		10
33	Replacing hybrid density functional theory: motivation and recent advances. 2021 , 50, 8470-8495		23
32	DFT investigation of solvent, substituent, and catalysis effects on the intramolecular Diels-Alder reaction. 2021 , 27, 125		5
31	Molecular modeling of organic corrosion inhibitors: calculations, pitfalls, and conceptualization of moleculeBurface bonding. 2021 , 109650		10
30	Conceptual Density Functional Theory in the Grand Canonical Ensemble. 2021, 191-211		1
29	Conceptual density functional theory based electronic structure principles. 2021 , 12, 6264-6279		26
28	Fukui Function. 2009,		31
27	Chemical Reactivity Concepts in Density Functional Theory. 2009,		10

26	Study of the Reactivity of (100) Felodipine Surface Model Based on DFT Concepts. 2019 , 09, 1-12		1
25	Periodicity by Peripheral Electrons and Density in Chemical Atom. 2016 , 163-362		
24	Density functional theory, chemical reactivity, and the Fukui functions. 1		1
23	Hammett constants from density functional calculations: charge transfer and perturbations. <i>Theoretical Chemistry Accounts</i> , 2022 , 141, 1	1.9	O
22	Finite Temperature Conceptual Density Functional Theory. 2022, 137-160		
21	Charge Transfer and Polarization in Force Fields: An Ab Initio Approach Based on the (Atom-Condensed) KohnBham Equations, Approximated by Second-Order Perturbation Theory About the Reference Atoms (ACKS2). 2022 , 603-629		
20	Constrained Iterative Hirshfeld Charges: A Variational Approach. Journal of Chemical Physics,	3.9	1
19	Selectivity: An Electron Density Perspective. 2022 , 187-208		
18	Basic Formalism. 2022 , 47-60		
17	The Hard/Soft Acid/Base Rule: A Perspective from Conceptual Density-Functional Theory. 2022 , 263-2	79	0
16	The Hard/Soft Acid/Base Rule: A Perspective from Conceptual Density-Functional Theory. 2022, 263-2 ChemTools: Gain Chemical Insight from Quantum Chemistry Calculations. 2022, 649-661	79	O
		79	O
16	ChemTools: Gain Chemical Insight from Quantum Chemistry Calculations. 2022 , 649-661	79	O
16	ChemTools: Gain Chemical Insight from Quantum Chemistry Calculations. 2022 , 649-661 Charge Transfer Models in Conceptual DFT. 2022 , 209-228	79	0
16 15	ChemTools: Gain Chemical Insight from Quantum Chemistry Calculations. 2022, 649-661 Charge Transfer Models in Conceptual DFT. 2022, 209-228 Basic Principles. 2022, 61-74	2.1	
16 15 14	ChemTools: Gain Chemical Insight from Quantum Chemistry Calculations. 2022, 649-661 Charge Transfer Models in Conceptual DFT. 2022, 209-228 Basic Principles. 2022, 61-74 Basic Functions. 2022, 17-46		O
16 15 14 13	ChemTools: Gain Chemical Insight from Quantum Chemistry Calculations. 2022, 649-661 Charge Transfer Models in Conceptual DFT. 2022, 209-228 Basic Principles. 2022, 61-74 Basic Functions. 2022, 17-46 Electronegativity: A Continuing Enigma. <i>Journal of Physical Organic Chemistry</i> , Molecular Interactions From the Density Functional Theory for Chemical Reactivity: The Interaction	2.1	0

natural bond orbital reactivity in the c-DFT background.

Hardness of Molecules and Bandgap of Solids from a Generalized Gradient Approximation Exchange Energy Functional.

Properties of the density functional response kernels and its implications on chemistry. 2022, 157, 114102 o

Charge transfer at finite temperature: the "|[I]big is good" principle.

Conceptual Density Functional Theory. 2022,

A conceptual density functional theory approach to substituent effects in fluorescence processes: The case of naphthalimide derivatives.

DFT+U-type functional derived to explicitly address the flat plane condition. 2023, 107,

A kinetic perspective of charge transfer reactions: the downfall of hard/soft acid/base interactions.

Introducing a new model based on electronegativity equalization principle for the analysis of the

2023, 142,